Full wwPDB EM Validation Report ⓘ

Sep 8, 2026 – 09:27 pm BST

PDB ID	:	7AK5 / pdb_00007ak5
EMDB ID	:	EMD-11810
Title	:	Cryo-EM structure of respiratory complex I in the deactive state from Mus musculus at 3.2 A
Authors	:	Yin, Z.; Bridges, H.R.; Grba, D.; Hirst, J.
Deposited on	:	2020-09-29
Resolution	:	3.17 Å(reported)

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

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

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

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

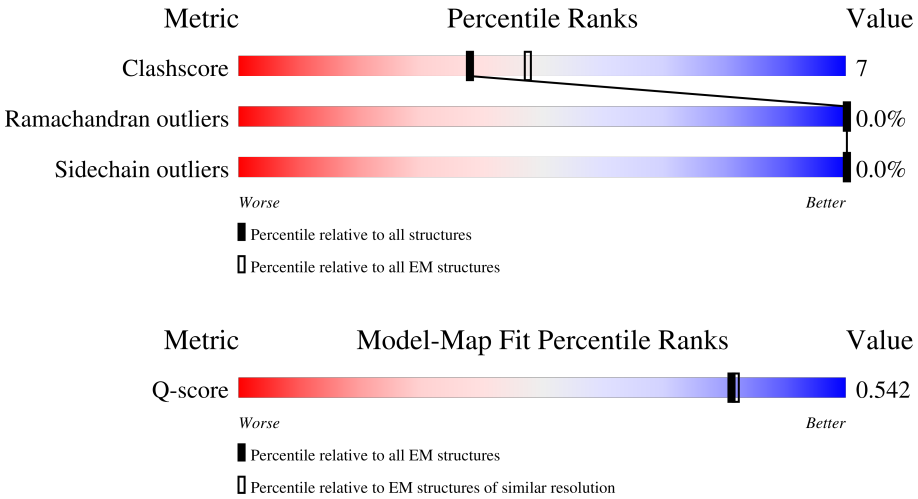
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.17 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	14465 (2.67 - 3.67)

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	115	63% 16% 22%
2	B	224	60% 8% 31%
3	C	263	65% 13% 22%
4	D	463	76% 14% 10%

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Mol	Chain	Length	Quality of chain
5	E	245	9% 67% 18% 14%
6	F	464	5% 73% 19% 8%
7	G	715	5% 80% 16%
8	H	318	76% 20%
9	I	212	66% 18% 16%
10	J	172	16% 74% 26%
11	K	98	77% 22%
12	L	607	76% 24%
13	M	459	80% 20%
14	N	345	74% 26%
15	O	355	5% 71% 19% 10%
16	P	377	7% 61% 16% 23%
17	Q	175	61% 11% 29%
18	R	114	70% 12% 18%
19	S	99	20% 73% 10% 17%
20	T	156	25% 33% 14% 53%
20	U	156	9% 48% 8% 44%
21	V	116	8% 70% 27%
22	W	131	8% 70% 17% 13%
23	X	172	5% 85% 14%
24	Y	143	5% 84% 14%
25	Z	144	88% 9%
26	a	68	88% 12%
27	b	83	8% 89% 11%
28	c	76	5% 46% 14% 39%

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Mol	Chain	Length	Quality of chain
29	d	120	92% 8%
30	e	106	89% 9%
31	f	57	12% 67% 21% 12%
32	g	151	5% 52% 15% 33%
33	h	189	65% 8% 28%
34	i	127	6% 54% 21% 24%
35	j	105	12% 50% 10% 40%
36	k	104	13% 61% 14% 25%
37	l	186	7% 73% 11% 16%
38	m	129	9% 78% 19%
39	n	179	10% 79% 20%
40	o	137	17% 68% 15% 17%
41	p	176	5% 81% 14% 5%
42	q	145	84% 14%
43	r	112	73% 12% 14%
44	s	104	27% 11% 62%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 65895 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	90	737	511	101	120	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	155	1241	793	222	212	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	206	1712	1105	294	310	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	419	3381	2163	578	616	24	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1639	1043	275	310	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	428	Total	C	N	O	S	0	0
			3301	2080	590	609	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total	C	N	O	S	0	0
			5287	3316	918	1012	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	308	Total	C	N	O	S	0	0
			2465	1659	373	411	22		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	178	Total	C	N	O	S	0	0
			1408	885	243	268	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1277	857	185	220	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	98	Total	C	N	O	S	0	0
			737	477	112	137	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	606	Total	C	N	O	S	0	0
			4800	3182	746	827	45		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	459	Total	C	N	O	S	0	0
			3632	2408	567	617	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2696	1791	416	452	37		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2607	1674	431	492	10		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	290	Total	C	N	O	S	0	0
			2297	1463	415	412	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	125	Total	C	N	O	S	0	0
			1015	642	179	190	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	94	Total	C	N	O	S	0	0
			738	458	135	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	82	Total	C	N	O	S	0	0
			659	413	125	118	3		

- Molecule 20 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	73	Total	C	N	O	S	0	0
			588	378	87	118	5		
20	U	88	Total	C	N	O	S	0	0
			706	453	104	144	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	171	Total	C	N	O	S	0	0
			1396	889	250	247	10		

- Molecule 24 is a protein called MCG5603.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	140	Total	C	N	O	S	0	0
			1037	662	175	192	8		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	68	Total	C	N	O	S	0	0
			556	360	99	93	4		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	83	Total	C	N	O	S	0	0
			651	427	105	115	4		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	46	Total	C	N	O	S	0	0
			381	249	66	65	1		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	119	Total	C	N	O	S	0	0
			985	645	167	164	9		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	104	Total	C	N	O	S	0	0
			870	550	161	151	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	50	Total	C	N	O	S	0	0
			424	273	76	73	2		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	101	Total	C	N	O	S	0	0
			850	549	136	161	4		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	137	Total	C	N	O	S	0	0
			1153	756	192	202	3		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	96	Total	C	N	O	S	0	0
			811	529	139	140	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	63	Total	C	N	O	S	0	0
			542	358	89	94	1		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	78	Total	C	N	O	S	0	0
			630	416	107	105	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	l	156	Total	C	N	O	S	0	0
			1312	846	219	236	11		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	m	125	Total	C	N	O	0	0
			1044	673	188	183		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	176	Total	C	N	O	S	0	0
			1527	976	274	266	11		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	114	Total	C	N	O	S	0	0
			984	620	185	171	8		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	168	Total	C	N	O	S	0	0
			1424	896	256	264	8		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	q	143	Total	C	N	O	S	0	0
			1192	766	212	210	4		

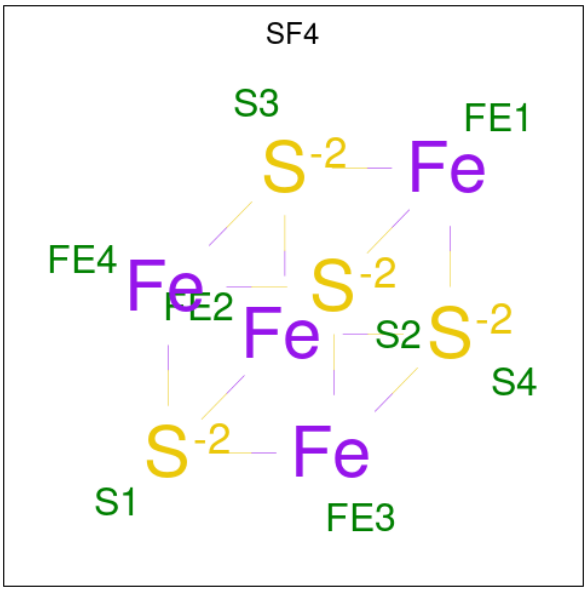
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	r	96	Total	C	N	O	S	0	0
			776	490	145	138	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

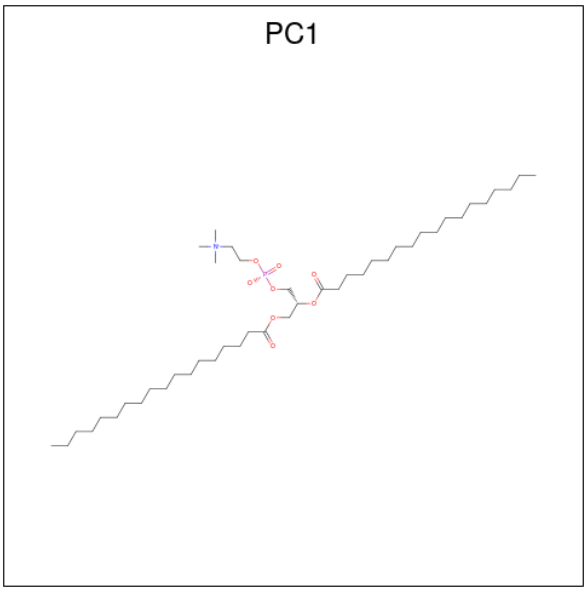
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	39	Total	C	N	O	0	0
			329	207	59	63		

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



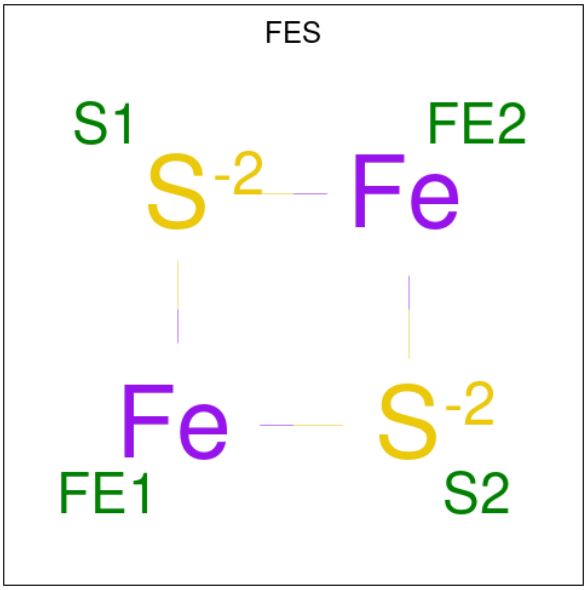
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



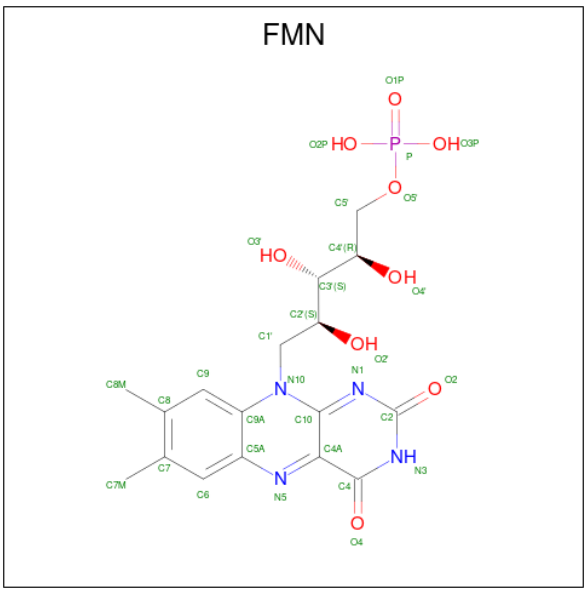
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
46	I	1	Total	C	N	O	P	0
			54	44	1	8	1	

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



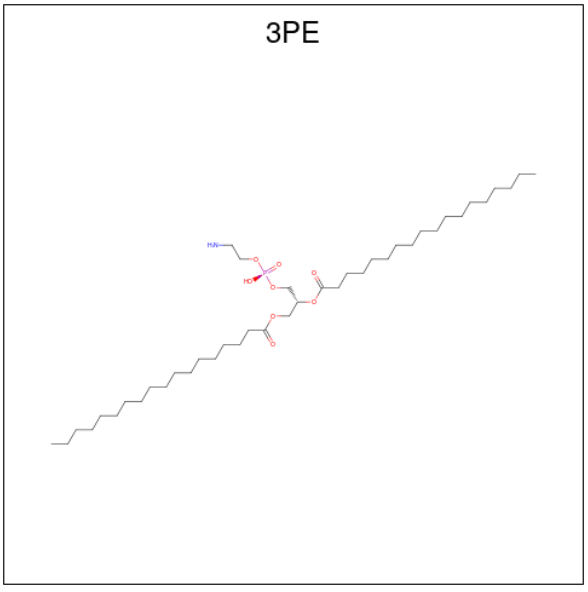
Mol	Chain	Residues	Atoms			AltConf
47	E	1	Total	Fe	S	0
			4	2	2	
47	G	1	Total	Fe	S	0
			4	2	2	

- 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	0
			31	17	4	9	1	

- Molecule 49 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



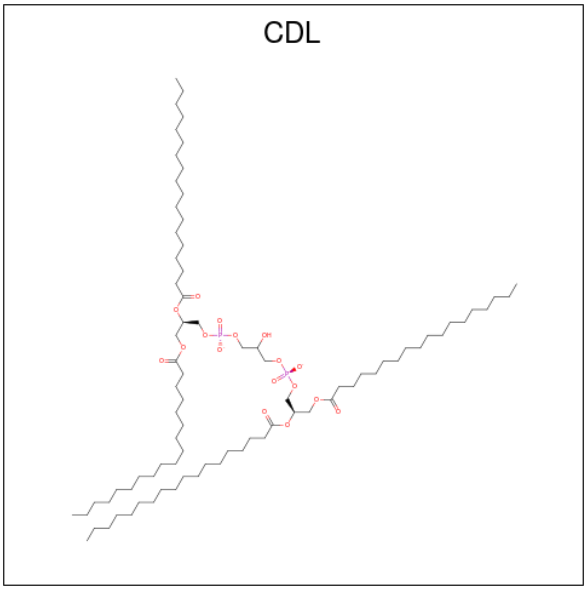
Mol	Chain	Residues	Atoms					AltConf
49	H	1	Total	C	N	O	P	0
			51	41	1	8	1	

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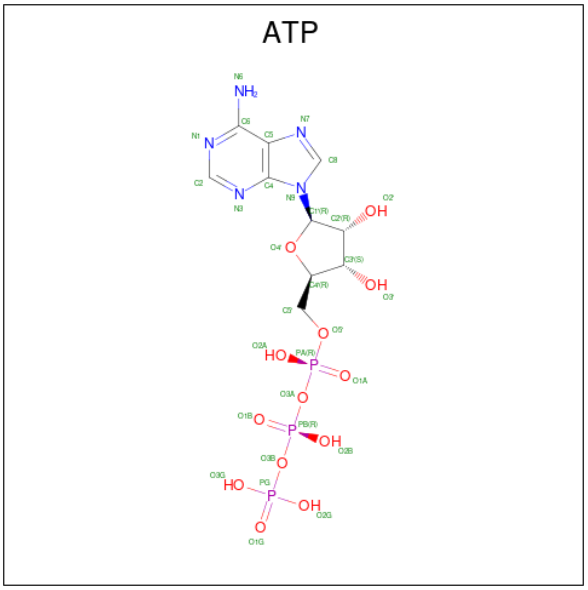
Mol	Chain	Residues	Atoms					AltConf
49	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	L	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	M	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	N	1	Total	C	N	O	P	0
			51	41	1	8	1	
49	f	1	Total	C	N	O	P	0
			39	29	1	8	1	
49	i	1	Total	C	N	O	P	0
			42	32	1	8	1	

- Molecule 50 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



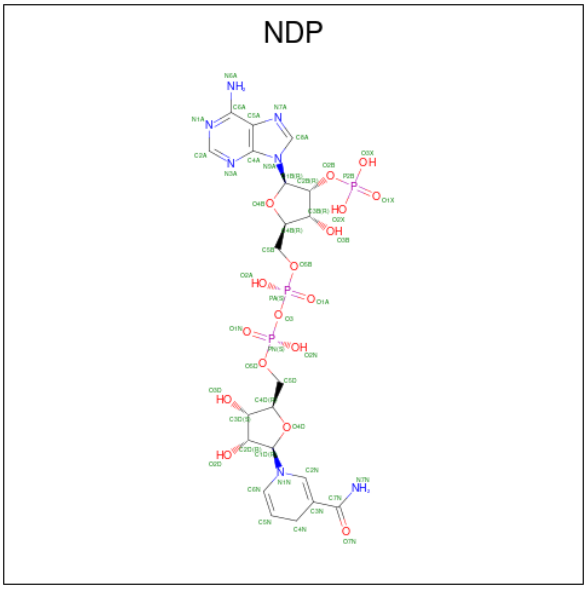
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O	P	0
			81	62	17	2	
50	d	1	Total	C	O	P	0
			100	81	17	2	
50	h	1	Total	C	O	P	0
			78	59	17	2	
50	q	1	Total	C	O	P	0
			69	50	17	2	

- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (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: $C_{21}H_{30}N_7O_{17}P_3$).

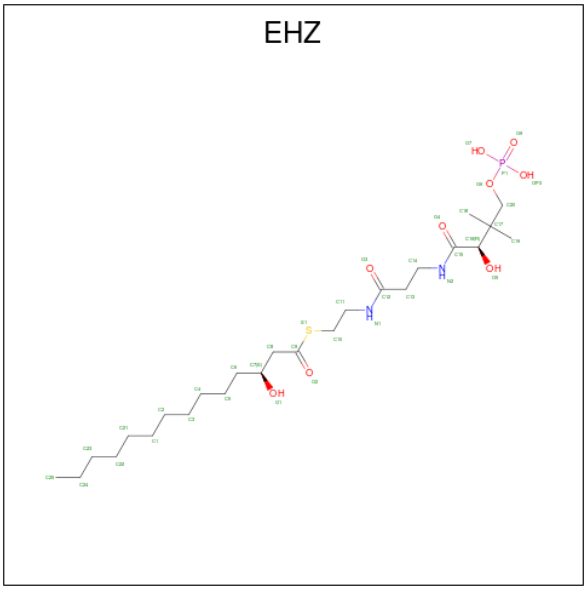


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

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

- 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 37 25 2 8 1 1	0
54	U	1	Total C N O P S 37 25 2 8 1 1	0

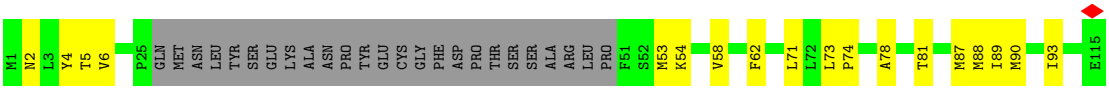
3 Residue-property plots (i)

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

• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A:

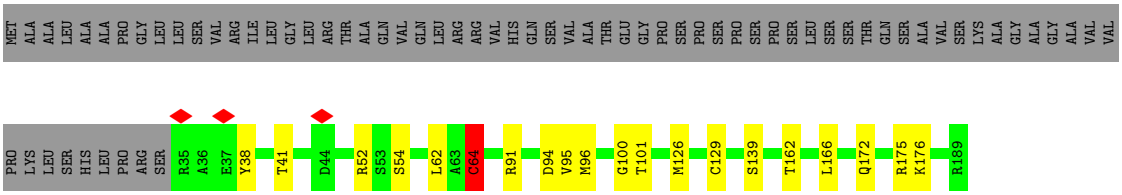




• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain B:

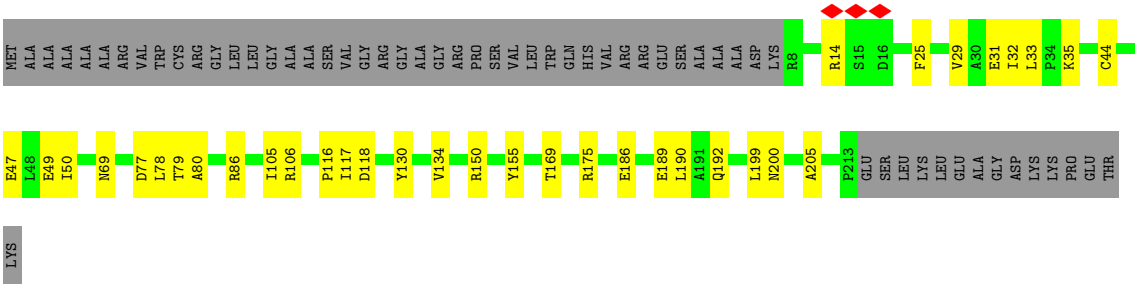




• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C:

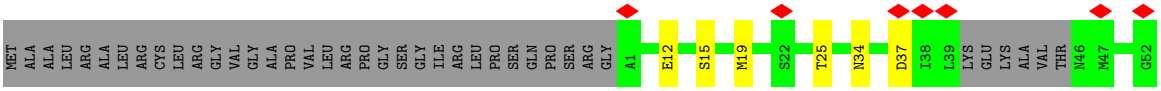


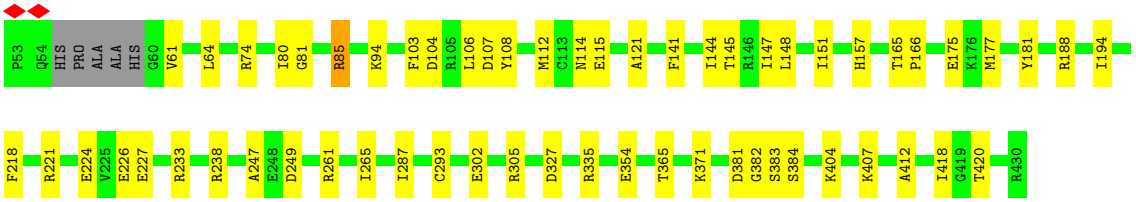


• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

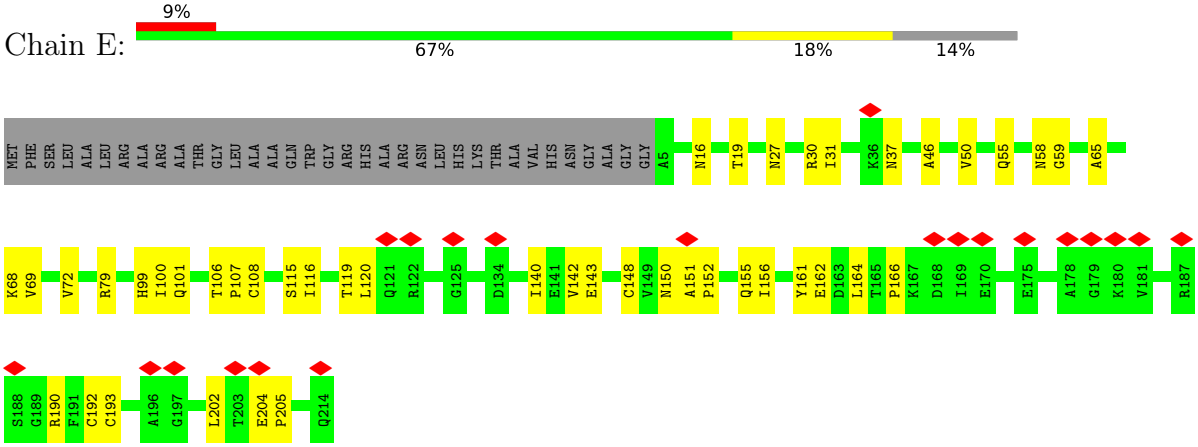
Chain D:



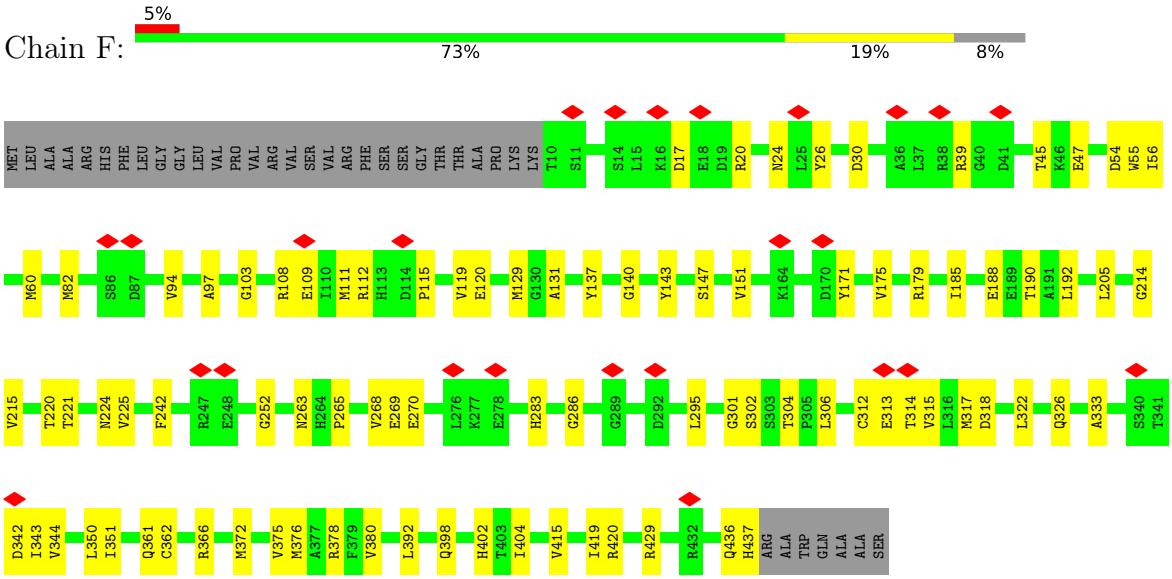




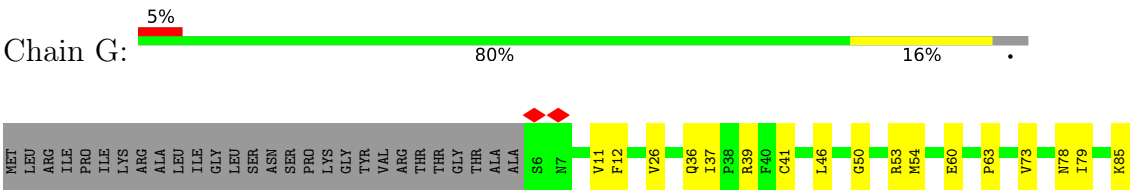
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

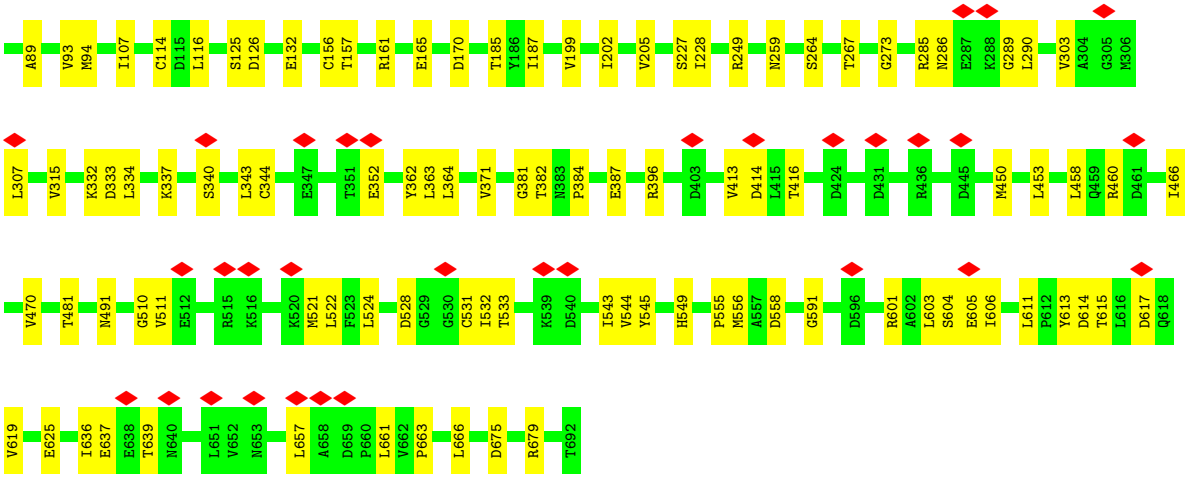


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



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

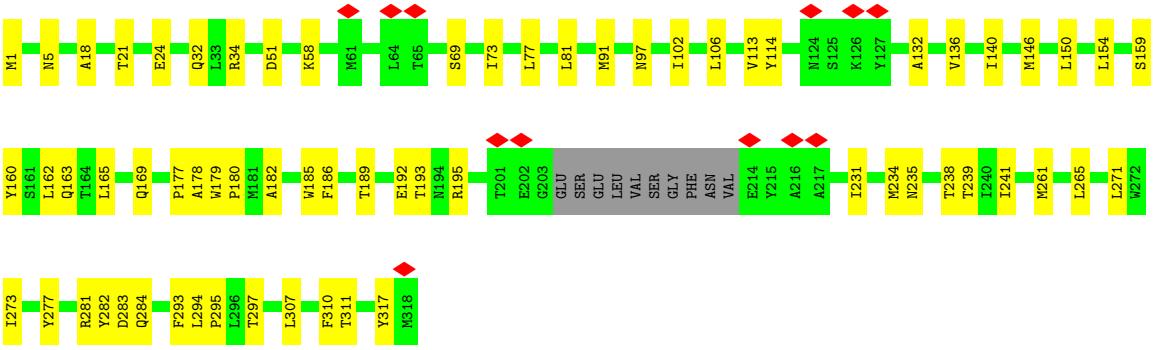




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:

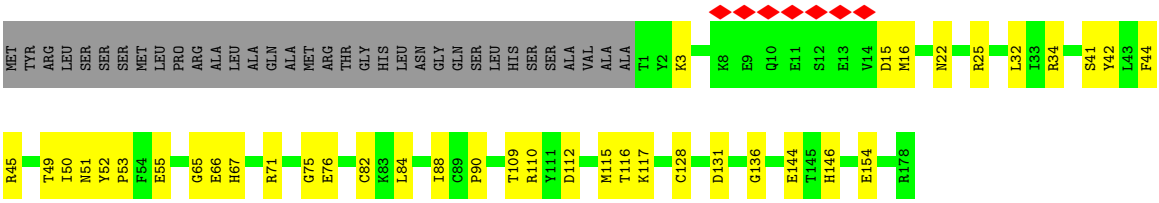




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:



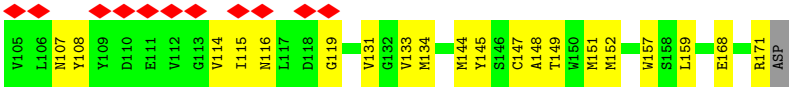


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:







• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

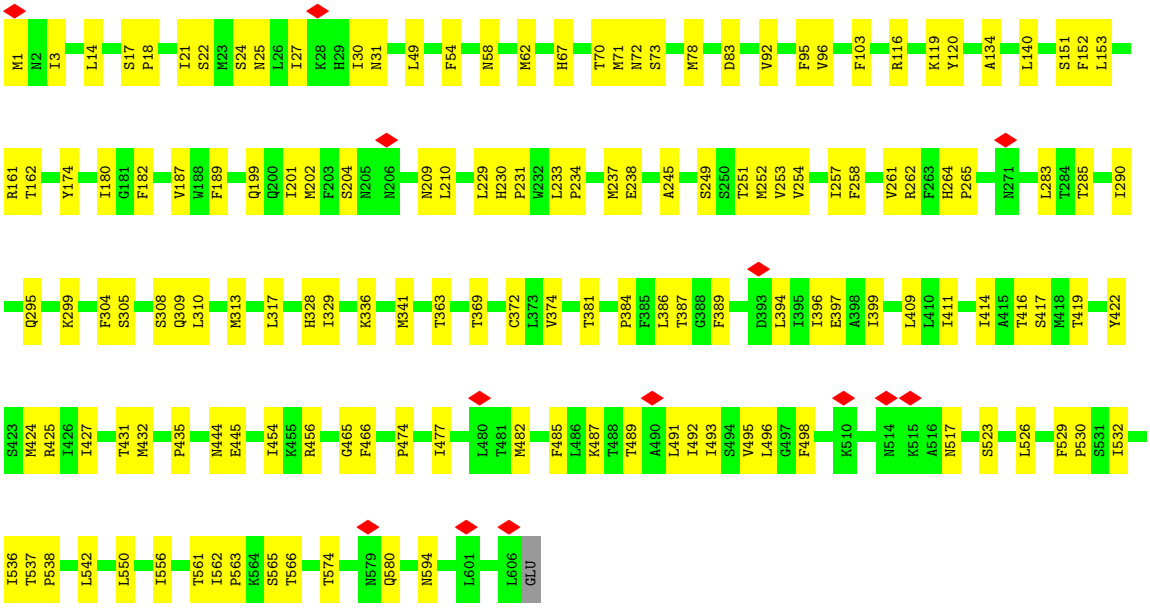




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:

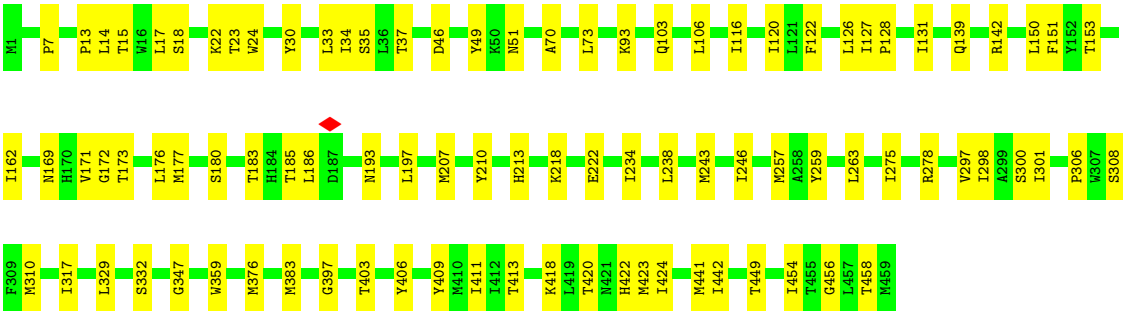




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:

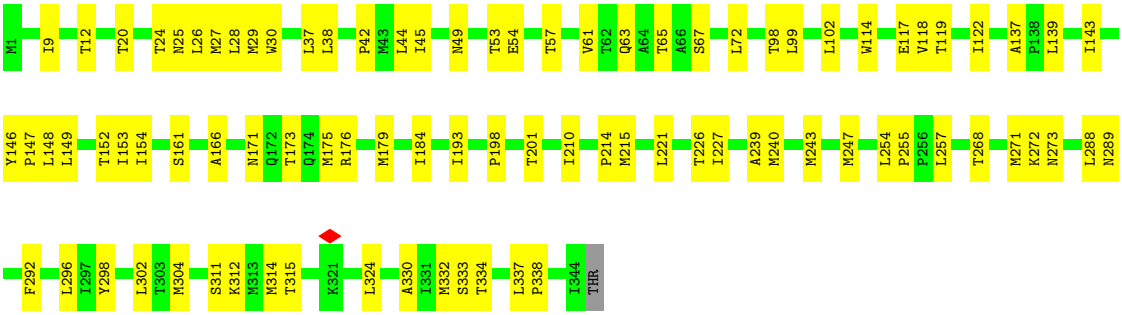




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:

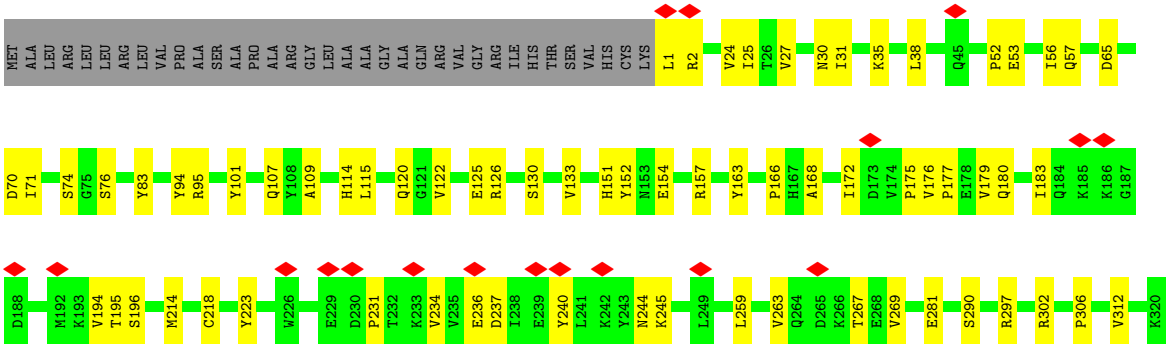




• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:

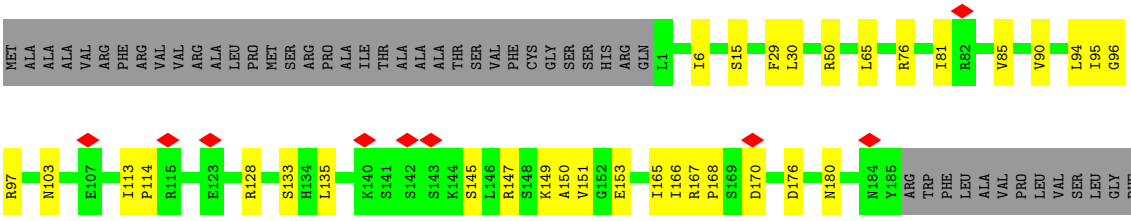


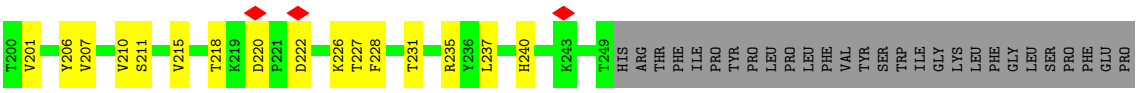


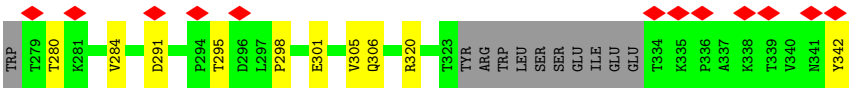
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:





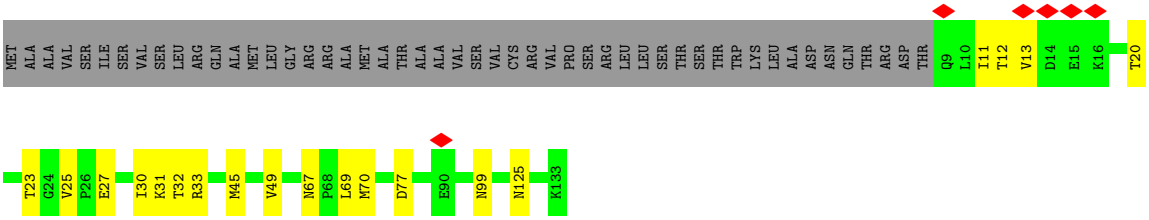




• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:





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

Chain R:

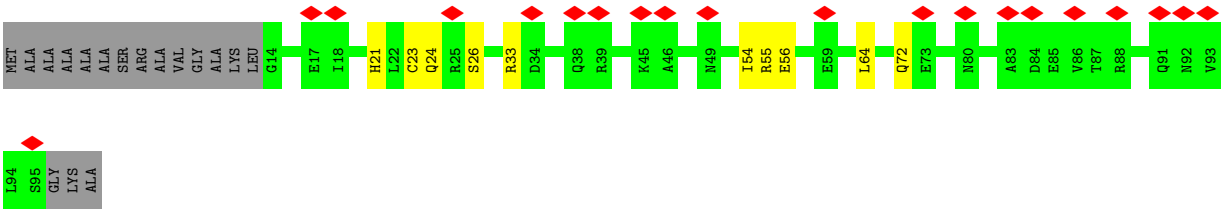




• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:

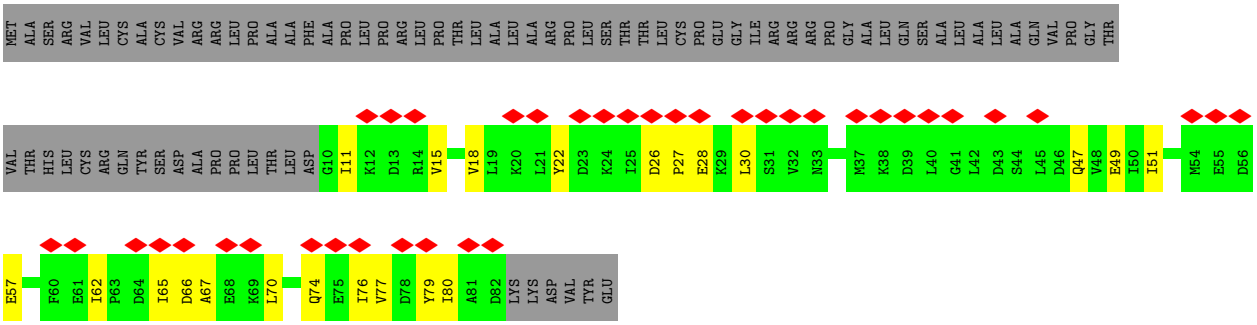




• Molecule 20: Acyl carrier protein, mitochondrial

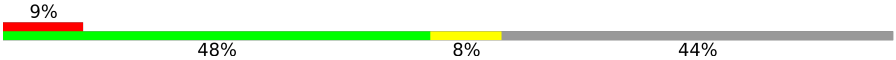
Chain T:

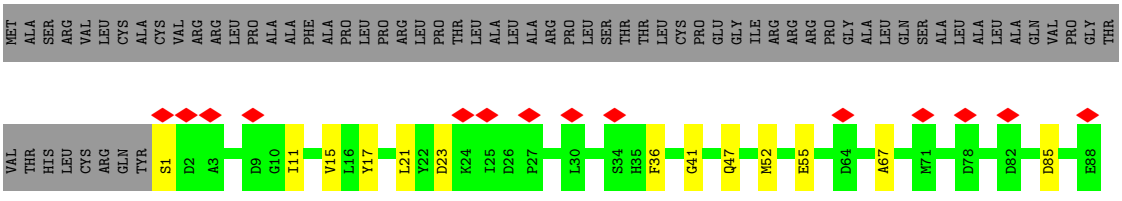




• Molecule 20: Acyl carrier protein, mitochondrial

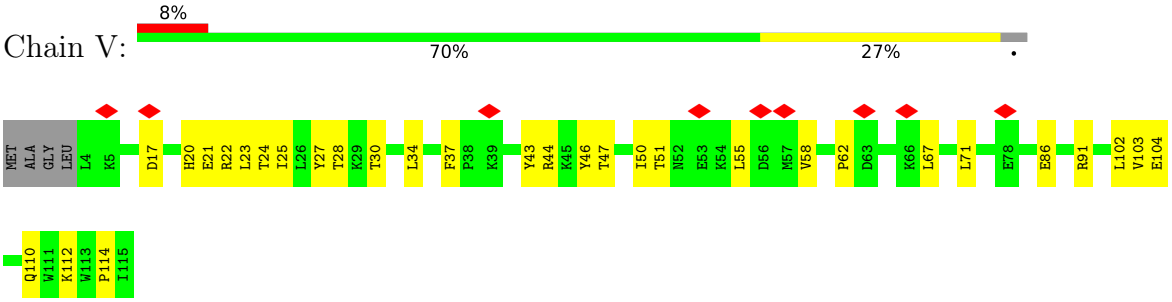
Chain U:





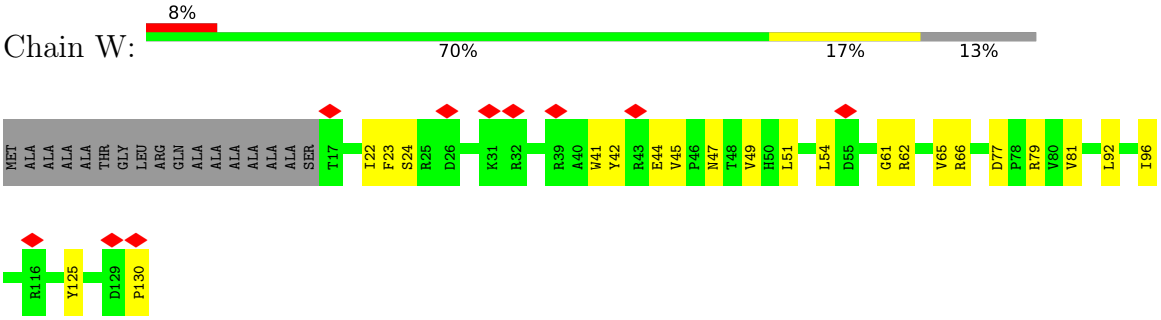
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



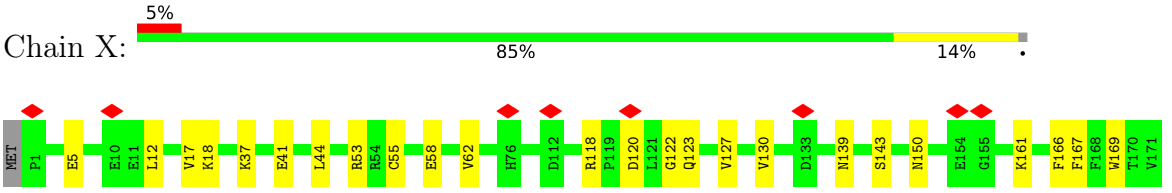
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



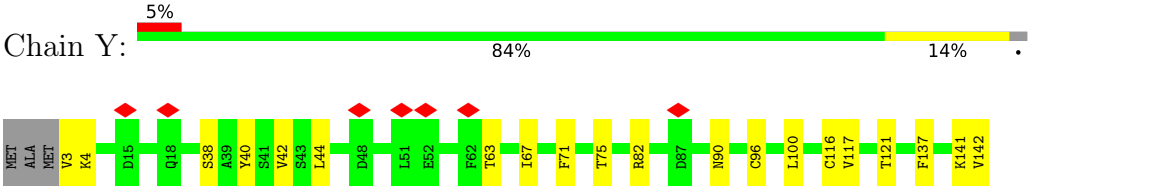
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



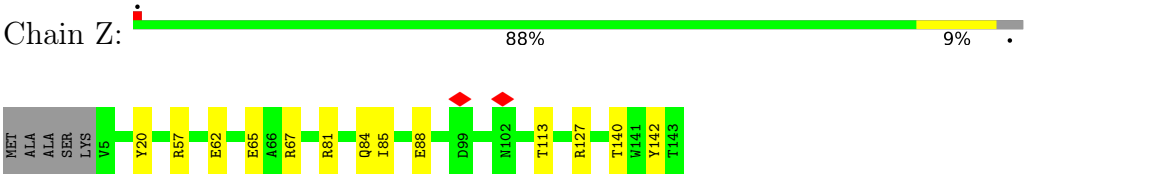
• Molecule 24: MCG5603

Chain Y:



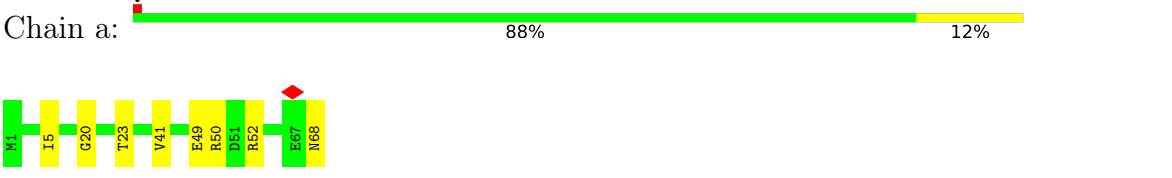
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

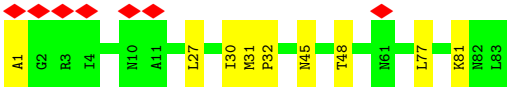
Chain a:



• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

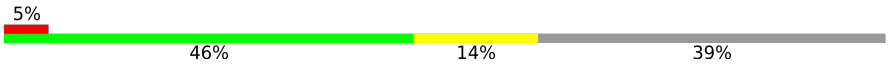
Chain b:

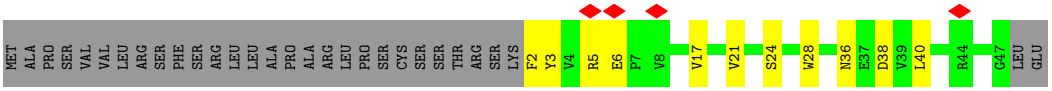




• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:

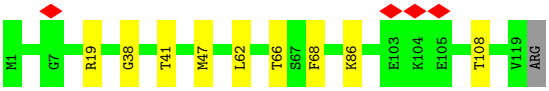




• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:

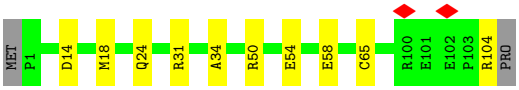




• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:

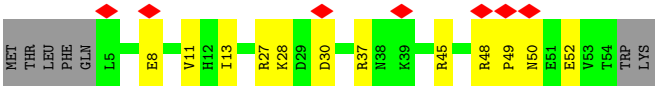




• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

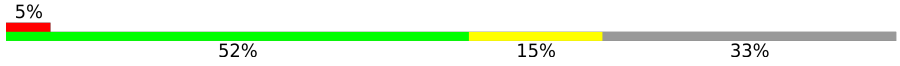
Chain f:

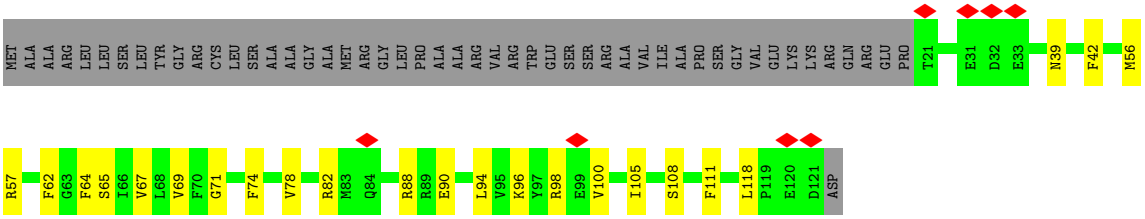




• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

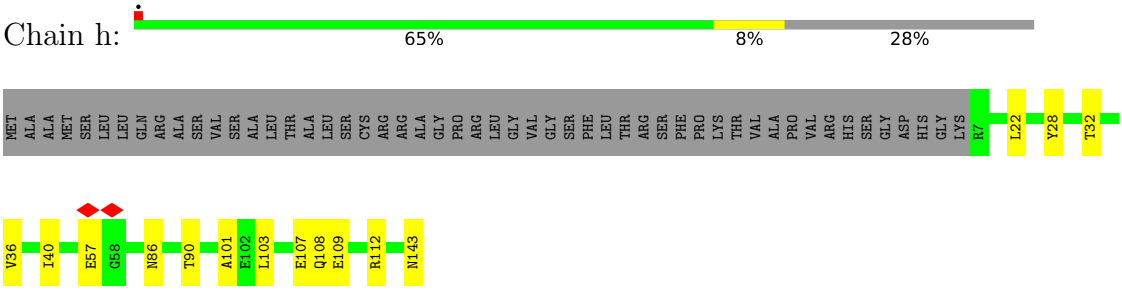
Chain g:





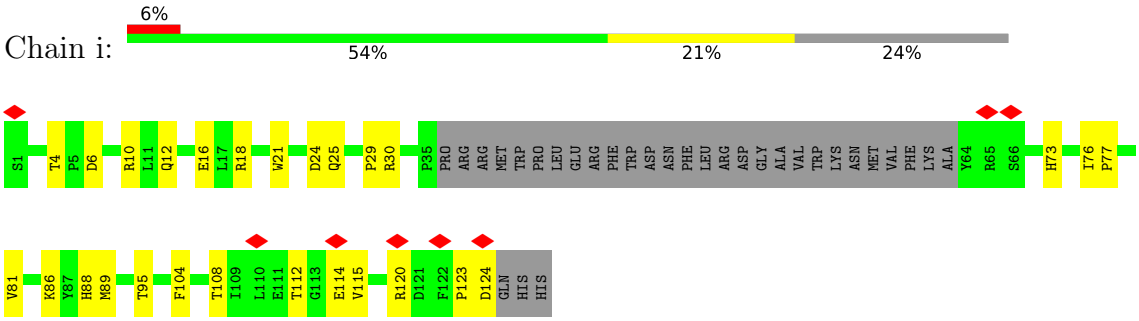
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



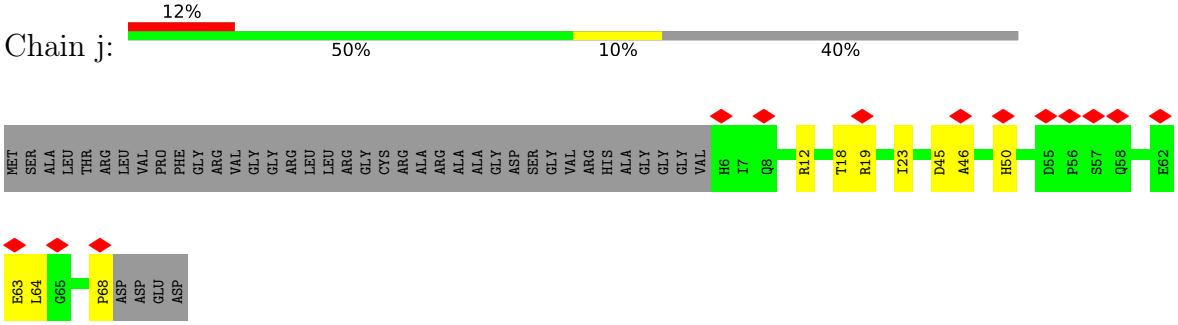
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



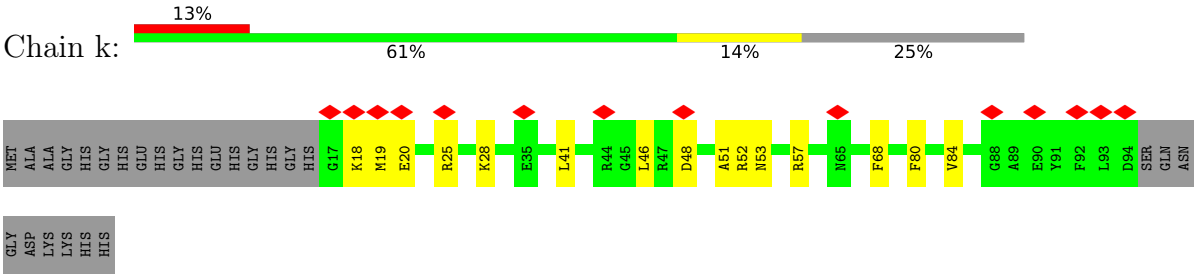
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

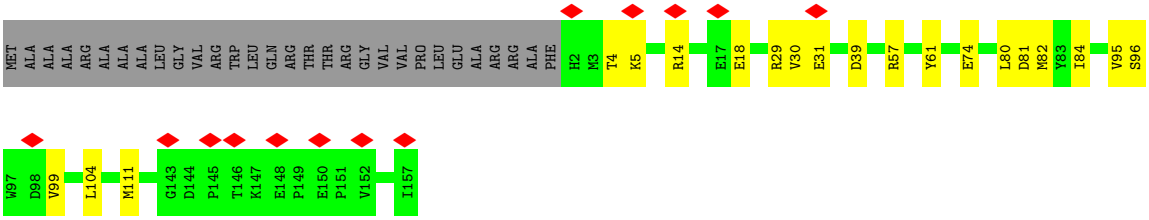
Chain k:



• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain l:

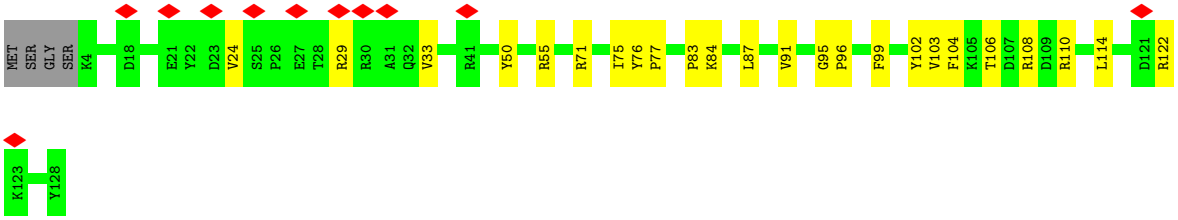




• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m:

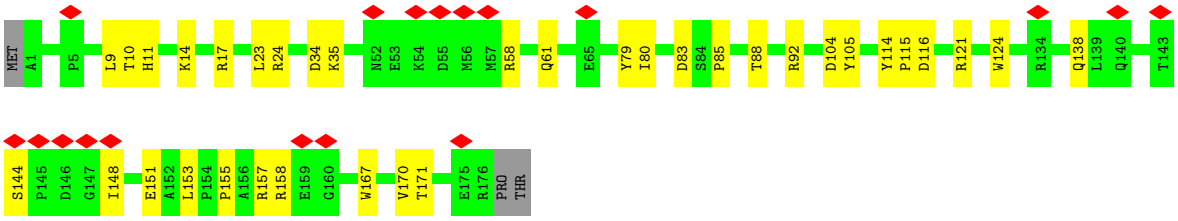




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:

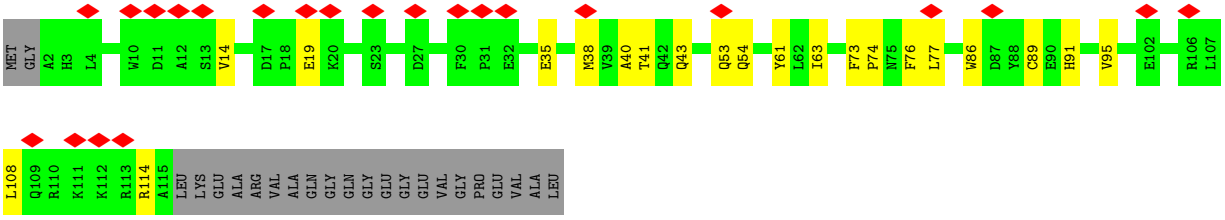




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:

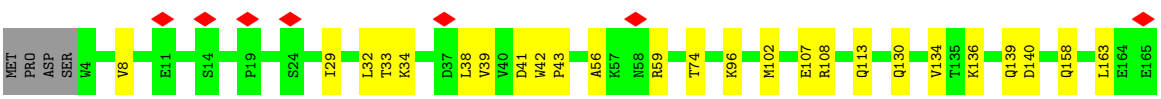


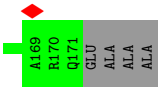


• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain p:



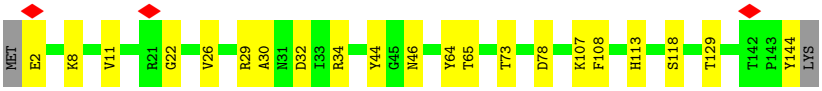




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:

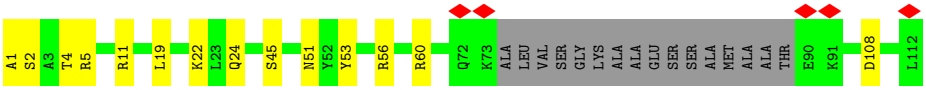




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

Chain r:

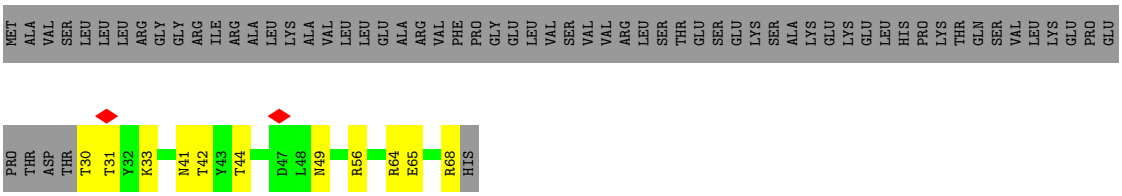




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	50184	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.271	Depositor
Minimum map value	-0.107	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.0355	Depositor
Map size (Å)	486.0, 486.0, 486.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.35, 1.35, 1.35	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, CDL, 2MR, FME, ATP, EHZ, AYA, SF4, FES, SAC, 3PE, PC1, NDP, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.16	0/746	0.35	0/1019
2	B	0.21	0/1272	0.39	0/1722
3	C	0.18	0/1762	0.34	0/2401
4	D	0.20	0/3452	0.35	0/4672
5	E	0.14	0/1679	0.33	0/2288
6	F	0.15	0/3376	0.34	0/4561
7	G	0.16	0/5374	0.33	0/7281
8	H	0.19	0/2530	0.34	0/3458
9	I	0.21	0/1438	0.33	0/1946
10	J	0.16	0/1297	0.31	0/1765
11	K	0.17	0/738	0.31	0/1002
12	L	0.16	0/4913	0.35	0/6686
13	M	0.19	0/3709	0.34	0/5052
14	N	0.19	0/2748	0.32	0/3741
15	O	0.14	0/2674	0.32	0/3626
16	P	0.15	0/2345	0.32	0/3166
17	Q	0.16	0/1038	0.30	0/1401
18	R	0.18	0/751	0.32	0/1011
19	S	0.13	0/670	0.32	0/904
20	T	0.12	0/597	0.36	0/804
20	U	0.15	0/718	0.27	0/970
21	V	0.15	0/937	0.32	0/1270
22	W	0.16	0/993	0.40	0/1335
23	X	0.16	0/1434	0.37	1/1937 (0.1%)
24	Y	0.15	0/1061	0.29	0/1439
25	Z	0.16	0/1183	0.32	0/1597
26	a	0.17	0/569	0.30	0/766
27	b	0.15	0/666	0.31	0/914
28	c	0.13	0/392	0.29	0/533
29	d	0.17	0/1017	0.27	0/1373
30	e	0.16	0/892	0.34	0/1187
31	f	0.15	0/434	0.36	0/584

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	g	0.15	0/878	0.36	0/1196
33	h	0.16	0/1188	0.32	0/1610
34	i	0.15	0/828	0.35	0/1125
35	j	0.12	0/566	0.30	0/775
36	k	0.13	0/650	0.31	0/878
37	l	0.15	0/1367	0.31	0/1866
38	m	0.15	0/1073	0.34	0/1455
39	n	0.15	0/1581	0.33	0/2140
40	o	0.17	0/1009	0.39	0/1355
41	p	0.15	0/1457	0.34	0/1969
42	q	0.17	0/1234	0.31	0/1681
43	r	0.16	0/786	0.32	0/1062
44	s	0.13	0/338	0.29	0/458
All	All	0.16	0/66360	0.33	1/89981 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	X	55	CYS	CA-CB-SG	5.91	128.00	114.40

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	737	0	787	14	0
2	B	1241	0	1250	18	0
3	C	1712	0	1667	25	0
4	D	3381	0	3330	52	0
5	E	1639	0	1631	37	0
6	F	3301	0	3252	64	0
7	G	5287	0	5316	80	0
8	H	2465	0	2556	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	I	1408	0	1344	35	0
10	J	1277	0	1288	31	0
11	K	737	0	768	19	0
12	L	4800	0	4985	113	0
13	M	3632	0	3853	69	0
14	N	2696	0	2895	67	0
15	O	2607	0	2566	47	0
16	P	2297	0	2325	42	0
17	Q	1015	0	1016	15	0
18	R	738	0	717	9	0
19	S	659	0	674	8	0
20	T	588	0	580	15	0
20	U	706	0	698	9	0
21	V	915	0	954	23	0
22	W	970	0	991	16	0
23	X	1396	0	1383	19	0
24	Y	1037	0	1024	13	0
25	Z	1152	0	1148	12	0
26	a	556	0	568	7	0
27	b	651	0	653	8	0
28	c	381	0	374	9	0
29	d	985	0	988	10	0
30	e	870	0	868	9	0
31	f	424	0	421	8	0
32	g	850	0	783	16	0
33	h	1153	0	1150	13	0
34	i	811	0	816	22	0
35	j	542	0	497	8	0
36	k	630	0	623	11	0
37	l	1312	0	1204	15	0
38	m	1044	0	1056	16	0
39	n	1527	0	1459	25	0
40	o	984	0	970	18	0
41	p	1424	0	1393	20	0
42	q	1192	0	1145	19	0
43	r	776	0	806	12	0
44	s	329	0	313	9	0
45	B	8	0	0	1	0
45	F	8	0	0	1	0
45	G	16	0	0	1	0
45	I	16	0	0	0	0
46	B	51	0	79	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	I	54	0	88	1	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	2	0
49	H	51	0	82	0	0
49	I	51	0	82	0	0
49	L	51	0	82	0	0
49	M	102	0	164	1	0
49	N	51	0	82	0	0
49	f	39	0	55	0	0
49	i	42	0	61	1	0
50	L	81	0	112	2	0
50	d	100	0	156	1	0
50	h	78	0	103	1	0
50	q	69	0	85	1	0
51	O	31	0	12	2	0
52	P	48	0	26	6	0
53	R	1	0	0	0	0
54	T	37	0	0	1	0
54	U	37	0	0	0	0
All	All	65895	0	66373	978	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 7.

All (978) 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)
8:H:293:PHE:O	8:H:297:THR:OG1	1.87	0.92
6:F:82:MET:SD	6:F:221:THR:OG1	2.28	0.91
12:L:245:ALA:O	12:L:249:SER:OG	1.87	0.91
8:H:307:LEU:O	8:H:311:THR:OG1	1.90	0.89
15:O:240:TYR:OH	21:V:22:ARG:NH2	2.05	0.89
16:P:176:ASP:OD1	16:P:180:ASN:ND2	2.09	0.86
7:G:63:PRO:O	7:G:85:LYS:NZ	2.09	0.85
13:M:278:ARG:O	38:m:71:ARG:NH2	2.09	0.85
3:C:205:ALA:O	43:r:60:ARG:NH1	2.09	0.84
7:G:528:ASP:OD1	7:G:545:TYR:OH	1.94	0.84
15:O:30:ASN:O	15:O:35:LYS:NZ	2.10	0.84
3:C:192:GLN:OE1	9:I:117:LYS:NZ	2.10	0.84
7:G:315:VAL:O	7:G:340:SER:OG	1.95	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:U:55:GLU:OE1	39:n:24:ARG:NH2	2.11	0.84
12:L:594:ASN:ND2	24:Y:40:TYR:OH	2.11	0.83
34:i:86:LYS:NZ	41:p:41:ASP:OD1	2.11	0.83
6:F:20:ARG:NH1	6:F:269:GLU:O	2.11	0.83
16:P:180:ASN:OD1	16:P:320:ARG:NH1	2.11	0.82
19:S:26:SER:O	19:S:33:ARG:NH2	2.12	0.82
12:L:474:PRO:O	40:o:54:GLN:NE2	2.12	0.82
34:i:89:MET:O	34:i:95:THR:OG1	1.98	0.82
6:F:380:VAL:O	6:F:429:ARG:NH1	2.13	0.81
37:l:61:TYR:OH	39:n:151:GLU:OE2	1.98	0.81
7:G:396:ARG:NH1	7:G:416:THR:O	2.13	0.81
8:H:169:GLN:NE2	8:H:241:ILE:O	2.14	0.81
37:l:81:ASP:OD2	38:m:71:ARG:NH1	2.14	0.81
3:C:31:GLU:OE2	21:V:46:TYR:OH	1.99	0.80
42:q:46:ASN:OD1	42:q:65:THR:OG1	1.98	0.80
3:C:14:ARG:NH1	3:C:44:CYS:O	2.15	0.80
9:I:55:GLU:OE2	42:q:34:ARG:NH2	2.16	0.79
48:F:501:FMN:N1	48:F:501:FMN:O3'	2.15	0.79
12:L:416:THR:O	12:L:419:THR:OG1	2.01	0.79
44:s:41:ASN:OD1	44:s:44:THR:OG1	2.00	0.79
21:V:112:LYS:NZ	21:V:114:PRO:O	2.15	0.79
20:U:23:ASP:OD1	36:k:52:ARG:NH2	2.16	0.79
19:S:23:CYS:SG	19:S:24:GLN:N	2.56	0.79
7:G:333:ASP:OD2	7:G:613:TYR:OH	2.00	0.78
7:G:364:LEU:HD23	7:G:491:ASN:HB3	1.66	0.78
12:L:62:MET:SD	12:L:199:GLN:NE2	2.56	0.78
20:T:49:GLU:OE2	22:W:66:ARG:NH2	2.16	0.78
15:O:83:TYR:OH	51:O:401:ATP:O2'	2.02	0.78
16:P:76:ARG:NH1	16:P:103:ASN:O	2.18	0.77
25:Z:20:TYR:OH	43:r:108:ASP:OD2	2.02	0.77
2:B:91:ARG:NH2	2:B:91:ARG:O	2.18	0.77
8:H:231:ILE:O	8:H:235:ASN:ND2	2.18	0.76
39:n:9:LEU:O	39:n:14:LYS:NZ	2.18	0.76
7:G:37:ILE:O	7:G:39:ARG:NH1	2.18	0.76
5:E:101:GLN:NE2	5:E:155:GLN:OE1	2.19	0.76
54:T:201:EHZ:O2	54:T:201:EHZ:O1	2.00	0.75
7:G:156:CYS:O	7:G:157:THR:OG1	2.03	0.75
15:O:83:TYR:HH	51:O:401:ATP:HO2'	1.35	0.75
32:g:82:ARG:O	41:p:96:LYS:NZ	2.19	0.75
34:i:12:GLN:NE2	34:i:16:GLU:OE1	2.20	0.75
9:I:53:PRO:O	42:q:64:TYR:OH	2.03	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:30:TRP:NE1	14:N:67:SER:OG	2.19	0.74
1:A:4:TYR:HH	10:J:4:TYR:HH	0.77	0.74
13:M:424:ILE:O	39:n:105:TYR:OH	2.05	0.74
15:O:38:LEU:HD23	15:O:172:ILE:HD11	1.69	0.74
1:A:54:LYS:O	1:A:58:VAL:HG23	1.87	0.74
12:L:305:SER:OG	12:L:336:LYS:NZ	2.21	0.74
7:G:285:ARG:NH1	7:G:555:PRO:O	2.21	0.74
10:J:107:ASN:OD1	10:J:108:TYR:N	2.21	0.73
15:O:76:SER:O	15:O:95:ARG:NH1	2.20	0.73
4:D:327:ASP:OD1	43:r:53:TYR:OH	2.03	0.73
10:J:22:LYS:NZ	11:K:21:MET:O	2.19	0.73
9:I:22:ASN:OD1	9:I:25:ARG:NH2	2.20	0.73
21:V:43:TYR:O	21:V:47:THR:HG22	1.88	0.73
12:L:134:ALA:O	12:L:262:ARG:NH2	2.21	0.73
25:Z:57:ARG:NH2	27:b:45:ASN:OD1	2.22	0.73
13:M:306:PRO:HA	13:M:458:THR:HG21	1.70	0.72
16:P:97:ARG:NH2	52:P:501:NDP:O1A	2.22	0.72
18:R:20:GLU:O	18:R:25:ARG:NH2	2.22	0.72
10:J:168:GLU:OE1	10:J:171:ARG:NH1	2.23	0.72
14:N:312:LYS:O	14:N:315:THR:OG1	2.07	0.72
9:I:34:ARG:NH1	46:I:201:PC1:O12	2.22	0.72
35:j:68:PRO:O	40:o:114:ARG:NH2	2.23	0.71
39:n:138:GLN:NE2	39:n:155:PRO:O	2.23	0.71
12:L:72:ASN:O	12:L:73:SER:OG	2.00	0.71
8:H:97:ASN:ND2	8:H:163:GLN:OE1	2.24	0.71
4:D:381:ASP:OD1	4:D:382:GLY:N	2.24	0.70
7:G:26:VAL:HG13	7:G:79:ILE:HD13	1.74	0.70
5:E:16:ASN:OD1	5:E:19:THR:OG1	2.06	0.70
16:P:95:ILE:O	52:P:501:NDP:O3D	2.08	0.70
50:q:201:CDL:O1	43:r:2:SER:O	2.08	0.70
33:h:57:GLU:N	33:h:57:GLU:OE1	2.24	0.70
38:m:50:TYR:O	38:m:55:ARG:NH1	2.25	0.70
15:O:31:ILE:HD11	15:O:183:ILE:HD11	1.74	0.70
13:M:420:THR:OG1	13:M:423:MET:SD	2.50	0.69
18:R:32:GLN:NE2	18:R:34:GLU:OE1	2.24	0.69
14:N:118:VAL:HG12	14:N:122:ILE:HD12	1.74	0.69
36:k:25:ARG:O	36:k:28:LYS:NZ	2.25	0.69
4:D:226:GLU:OE1	4:D:305:ARG:NH2	2.25	0.69
33:h:109:GLU:OE1	33:h:112:ARG:NH1	2.25	0.69
44:s:65:GLU:OE1	44:s:68:ARG:NH1	2.26	0.69
4:D:107:ASP:OD1	4:D:371:LYS:NZ	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:302:GLU:OE2	9:I:3:LYS:NZ	2.20	0.69
20:T:47:GLN:NE2	20:T:67:ALA:O	2.25	0.69
34:i:120:ARG:NH2	40:o:38:MET:O	2.25	0.69
7:G:307:LEU:HB2	7:G:521:MET:HE1	1.74	0.69
9:I:116:THR:HG21	9:I:146:HIS:NE2	2.08	0.68
15:O:306:PRO:O	28:c:3:TYR:OH	2.09	0.68
8:H:154:LEU:HD12	8:H:159:SER:O	1.94	0.68
23:X:37:LYS:NZ	23:X:41:GLU:OE2	2.25	0.68
39:n:144:SER:OG	39:n:148:ILE:O	2.10	0.68
9:I:71:ARG:NH1	9:I:75:GLY:O	2.26	0.68
25:Z:84:GLN:OE1	30:e:104:ARG:NH2	2.26	0.68
30:e:31:ARG:NH2	30:e:65:CYS:O	2.27	0.68
5:E:68:LYS:O	5:E:72:VAL:HG23	1.94	0.68
6:F:45:THR:OG1	6:F:120:GLU:OE1	2.10	0.68
21:V:27:TYR:O	21:V:30:THR:OG1	2.11	0.68
36:k:80:PHE:O	36:k:84:VAL:HG23	1.94	0.68
12:L:290:ILE:O	12:L:523:SER:OG	2.10	0.68
9:I:51:ASN:N	9:I:55:GLU:OE1	2.26	0.68
23:X:58:GLU:N	23:X:58:GLU:OE1	2.26	0.67
14:N:221:LEU:HD22	14:N:240:MET:HE1	1.76	0.67
42:q:29:ARG:NH2	42:q:73:THR:O	2.26	0.67
39:n:9:LEU:HD21	39:n:17:ARG:NH1	2.10	0.67
4:D:106:LEU:O	4:D:114:ASN:ND2	2.28	0.67
15:O:65:ASP:OD1	28:c:2:PHE:N	2.28	0.67
16:P:235:ARG:NH1	16:P:291:ASP:O	2.27	0.67
3:C:150:ARG:NH1	3:C:155:TYR:O	2.28	0.67
12:L:363:THR:OG1	12:L:431:THR:O	2.09	0.67
2:B:139:SER:OG	4:D:85:2MR:O	2.05	0.67
32:g:108:SER:OG	41:p:140:ASP:OD2	2.13	0.67
2:B:176:LYS:NZ	9:I:144:GLU:OE1	2.27	0.67
10:J:96:VAL:O	10:J:100:VAL:HG23	1.93	0.67
12:L:116:ARG:NH2	12:L:120:TYR:OH	2.28	0.66
1:A:73:LEU:O	8:H:160:TYR:OH	2.11	0.66
23:X:118:ARG:NH1	25:Z:62:GLU:OE1	2.28	0.66
14:N:198:PRO:O	14:N:201:THR:OG1	2.12	0.66
15:O:281:GLU:N	15:O:281:GLU:OE1	2.29	0.66
12:L:561:THR:O	12:L:565:SER:OG	2.09	0.66
16:P:81:ILE:O	16:P:85:VAL:HG22	1.95	0.66
12:L:466:PHE:CZ	40:o:77:LEU:HD21	2.31	0.66
4:D:141:PHE:O	4:D:145:THR:HG23	1.96	0.65
9:I:116:THR:HG21	9:I:146:HIS:CD2	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:p:29:ILE:O	41:p:33:THR:HG23	1.96	0.65
12:L:381:THR:HG21	12:L:498:PHE:CZ	2.30	0.65
13:M:317:ILE:HG13	13:M:454:ILE:HD11	1.78	0.65
5:E:150:ASN:OD1	5:E:190:ARG:NH1	2.30	0.65
8:H:32:GLN:OE1	8:H:34:ARG:NH2	2.29	0.65
14:N:44:LEU:HD22	14:N:122:ILE:HD13	1.77	0.65
12:L:204:SER:O	12:L:209:ASN:ND2	2.30	0.65
15:O:94:TYR:HH	15:O:151:HIS:HD1	0.66	0.65
15:O:223:TYR:OH	15:O:237:ASP:OD2	2.14	0.65
6:F:30:ASP:O	6:F:39:ARG:NH2	2.30	0.65
12:L:257:ILE:CG2	12:L:329:ILE:HD11	2.27	0.65
21:V:37:PHE:O	21:V:44:ARG:NH2	2.29	0.65
17:Q:27:GLU:HA	17:Q:30:ILE:HG22	1.77	0.65
30:e:58:GLU:N	30:e:58:GLU:OE1	2.30	0.65
38:m:99:PHE:O	38:m:103:VAL:HG23	1.97	0.65
7:G:533:THR:HA	7:G:556:MET:HE1	1.78	0.64
12:L:78:MET:HE1	49:i:201:3PE:H382	1.77	0.64
13:M:73:LEU:HD22	13:M:103:GLN:OE1	1.97	0.64
14:N:311:SER:O	14:N:315:THR:HG23	1.96	0.64
32:g:118:LEU:HD23	41:p:163:LEU:HD12	1.79	0.64
3:C:130:TYR:O	3:C:134:VAL:HG23	1.96	0.64
6:F:392:LEU:HD23	6:F:419:ILE:HD11	1.78	0.64
23:X:120:ASP:OD2	27:b:81:LYS:NZ	2.29	0.64
13:M:173:THR:HG23	33:h:101:ALA:HB2	1.79	0.64
28:c:38:ASP:OD1	29:d:19:ARG:NH1	2.31	0.64
12:L:556:ILE:HD11	38:m:75:ILE:HG22	1.81	0.63
13:M:300:SER:O	13:M:308:SER:OG	2.15	0.63
11:K:43:MET:O	11:K:47:THR:HG23	1.98	0.63
39:n:80:ILE:HG21	39:n:85:PRO:O	1.98	0.63
8:H:235:ASN:O	8:H:239:THR:HG23	1.98	0.63
13:M:33:LEU:O	13:M:37:THR:HG23	1.99	0.63
6:F:54:ASP:OD1	6:F:55:TRP:N	2.32	0.63
17:Q:20:THR:HG22	17:Q:99:ASN:O	1.98	0.63
6:F:175:VAL:O	44:s:56:ARG:NH1	2.32	0.63
14:N:53:THR:O	14:N:57:THR:HG23	1.98	0.62
8:H:283:ASP:OD1	8:H:284:GLN:N	2.32	0.62
12:L:424:MET:HE1	36:k:68:PHE:CD1	2.34	0.62
29:d:108:THR:OG1	41:p:74:THR:O	2.15	0.62
4:D:293:CYS:SG	4:D:420:THR:HG21	2.40	0.62
6:F:131:ALA:O	6:F:171:TYR:OH	2.14	0.62
2:B:54:SER:OG	8:H:51:ASP:OD2	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:326:GLN:OE1	6:F:420:ARG:NH1	2.32	0.62
4:D:112:MET:HB3	4:D:145:THR:HG21	1.81	0.62
32:g:88:ARG:NH2	41:p:107:GLU:OE1	2.33	0.62
41:p:8:VAL:O	41:p:108:ARG:NH2	2.32	0.62
13:M:15:THR:O	13:M:93:LYS:NZ	2.33	0.61
34:i:77:PRO:O	34:i:81:VAL:HG23	1.98	0.61
29:d:62:LEU:O	29:d:66:THR:HG23	2.01	0.61
37:l:80:LEU:O	37:l:84:ILE:HG23	2.00	0.61
34:i:4:THR:OG1	34:i:6:ASP:OD1	2.12	0.61
24:Y:82:ARG:NH2	24:Y:90:ASN:OD1	2.34	0.60
13:M:127:ILE:HD11	14:N:254:LEU:HD23	1.83	0.60
38:m:102:TYR:O	38:m:106:THR:HG23	2.02	0.60
15:O:223:TYR:CE2	15:O:234:VAL:HG22	2.37	0.60
5:E:46:ALA:O	5:E:50:VAL:HG23	2.00	0.60
6:F:372:MET:SD	6:F:415:VAL:HG21	2.41	0.60
12:L:435:PRO:O	36:k:57:ARG:NE	2.32	0.60
12:L:491:LEU:O	12:L:495:VAL:HG23	2.01	0.60
14:N:292:PHE:O	14:N:296:LEU:HD13	2.00	0.60
9:I:110:ARG:NH2	17:Q:70:MET:O	2.34	0.60
12:L:387:THR:HG22	12:L:465:GLY:H	1.67	0.60
34:i:104:PHE:CD1	40:o:63:ILE:HG23	2.37	0.60
6:F:143:TYR:OH	44:s:41:ASN:O	2.19	0.59
8:H:18:ALA:O	8:H:21:THR:OG1	2.19	0.59
12:L:580:GLN:OE1	24:Y:44:LEU:HD22	2.03	0.59
39:n:34:ASP:OD1	39:n:35:LYS:N	2.34	0.59
4:D:151:ILE:HD11	4:D:218:PHE:CZ	2.37	0.59
9:I:66:GLU:O	9:I:136:GLY:N	2.33	0.59
13:M:51:ASN:OD1	33:h:90:THR:OG1	2.19	0.59
15:O:154:GLU:OE2	15:O:157:ARG:NH2	2.34	0.59
1:A:53:MET:HE1	11:K:79:VAL:HG11	1.84	0.59
5:E:140:ILE:HG22	5:E:142:VAL:HG23	1.84	0.59
13:M:150:LEU:HD23	13:M:151:PHE:CE1	2.38	0.59
14:N:221:LEU:HD22	14:N:240:MET:CE	2.33	0.59
16:P:166:ILE:HG22	16:P:168:PRO:HD3	1.85	0.59
13:M:278:ARG:NH1	37:l:82:MET:SD	2.76	0.59
7:G:46:LEU:HD11	7:G:202:ILE:HD11	1.84	0.58
24:Y:117:VAL:O	24:Y:121:THR:HG23	2.03	0.58
30:e:34:ALA:HB2	33:h:143:ASN:OD1	2.03	0.58
40:o:38:MET:HE2	40:o:40:ALA:HB3	1.85	0.58
1:A:2:ASN:O	1:A:6:VAL:HG23	2.03	0.58
12:L:22:SER:HA	12:L:27:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:153:GLU:OE1	16:P:167:ARG:NH1	2.32	0.58
3:C:49:GLU:OE2	3:C:106:ARG:NH1	2.35	0.58
28:c:28:TRP:HE1	29:d:66:THR:HG22	1.68	0.58
7:G:371:VAL:HG22	7:G:450:MET:HE1	1.84	0.58
23:X:44:LEU:HD22	23:X:130:VAL:CG1	2.33	0.58
8:H:5:ASN:HD21	26:a:23:THR:HG23	1.69	0.58
23:X:161:LYS:HD3	33:h:103:LEU:HD11	1.85	0.58
37:l:14:ARG:N	37:l:18:GLU:OE2	2.34	0.58
42:q:65:THR:O	42:q:73:THR:OG1	2.21	0.58
6:F:188:GLU:OE1	6:F:190:THR:OG1	2.21	0.57
25:Z:88:GLU:OE1	25:Z:127:ARG:NH2	2.37	0.57
4:D:112:MET:CG	4:D:194:ILE:HD12	2.34	0.57
13:M:35:SER:OG	13:M:70:ALA:O	2.22	0.57
15:O:115:LEU:O	15:O:115:LEU:HD23	2.04	0.57
22:W:49:VAL:HG12	22:W:54:LEU:HD12	1.86	0.57
4:D:354:GLU:OE2	4:D:384:SER:OG	2.22	0.57
6:F:263:ASN:ND2	6:F:286:GLY:O	2.38	0.57
5:E:151:ALA:HB3	5:E:152:PRO:HD3	1.85	0.57
15:O:175:PRO:O	15:O:179:VAL:HG23	2.03	0.57
6:F:143:TYR:OH	44:s:42:THR:O	2.17	0.57
4:D:145:THR:HG22	4:D:181:TYR:OH	2.04	0.57
14:N:243:MET:SD	14:N:330:ALA:HB1	2.45	0.57
26:a:49:GLU:OE1	26:a:52:ARG:NH1	2.36	0.57
34:i:104:PHE:HD1	40:o:63:ILE:HG23	1.68	0.57
44:s:30:THR:OG1	44:s:33:LYS:NZ	2.38	0.57
12:L:304:PHE:CZ	12:L:526:LEU:HD11	2.40	0.57
14:N:117:GLU:OE1	14:N:117:GLU:N	2.36	0.57
7:G:522:LEU:HB2	7:G:543:ILE:HG22	1.87	0.57
15:O:70:ASP:OD1	15:O:71:ILE:N	2.38	0.57
41:p:130:GLN:O	41:p:134:VAL:HG23	2.05	0.57
3:C:86:ARG:NH1	21:V:110:GLN:O	2.38	0.57
7:G:53:ARG:O	7:G:93:VAL:HG21	2.04	0.57
12:L:386:LEU:O	12:L:387:THR:OG1	2.23	0.57
13:M:329:LEU:O	13:M:332:SER:OG	2.23	0.57
17:Q:13:VAL:O	17:Q:13:VAL:HG13	2.05	0.57
20:U:47:GLN:NE2	20:U:67:ALA:O	2.37	0.57
32:g:62:PHE:O	32:g:67:VAL:HG23	2.05	0.57
7:G:615:THR:OG1	7:G:617:ASP:OD1	2.12	0.56
14:N:44:LEU:HD22	14:N:122:ILE:CD1	2.35	0.56
4:D:19:MET:HG2	14:N:173:THR:HG23	1.86	0.56
6:F:24:ASN:ND2	6:F:30:ASP:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:115:PRO:O	6:F:119:VAL:HG23	2.05	0.56
6:F:214:GLY:HA3	6:F:220:THR:HG22	1.87	0.56
14:N:148:LEU:HD12	14:N:148:LEU:O	2.06	0.56
34:i:21:TRP:NE1	34:i:25:GLN:OE1	2.38	0.56
4:D:249:ASP:OD2	4:D:404:LYS:NZ	2.29	0.56
17:Q:30:ILE:HG23	17:Q:31:LYS:HG3	1.87	0.56
5:E:150:ASN:ND2	5:E:192:CYS:O	2.38	0.56
12:L:202:MET:HE3	12:L:265:PRO:HG2	1.88	0.56
10:J:131:VAL:O	25:Z:67:ARG:NH1	2.34	0.56
7:G:531:CYS:SG	7:G:532:ILE:N	2.78	0.56
13:M:22:LYS:NZ	31:f:8:GLU:OE2	2.33	0.56
15:O:312:VAL:O	15:O:312:VAL:HG22	2.06	0.56
23:X:167:PHE:O	23:X:169:TRP:CE3	2.59	0.56
25:Z:140:THR:HG22	25:Z:140:THR:O	2.05	0.56
38:m:29:ARG:O	38:m:33:VAL:HG23	2.05	0.56
12:L:381:THR:HG21	12:L:498:PHE:HZ	1.71	0.56
12:L:71:MET:HE1	13:M:376:MET:HE3	1.88	0.56
14:N:210:ILE:HG22	14:N:333:SER:HB2	1.88	0.56
1:A:78:ALA:O	1:A:81:THR:HG22	2.06	0.55
12:L:283:LEU:HD13	37:l:111:MET:HG2	1.88	0.55
15:O:297:ARG:NH1	15:O:302:ARG:O	2.37	0.55
17:Q:125:ASN:O	44:s:64:ARG:NH1	2.39	0.55
7:G:362:TYR:O	7:G:363:LEU:HD23	2.06	0.55
15:O:53:GLU:OE1	15:O:126:ARG:NH1	2.39	0.55
12:L:17:SER:O	12:L:21:ILE:HD12	2.06	0.55
20:T:65:ILE:HD12	20:T:65:ILE:H	1.71	0.55
14:N:98:THR:O	14:N:102:LEU:HD23	2.06	0.55
23:X:58:GLU:O	23:X:62:VAL:HG23	2.07	0.55
5:E:148:CYS:SG	6:F:103:GLY:N	2.78	0.55
22:W:44:GLU:HG2	22:W:96:ILE:HG22	1.87	0.55
10:J:133:VAL:HG12	26:a:41:VAL:HG21	1.89	0.55
14:N:61:VAL:O	14:N:65:THR:HG23	2.07	0.55
34:i:76:ILE:HB	34:i:77:PRO:HD3	1.89	0.55
5:E:100:ILE:HG21	5:E:120:LEU:HD21	1.89	0.55
12:L:237:MET:O	12:L:299:LYS:NZ	2.40	0.55
39:n:104:ASP:OD1	39:n:121:ARG:NH2	2.34	0.55
7:G:511:VAL:HG12	7:G:511:VAL:O	2.06	0.55
12:L:477:ILE:HG22	40:o:86:TRP:HZ2	1.72	0.55
7:G:352:GLU:OE1	7:G:352:GLU:N	2.35	0.54
16:P:90:VAL:HG11	16:P:218:THR:HG23	1.89	0.54
32:g:98:ARG:NH1	32:g:105:ILE:O	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:127:VAL:HG23	23:X:127:VAL:O	2.07	0.54
32:g:39:ASN:O	32:g:42:PHE:N	2.39	0.54
19:S:54:ILE:O	19:S:55:ARG:NH2	2.41	0.54
22:W:47:ASN:O	22:W:51:LEU:HD23	2.07	0.54
30:e:50:ARG:NE	30:e:54:GLU:OE2	2.41	0.54
12:L:411:ILE:HA	12:L:414:ILE:HD12	1.89	0.54
13:M:176:LEU:O	13:M:177:MET:HG2	2.07	0.54
17:Q:67:ASN:OD1	17:Q:69:LEU:N	2.41	0.54
2:B:126:MET:SD	2:B:166:LEU:HD22	2.48	0.54
3:C:32:ILE:HG22	3:C:33:LEU:HD12	1.89	0.54
4:D:37:ASP:OD2	11:K:95:LEU:HD13	2.07	0.54
4:D:121:ALA:HA	4:D:365:THR:HG21	1.90	0.54
6:F:94:VAL:HG11	6:F:192:LEU:HD21	1.90	0.54
8:H:24:GLU:HG3	8:H:271:LEU:HD22	1.90	0.54
4:D:74:ARG:O	4:D:407:LYS:NZ	2.40	0.54
32:g:56:MET:SD	32:g:57:ARG:N	2.81	0.54
7:G:558:ASP:OD1	42:q:144:TYR:OH	2.24	0.53
8:H:193:THR:HG22	8:H:193:THR:O	2.08	0.53
17:Q:23:THR:OG1	17:Q:25:VAL:HG12	2.08	0.53
4:D:247:ALA:HB1	4:D:265:ILE:HD11	1.89	0.53
12:L:532:ILE:HD11	37:l:104:LEU:HD23	1.91	0.53
13:M:139:GLN:O	13:M:142:ARG:NH1	2.41	0.53
6:F:295:LEU:HD23	6:F:343:ILE:HD11	1.90	0.53
6:F:313:GLU:HG3	6:F:314:THR:HG23	1.90	0.53
15:O:231:PRO:O	15:O:234:VAL:N	2.42	0.53
28:c:36:ASN:O	28:c:40:LEU:HD23	2.08	0.53
42:q:22:GLY:O	42:q:26:VAL:HG23	2.07	0.53
28:c:28:TRP:NE1	29:d:66:THR:HG22	2.22	0.53
35:j:45:ASP:OD1	35:j:46:ALA:N	2.42	0.53
9:I:146:HIS:HB3	16:P:65:LEU:HD11	1.90	0.53
38:m:110:ARG:O	38:m:114:LEU:HD23	2.08	0.53
4:D:12:GLU:O	4:D:15:SER:OG	2.27	0.53
6:F:109:GLU:OE2	6:F:112:ARG:NH2	2.38	0.53
8:H:146:MET:HE1	8:H:192:GLU:HG2	1.90	0.53
10:J:39:GLY:O	10:J:43:VAL:HG23	2.08	0.53
32:g:65:SER:OG	33:h:28:TYR:O	2.13	0.53
14:N:24:THR:N	30:e:14:ASP:OD2	2.41	0.53
18:R:22:ASP:OD2	18:R:24:ARG:NH2	2.40	0.53
32:g:90:GLU:O	32:g:94:LEU:HD23	2.08	0.53
9:I:110:ARG:NE	9:I:112:ASP:OD2	2.42	0.53
13:M:122:PHE:HD1	13:M:238:LEU:HD23	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:92:LEU:O	22:W:96:ILE:HG23	2.09	0.53
7:G:227:SER:OG	7:G:228:ILE:N	2.40	0.52
17:Q:49:VAL:HG12	17:Q:49:VAL:O	2.07	0.52
21:V:24:THR:O	21:V:28:THR:HG23	2.08	0.52
21:V:47:THR:O	21:V:51:THR:HG23	2.08	0.52
5:E:116:ILE:O	5:E:119:THR:OG1	2.24	0.52
12:L:397:GLU:HB3	12:L:482:MET:HE1	1.91	0.52
22:W:61:GLY:O	22:W:65:VAL:HG23	2.10	0.52
24:Y:71:PHE:O	24:Y:75:THR:HG23	2.09	0.52
3:C:25:PHE:O	3:C:29:VAL:HG23	2.10	0.52
12:L:71:MET:HE2	13:M:310:MET:SD	2.49	0.52
13:M:162:ILE:HG23	14:N:271:MET:HE3	1.92	0.52
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.09	0.52
15:O:176:VAL:HG13	15:O:177:PRO:HD3	1.91	0.52
16:P:30:LEU:HD23	16:P:94:LEU:HD22	1.92	0.52
23:X:150:ASN:OD1	30:e:50:ARG:NH2	2.43	0.52
42:q:44:TYR:OH	42:q:113:HIS:N	2.39	0.52
14:N:37:LEU:HD13	14:N:63:GLN:HB2	1.92	0.52
13:M:210:TYR:O	13:M:213:HIS:ND1	2.36	0.52
28:c:24:SER:HB3	29:d:66:THR:HG21	1.91	0.52
6:F:344:VAL:HG12	6:F:380:VAL:HG22	1.92	0.51
20:T:77:VAL:HA	20:T:80:ILE:HG22	1.92	0.51
3:C:69:ASN:OD1	21:V:50:ILE:HD11	2.09	0.51
15:O:180:GLN:NE2	15:O:196:SER:OG	2.42	0.51
23:X:120:ASP:N	23:X:123:GLN:OE1	2.42	0.51
6:F:129:MET:HE2	6:F:221:THR:HG21	1.93	0.51
6:F:205:LEU:HD11	7:G:50:GLY:HA3	1.93	0.51
6:F:270:GLU:OE2	6:F:283:HIS:NE2	2.35	0.51
7:G:524:LEU:HD23	7:G:544:VAL:O	2.10	0.51
14:N:42:PRO:HA	14:N:45:ILE:HG22	1.92	0.51
15:O:214:MET:HE3	15:O:218:CYS:SG	2.50	0.51
11:K:55:SER:OG	30:e:24:GLN:NE2	2.44	0.51
12:L:67:HIS:NE2	12:L:70:THR:OG1	2.39	0.51
20:T:26:ASP:N	20:T:27:PRO:CD	2.73	0.51
39:n:88:THR:O	39:n:92:ARG:NH1	2.44	0.51
4:D:151:ILE:HD11	4:D:218:PHE:HZ	1.76	0.51
9:I:154:GLU:OE2	18:R:36:ASN:N	2.37	0.51
36:k:41:LEU:O	36:k:46:LEU:N	2.39	0.51
40:o:73:PHE:HB3	40:o:74:PRO:HD3	1.93	0.51
6:F:94:VAL:HG11	6:F:192:LEU:CD2	2.41	0.51
6:F:306:LEU:HD23	6:F:306:LEU:H	1.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:261:MET:O	8:H:265:LEU:HD23	2.11	0.51
12:L:72:ASN:C	12:L:73:SER:HG	2.04	0.51
12:L:372:CYS:SG	12:L:454:ILE:HG22	2.51	0.51
20:T:18:VAL:HG22	20:T:57:GLU:HG3	1.92	0.51
5:E:99:HIS:NE2	5:E:140:ILE:HD12	2.26	0.51
8:H:150:LEU:O	8:H:154:LEU:HD23	2.11	0.51
8:H:317:TYR:CD1	10:J:134:MET:HE2	2.46	0.51
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.92	0.51
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.46	0.51
12:L:202:MET:HE3	12:L:265:PRO:CG	2.41	0.51
34:i:108:THR:HG22	34:i:115:VAL:HG23	1.92	0.50
12:L:295:GLN:O	12:L:425:ARG:NH1	2.44	0.50
20:T:11:ILE:O	20:T:15:VAL:HG23	2.11	0.50
32:g:111:PHE:O	41:p:158:GLN:NE2	2.43	0.50
43:r:51:ASN:OD1	43:r:56:ARG:NE	2.44	0.50
4:D:112:MET:HG2	4:D:194:ILE:HD12	1.93	0.50
7:G:185:THR:OG1	7:G:187:ILE:O	2.29	0.50
7:G:625:GLU:O	19:S:21:HIS:NE2	2.43	0.50
17:Q:32:THR:O	17:Q:32:THR:HG22	2.12	0.50
31:f:13:ILE:HG22	31:f:13:ILE:O	2.11	0.50
10:J:151:MET:SD	14:N:28:LEU:HD21	2.52	0.50
31:f:27:ARG:O	31:f:30:ASP:OD1	2.29	0.50
7:G:601:ARG:NH1	7:G:605:GLU:OE1	2.40	0.50
12:L:151:SER:CB	12:L:252:MET:HE1	2.41	0.50
6:F:375:VAL:HG11	6:F:392:LEU:HD13	1.92	0.50
6:F:398:GLN:O	6:F:402:HIS:ND1	2.42	0.50
10:J:157:TRP:HE1	14:N:12:THR:HG22	1.77	0.50
12:L:257:ILE:HG22	12:L:329:ILE:HD11	1.92	0.50
14:N:20:THR:HG21	14:N:137:ALA:HB1	1.94	0.50
20:U:11:ILE:O	20:U:15:VAL:HG23	2.10	0.50
12:L:309:GLN:OE1	12:L:328:HIS:NE2	2.42	0.50
2:B:38:TYR:O	2:B:41:THR:OG1	2.28	0.50
6:F:137:TYR:HB3	6:F:192:LEU:HD11	1.93	0.50
8:H:179:TRP:N	8:H:180:PRO:CD	2.75	0.50
10:J:107:ASN:OD1	10:J:107:ASN:C	2.55	0.50
38:m:24:VAL:HG12	38:m:24:VAL:O	2.12	0.50
4:D:64:LEU:HD11	4:D:418:ILE:HD11	1.94	0.49
12:L:304:PHE:HZ	12:L:526:LEU:HD11	1.76	0.49
13:M:422:HIS:O	13:M:422:HIS:ND1	2.45	0.49
40:o:76:PHE:O	40:o:77:LEU:HB2	2.12	0.49
42:q:30:ALA:O	42:q:32:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:397:GLU:OE2	12:L:487:LYS:NZ	2.45	0.49
13:M:49:TYR:O	33:h:86:ASN:ND2	2.40	0.49
4:D:224:GLU:OE1	9:I:42:TYR:OH	2.22	0.49
4:D:233:ARG:NH1	9:I:32:LEU:HD11	2.27	0.49
15:O:57:GLN:NE2	15:O:74:SER:OG	2.45	0.49
16:P:201:VAL:HG22	16:P:237:LEU:HD23	1.92	0.49
40:o:35:GLU:OE1	40:o:35:GLU:N	2.44	0.49
6:F:362:CYS:SG	6:F:404:ILE:HD12	2.52	0.49
14:N:193:ILE:HG23	14:N:201:THR:HG23	1.95	0.49
1:A:71:LEU:O	10:J:145:TYR:OH	2.24	0.49
3:C:79:THR:HG22	3:C:80:ALA:N	2.27	0.49
11:K:8:LEU:HD13	11:K:43:MET:HG2	1.94	0.49
23:X:5:GLU:O	23:X:53:ARG:NH1	2.46	0.49
5:E:202:LEU:HD23	6:F:17:ASP:OD1	2.13	0.49
6:F:376:MET:O	6:F:380:VAL:HG23	2.13	0.49
7:G:332:LYS:HA	7:G:343:LEU:HD21	1.95	0.49
13:M:456:GLY:O	32:g:82:ARG:NH2	2.45	0.49
7:G:591:GLY:HA2	16:P:6:ILE:HG21	1.95	0.49
12:L:264:HIS:N	12:L:265:PRO:CD	2.75	0.49
16:P:145:SER:O	16:P:149:LYS:HG3	2.12	0.49
3:C:189:GLU:OE1	16:P:15:SER:OG	2.28	0.49
16:P:97:ARG:HE	52:P:501:NDP:H8A	1.77	0.49
2:B:101:THR:OG1	2:B:129:CYS:SG	2.67	0.49
28:c:17:VAL:O	28:c:21:VAL:HG23	2.13	0.49
3:C:47:GLU:OE1	3:C:106:ARG:NH2	2.43	0.48
4:D:25:THR:HG22	4:D:25:THR:O	2.12	0.48
5:E:148:CYS:O	5:E:151:ALA:HB2	2.13	0.48
12:L:492:ILE:O	12:L:496:LEU:HD23	2.12	0.48
36:k:48:ASP:OD2	36:k:51:ALA:N	2.46	0.48
40:o:61:TYR:CE2	40:o:89:CYS:SG	3.06	0.48
6:F:301:GLY:O	6:F:304:THR:OG1	2.30	0.48
12:L:161:ARG:NE	12:L:238:GLU:OE1	2.46	0.48
2:B:172:GLN:NE2	42:q:118:SER:OG	2.46	0.48
8:H:113:VAL:HG13	8:H:136:VAL:HG13	1.95	0.48
14:N:30:TRP:NE1	14:N:67:SER:HG	2.09	0.48
14:N:257:LEU:HD23	14:N:334:THR:O	2.12	0.48
22:W:22:ILE:O	22:W:22:ILE:HG23	2.12	0.48
38:m:122:ARG:O	41:p:139:GLN:NE2	2.45	0.48
25:Z:57:ARG:NH1	27:b:48:THR:HG21	2.27	0.48
1:A:90:MET:HE2	10:J:149:THR:HB	1.95	0.48
3:C:117:ILE:HG22	3:C:118:ASP:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:89:ALA:O	7:G:93:VAL:HG23	2.13	0.48
8:H:24:GLU:CG	8:H:271:LEU:HD22	2.44	0.48
17:Q:11:ILE:HG22	17:Q:12:THR:N	2.28	0.48
4:D:335:ARG:NH2	9:I:131:ASP:OD1	2.40	0.48
7:G:606:ILE:HD11	22:W:125:TYR:OH	2.14	0.48
13:M:207:MET:HG3	13:M:298:ILE:HD11	1.95	0.48
16:P:176:ASP:O	16:P:180:ASN:ND2	2.46	0.48
44:s:31:THR:O	44:s:33:LYS:NZ	2.42	0.48
2:B:52:ARG:NH1	46:B:202:PC1:O14	2.47	0.48
7:G:615:THR:O	7:G:619:VAL:HG23	2.14	0.48
11:K:59:ILE:HB	11:K:60:PRO:HD3	1.95	0.48
12:L:257:ILE:HG23	12:L:317:LEU:HD11	1.95	0.48
14:N:273:ASN:HD21	24:Y:142:VAL:HG13	1.78	0.48
3:C:116:PRO:CG	22:W:22:ILE:HD12	2.44	0.48
4:D:112:MET:SD	4:D:141:PHE:HB3	2.54	0.48
5:E:119:THR:HG21	5:E:166:PRO:HB3	1.96	0.48
9:I:44:PHE:O	43:r:11:ARG:NH2	2.47	0.48
12:L:532:ILE:O	12:L:536:ILE:HG12	2.14	0.48
35:j:18:THR:HG22	35:j:19:ARG:H	1.78	0.48
8:H:106:LEU:HD11	8:H:150:LEU:HD12	1.95	0.48
12:L:189:PHE:CE1	12:L:201:ILE:HG23	2.48	0.48
15:O:259:LEU:O	15:O:263:VAL:HG23	2.14	0.48
21:V:20:HIS:NE2	21:V:62:PRO:O	2.46	0.48
27:b:77:LEU:HD23	27:b:77:LEU:H	1.78	0.48
32:g:96:LYS:O	32:g:100:VAL:HG23	2.13	0.48
10:J:67:PHE:O	10:J:71:THR:OG1	2.27	0.48
14:N:298:TYR:CD1	14:N:302:LEU:HD12	2.49	0.48
15:O:194:VAL:HG22	15:O:195:THR:H	1.79	0.48
39:n:58:ARG:NH1	39:n:61:GLN:OE1	2.46	0.48
3:C:116:PRO:HG2	22:W:22:ILE:HD12	1.96	0.47
3:C:175:ARG:NH2	3:C:186:GLU:OE2	2.44	0.47
5:E:190:ARG:NH2	6:F:265:PRO:O	2.42	0.47
7:G:60:GLU:OE1	7:G:78:ASN:ND2	2.41	0.47
7:G:663:PRO:HG2	7:G:666:LEU:HD23	1.96	0.47
13:M:297:VAL:O	13:M:301:ILE:HG12	2.14	0.47
29:d:86:LYS:NZ	33:h:107:GLU:OE2	2.37	0.47
5:E:162:GLU:OE2	6:F:108:ARG:NH2	2.44	0.47
14:N:114:TRP:O	14:N:118:VAL:HG23	2.13	0.47
23:X:12:LEU:HD12	23:X:12:LEU:O	2.14	0.47
5:E:37:ASN:ND2	44:s:49:ASN:OD1	2.46	0.47
6:F:140:GLY:O	6:F:179:ARG:NH2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:449:THR:HG21	49:M:502:3PE:O22	2.14	0.47
16:P:113:ILE:HB	16:P:114:PRO:HD3	1.96	0.47
16:P:128:ARG:NH1	16:P:220:ASP:O	2.38	0.47
34:i:6:ASP:OD1	34:i:6:ASP:N	2.48	0.47
1:A:53:MET:HE1	11:K:79:VAL:CG1	2.44	0.47
8:H:162:LEU:N	8:H:162:LEU:HD12	2.30	0.47
16:P:206:TYR:O	16:P:210:VAL:HG23	2.15	0.47
7:G:511:VAL:O	7:G:511:VAL:CG1	2.62	0.47
13:M:30:TYR:O	13:M:34:ILE:HG12	2.15	0.47
16:P:170:ASP:OD1	16:P:170:ASP:N	2.47	0.47
17:Q:12:THR:HG23	17:Q:12:THR:O	2.14	0.47
24:Y:96:CYS:O	24:Y:100:LEU:HD13	2.14	0.47
12:L:210:LEU:HD23	12:L:210:LEU:C	2.39	0.47
13:M:13:PRO:O	13:M:14:LEU:C	2.58	0.47
13:M:106:LEU:HD22	13:M:234:ILE:CG2	2.44	0.47
15:O:56:ILE:HG21	15:O:71:ILE:HD11	1.97	0.47
20:U:17:TYR:O	20:U:21:LEU:HD23	2.14	0.47
23:X:122:GLY:N	25:Z:65:GLU:OE2	2.42	0.47
12:L:151:SER:HB3	12:L:252:MET:HE1	1.95	0.47
12:L:529:PHE:HB3	12:L:530:PRO:HD3	1.96	0.47
12:L:532:ILE:HD11	37:l:104:LEU:CD2	2.45	0.47
13:M:259:TYR:O	13:M:263:LEU:HD23	2.15	0.47
14:N:254:LEU:HD12	14:N:255:PRO:HD2	1.97	0.47
15:O:114:HIS:NE2	15:O:120:GLN:OE1	2.45	0.47
16:P:165:ILE:HB	16:P:227:THR:HG22	1.96	0.47
25:Z:113:THR:HG22	25:Z:113:THR:O	2.15	0.47
6:F:224:ASN:OD1	6:F:225:VAL:N	2.46	0.47
12:L:199:GLN:OE1	12:L:199:GLN:N	2.43	0.47
14:N:215:MET:SD	14:N:247:MET:HE3	2.55	0.47
28:c:5:ARG:O	28:c:6:GLU:C	2.57	0.47
41:p:34:LYS:O	41:p:38:LEU:HD23	2.14	0.47
4:D:165:THR:OG1	4:D:166:PRO:HD3	2.15	0.47
7:G:94:MET:HE1	7:G:116:LEU:HD12	1.96	0.47
7:G:481:THR:O	7:G:481:THR:HG23	2.15	0.47
1:A:87:MET:SD	1:A:88:MET:N	2.88	0.47
7:G:11:VAL:HG12	7:G:12:PHE:N	2.29	0.47
13:M:317:ILE:CG1	13:M:454:ILE:HD11	2.42	0.47
15:O:38:LEU:CD2	15:O:172:ILE:HD11	2.42	0.47
15:O:236:GLU:OE2	21:V:91:ARG:NH2	2.45	0.47
38:m:87:LEU:O	38:m:91:VAL:HG23	2.14	0.47
13:M:185:THR:C	13:M:186:LEU:HD12	2.41	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:O	1:A:93:ILE:HG12	2.15	0.46
2:B:175:ARG:NH1	42:q:78:ASP:OD1	2.49	0.46
4:D:238:ARG:NH2	4:D:412:ALA:O	2.48	0.46
4:D:335:ARG:NH2	9:I:128:CYS:O	2.39	0.46
6:F:268:VAL:HG12	6:F:269:GLU:N	2.30	0.46
7:G:639:THR:HA	19:S:56:GLU:OE2	2.15	0.46
6:F:242:PHE:CZ	6:F:252:GLY:HA3	2.51	0.46
6:F:313:GLU:O	6:F:314:THR:OG1	2.20	0.46
9:I:84:LEU:O	9:I:88:ILE:HG22	2.15	0.46
12:L:152:PHE:HD1	12:L:153:LEU:HD12	1.80	0.46
12:L:562:ILE:HB	12:L:563:PRO:CD	2.45	0.46
16:P:280:THR:O	16:P:284:VAL:HG23	2.14	0.46
2:B:162:THR:HG22	4:D:188:ARG:HD2	1.98	0.46
3:C:77:ASP:OD1	3:C:78:LEU:N	2.48	0.46
4:D:144:ILE:HG23	4:D:177:MET:SD	2.55	0.46
5:E:150:ASN:ND2	5:E:162:GLU:OE1	2.41	0.46
6:F:378:ARG:NE	7:G:132:GLU:OE1	2.39	0.46
9:I:146:HIS:CD2	9:I:146:HIS:O	2.68	0.46
12:L:409:LEU:HD12	12:L:409:LEU:O	2.16	0.46
23:X:166:PHE:CD2	23:X:169:TRP:CZ3	3.04	0.46
12:L:140:LEU:HD22	12:L:182:PHE:CZ	2.50	0.46
12:L:254:VAL:HG11	12:L:329:ILE:HG23	1.98	0.46
15:O:52:PRO:O	15:O:107:GLN:NE2	2.40	0.46
21:V:102:LEU:HD23	21:V:104:GLU:N	2.31	0.46
5:E:27:ASN:OD1	5:E:30:ARG:NH1	2.48	0.46
5:E:55:GLN:O	5:E:58:ASN:O	2.33	0.46
7:G:675:ASP:C	7:G:679:ARG:HE	2.23	0.46
8:H:185:TRP:HE1	8:H:238:THR:HG22	1.81	0.46
12:L:230:HIS:N	12:L:231:PRO:HD3	2.31	0.46
14:N:332:MET:HE3	29:d:68:PHE:HE2	1.80	0.46
16:P:133:SER:O	52:P:501:NDP:H6N	2.16	0.46
4:D:381:ASP:O	4:D:383:SER:N	2.44	0.46
5:E:192:CYS:SG	5:E:193:CYS:N	2.89	0.46
7:G:249:ARG:NH1	17:Q:45:MET:HE3	2.30	0.46
12:L:30:ILE:HG22	12:L:31:ASN:N	2.29	0.46
18:R:2:VAL:O	18:R:2:VAL:HG23	2.15	0.46
24:Y:96:CYS:HA	24:Y:116:CYS:HA	1.98	0.46
31:f:45:ARG:NH2	31:f:50:ASN:OD1	2.48	0.46
33:h:36:VAL:O	33:h:40:ILE:HG12	2.16	0.46
41:p:42:TRP:HB3	41:p:43:PRO:HD3	1.96	0.46
5:E:55:GLN:O	5:E:59:GLY:HA2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:466:ILE:O	7:G:470:VAL:HG23	2.15	0.46
8:H:114:TYR:OH	10:J:60:LEU:O	2.27	0.46
12:L:537:THR:HB	12:L:538:PRO:HD3	1.98	0.46
22:W:23:PHE:O	22:W:24:SER:OG	2.27	0.46
41:p:56:ALA:HA	41:p:59:ARG:HD3	1.98	0.46
4:D:148:LEU:CD2	4:D:177:MET:HE3	2.46	0.46
6:F:215:VAL:HG12	6:F:220:THR:HB	1.97	0.46
7:G:36:GLN:HG3	7:G:39:ARG:HH12	1.80	0.46
12:L:71:MET:HE1	13:M:376:MET:CE	2.46	0.46
13:M:7:PRO:HB2	13:M:34:ILE:HD11	1.96	0.46
14:N:139:LEU:O	14:N:143:ILE:HG12	2.16	0.46
14:N:214:PRO:HB2	14:N:247:MET:HE1	1.98	0.46
41:p:102:MET:SD	41:p:134:VAL:HG12	2.56	0.46
6:F:361:GLN:O	6:F:366:ARG:NH2	2.43	0.46
7:G:413:VAL:HG12	7:G:414:ASP:N	2.30	0.46
10:J:114:VAL:HG12	10:J:115:ILE:HG23	1.98	0.46
12:L:103:PHE:CG	12:L:341:MET:SD	3.09	0.46
12:L:574:THR:CG2	14:N:171:ASN:HB2	2.46	0.46
13:M:23:THR:HG23	13:M:24:TRP:N	2.30	0.46
21:V:20:HIS:O	21:V:24:THR:HG23	2.17	0.46
39:n:167:TRP:O	39:n:171:THR:OG1	2.30	0.46
2:B:101:THR:HA	2:B:129:CYS:HB3	1.97	0.45
10:J:159:LEU:HD21	11:K:65:VAL:HG13	1.98	0.45
16:P:95:ILE:HG22	16:P:96:GLY:N	2.31	0.45
20:T:28:GLU:OE1	20:T:28:GLU:N	2.47	0.45
6:F:103:GLY:O	6:F:333:ALA:HB1	2.16	0.45
14:N:298:TYR:HD1	14:N:302:LEU:HD12	1.80	0.45
21:V:17:ASP:OD1	21:V:17:ASP:N	2.49	0.45
4:D:148:LEU:HD23	4:D:177:MET:HE3	1.98	0.45
12:L:202:MET:SD	41:p:113:GLN:NE2	2.89	0.45
12:L:550:LEU:HD22	13:M:275:ILE:HG23	1.98	0.45
14:N:26:LEU:HD23	14:N:29:MET:SD	2.56	0.45
20:T:30:LEU:HD23	20:T:30:LEU:H	1.82	0.45
7:G:259:ASN:N	7:G:259:ASN:OD1	2.50	0.45
13:M:176:LEU:O	13:M:177:MET:CG	2.64	0.45
15:O:27:VAL:HG23	15:O:27:VAL:O	2.16	0.45
16:P:301:GLU:OE1	16:P:301:GLU:N	2.45	0.45
2:B:62:LEU:HD23	4:D:61:VAL:HG12	1.98	0.45
10:J:60:LEU:O	10:J:65:VAL:HG23	2.17	0.45
12:L:233:LEU:HB3	12:L:234:PRO:HD3	1.97	0.45
12:L:253:VAL:HB	12:L:310:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:243:MET:CG	14:N:330:ALA:HB1	2.46	0.45
21:V:55:LEU:HA	21:V:58:VAL:HG22	1.98	0.45
38:m:24:VAL:HG13	38:m:29:ARG:HE	1.80	0.45
5:E:31:ILE:CD1	5:E:50:VAL:HG13	2.46	0.45
6:F:185:ILE:HD13	45:F:502:SF4:S1	2.56	0.45
10:J:116:ASN:O	10:J:119:GLY:N	2.49	0.45
12:L:83:ASP:OD1	12:L:83:ASP:N	2.47	0.45
15:O:115:LEU:HD23	15:O:115:LEU:C	2.41	0.45
16:P:222:ASP:O	16:P:226:LYS:NZ	2.27	0.45
23:X:18:LYS:HB3	26:a:68:ASN:ND2	2.32	0.45
3:C:169:THR:HG21	3:C:190:LEU:HD11	1.98	0.45
7:G:205:VAL:HB	45:G:801:SF4:S2	2.57	0.45
10:J:92:LEU:O	10:J:96:VAL:HG23	2.17	0.45
11:K:63:ILE:HG22	14:N:27:MET:HE1	1.99	0.45
13:M:7:PRO:HB2	13:M:34:ILE:CD1	2.47	0.45
13:M:127:ILE:HG22	13:M:131:ILE:HD12	1.98	0.45
13:M:162:ILE:HG23	14:N:271:MET:CE	2.46	0.45
34:i:24:ASP:OD2	39:n:124:TRP:NE1	2.40	0.45
34:i:29:PRO:O	34:i:30:ARG:HG3	2.16	0.45
7:G:125:SER:OG	7:G:126:ASP:N	2.50	0.45
8:H:294:LEU:HB3	8:H:295:PRO:HD3	1.99	0.45
12:L:466:PHE:HZ	40:o:77:LEU:HD21	1.80	0.45
13:M:46:ASP:N	13:M:46:ASP:OD1	2.49	0.45
22:W:41:TRP:O	22:W:45:VAL:HG23	2.17	0.45
42:q:107:LYS:O	42:q:108:PHE:CG	2.69	0.45
7:G:156:CYS:C	7:G:157:THR:HG1	2.15	0.45
7:G:661:LEU:O	7:G:661:LEU:HG	2.16	0.45
14:N:268:THR:HG22	14:N:272:LYS:HE3	1.99	0.45
16:P:133:SER:HA	16:P:149:LYS:HE3	1.99	0.45
5:E:115:SER:O	5:E:119:THR:HG23	2.17	0.45
7:G:114:CYS:SG	7:G:116:LEU:HB3	2.57	0.45
12:L:174:TYR:HD1	12:L:229:LEU:HD22	1.81	0.45
14:N:152:THR:HG23	24:Y:137:PHE:CD2	2.52	0.45
16:P:135:LEU:HD22	16:P:231:THR:HG22	1.99	0.45
16:P:228:PHE:HA	16:P:298:PRO:O	2.17	0.45
6:F:318:ASP:N	6:F:318:ASP:OD1	2.50	0.44
7:G:334:LEU:HD23	7:G:334:LEU:C	2.42	0.44
12:L:17:SER:HB2	12:L:18:PRO:HD3	1.97	0.44
13:M:218:LYS:O	13:M:222:GLU:OE1	2.36	0.44
13:M:409:TYR:CE1	13:M:413:THR:HG21	2.51	0.44
15:O:130:SER:O	15:O:133:VAL:HG22	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:LYS:HE3	21:V:103:VAL:HG22	1.99	0.44
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.99	0.44
11:K:12:PHE:CE1	14:N:72:LEU:HD22	2.51	0.44
12:L:119:LYS:NZ	50:L:702:CDL:OB7	2.34	0.44
15:O:244:ASN:O	15:O:245:LYS:HG2	2.18	0.44
16:P:235:ARG:NH2	16:P:342:TYR:OH	2.51	0.44
37:l:96:SER:O	37:l:99:VAL:HG22	2.17	0.44
4:D:80:ILE:HG22	4:D:81:GLY:N	2.32	0.44
5:E:116:ILE:CD1	5:E:164:LEU:HD11	2.47	0.44
6:F:94:VAL:CG1	6:F:192:LEU:HD21	2.47	0.44
7:G:165:GLU:O	7:G:396:ARG:NE	2.51	0.44
7:G:285:ARG:NH2	7:G:289:GLY:O	2.42	0.44
9:I:15:ASP:OD1	9:I:16:MET:N	2.51	0.44
11:K:53:SER:O	11:K:53:SER:OG	2.33	0.44
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.99	0.44
14:N:143:ILE:HD12	14:N:198:PRO:HB2	1.98	0.44
14:N:314:MET:SD	15:O:267:THR:HG22	2.57	0.44
5:E:55:GLN:O	5:E:58:ASN:C	2.61	0.44
8:H:182:ALA:O	8:H:185:TRP:N	2.49	0.44
9:I:82:CYS:SG	9:I:84:LEU:HD13	2.57	0.44
12:L:374:VAL:HG22	12:L:427:ILE:HD12	1.99	0.44
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.99	0.44
31:f:48:ARG:HB2	31:f:49:PRO:HD3	2.00	0.44
39:n:157:ARG:O	39:n:158:ARG:CG	2.65	0.44
5:E:108:CYS:SG	5:E:151:ALA:HB1	2.57	0.44
15:O:109:ALA:O	15:O:263:VAL:CG1	2.65	0.44
10:J:54:MET:HG2	10:J:58:ILE:HD13	1.98	0.44
12:L:14:LEU:HD21	34:i:73:HIS:O	2.18	0.44
12:L:95:PHE:CZ	12:L:456:ARG:HG2	2.52	0.44
12:L:563:PRO:O	12:L:566:THR:OG1	2.31	0.44
21:V:43:TYR:OH	21:V:86:GLU:OE2	2.32	0.44
24:Y:63:THR:O	24:Y:67:ILE:HG12	2.17	0.44
35:j:50:HIS:O	35:j:50:HIS:ND1	2.51	0.44
4:D:157:HIS:CE1	4:D:420:THR:HG23	2.53	0.44
6:F:376:MET:SD	6:F:392:LEU:HD21	2.57	0.44
12:L:396:ILE:O	12:L:399:ILE:HG22	2.18	0.44
16:P:211:SER:O	16:P:215:VAL:HG23	2.18	0.44
20:T:70:LEU:HD21	20:T:79:TYR:HB2	1.99	0.44
4:D:147:ILE:HG22	4:D:177:MET:HE1	2.00	0.44
5:E:142:VAL:CG1	5:E:143:GLU:N	2.81	0.44
7:G:603:LEU:C	7:G:603:LEU:HD23	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:186:PHE:O	8:H:189:THR:OG1	2.36	0.44
9:I:76:GLU:HA	18:R:40:ALA:HB1	1.98	0.44
23:X:139:ASN:OD1	23:X:143:SER:N	2.41	0.44
34:i:123:PRO:O	34:i:124:ASP:HB2	2.18	0.44
42:q:8:LYS:HA	42:q:11:VAL:HG12	2.00	0.44
5:E:16:ASN:OD1	5:E:19:THR:N	2.50	0.44
7:G:26:VAL:HG13	7:G:79:ILE:CD1	2.46	0.44
7:G:107:ILE:HG22	7:G:107:ILE:O	2.17	0.44
14:N:119:THR:HG22	14:N:176:ARG:HB3	2.00	0.44
20:T:66:ASP:OD1	20:T:66:ASP:N	2.50	0.44
40:o:19:GLU:OE1	40:o:19:GLU:N	2.51	0.44
9:I:49:THR:HG22	9:I:50:ILE:N	2.33	0.43
10:J:147:CYS:O	10:J:148:ALA:HB3	2.17	0.43
12:L:54:PHE:O	12:L:58:ASN:N	2.45	0.43
13:M:171:VAL:HG12	13:M:172:GLY:N	2.33	0.43
21:V:67:LEU:O	21:V:71:LEU:HD13	2.17	0.43
27:b:30:ILE:HG23	27:b:31:MET:N	2.33	0.43
34:i:30:ARG:NH2	39:n:116:ASP:OD2	2.51	0.43
8:H:234:MET:O	8:H:238:THR:HG23	2.17	0.43
13:M:180:SER:O	13:M:183:THR:HG22	2.18	0.43
14:N:324:LEU:HD12	14:N:324:LEU:H	1.83	0.43
15:O:1:LEU:HD12	15:O:2:ARG:O	2.18	0.43
15:O:24:VAL:HG23	15:O:122:VAL:HG23	1.99	0.43
20:U:52:MET:HE1	39:n:23:LEU:HD13	2.01	0.43
21:V:23:LEU:HD13	21:V:58:VAL:HG11	2.00	0.43
39:n:170:VAL:HG12	39:n:171:THR:N	2.33	0.43
2:B:95:VAL:HG22	2:B:96:MET:N	2.32	0.43
6:F:436:GLN:O	6:F:437:HIS:C	2.61	0.43
7:G:453:LEU:HD21	7:G:458:LEU:HD21	2.00	0.43
13:M:171:VAL:HG12	13:M:172:GLY:H	1.83	0.43
20:T:70:LEU:HD22	20:T:76:ILE:HA	2.00	0.43
4:D:227:GLU:OE2	9:I:34:ARG:NH2	2.52	0.43
10:J:34:VAL:O	10:J:38:VAL:HG23	2.18	0.43
12:L:285:THR:HG22	12:L:308:SER:O	2.18	0.43
12:L:396:ILE:O	12:L:396:ILE:HG22	2.18	0.43
13:M:359:TRP:O	13:M:411:ILE:HD11	2.18	0.43
13:M:403:THR:HA	13:M:406:TYR:CE2	2.53	0.43
14:N:239:ALA:O	29:d:47:MET:HE2	2.18	0.43
26:a:5:ILE:O	26:a:5:ILE:HG22	2.17	0.43
39:n:114:TYR:N	39:n:115:PRO:CD	2.82	0.43
39:n:170:VAL:O	39:n:171:THR:OG1	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:79:ARG:NH2	7:G:170:ASP:OD1	2.50	0.43
7:G:601:ARG:NH2	7:G:614:ASP:OD1	2.48	0.43
14:N:226:THR:HG22	14:N:227:ILE:N	2.34	0.43
38:m:83:PRO:O	38:m:84:LYS:HB3	2.18	0.43
8:H:235:ASN:O	8:H:238:THR:OG1	2.29	0.43
14:N:24:THR:HG22	30:e:18:MET:HE1	2.00	0.43
16:P:305:VAL:HG12	16:P:306:GLN:N	2.33	0.43
32:g:74:PHE:O	32:g:78:VAL:HG23	2.19	0.43
38:m:104:PHE:O	38:m:108:ARG:HG2	2.18	0.43
1:A:73:LEU:N	1:A:74:PRO:CD	2.81	0.43
7:G:199:VAL:HA	7:G:202:ILE:HG22	1.99	0.43
12:L:187:VAL:HG22	13:M:383:MET:HG3	1.99	0.43
12:L:313:MET:SD	12:L:329:ILE:HG13	2.59	0.43
13:M:17:LEU:CD1	31:f:11:VAL:HG12	2.49	0.43
14:N:49:ASN:O	14:N:53:THR:HG23	2.18	0.43
14:N:146:TYR:N	14:N:147:PRO:CD	2.81	0.43
15:O:24:VAL:HG13	15:O:166:PRO:HA	2.01	0.43
21:V:21:GLU:O	21:V:25:ILE:HG12	2.19	0.43
39:n:157:ARG:O	39:n:158:ARG:HG3	2.19	0.43
3:C:50:ILE:HD12	3:C:105:ILE:HD11	2.01	0.43
4:D:221:ARG:NH1	43:r:22:LYS:O	2.52	0.43
8:H:165:LEU:HD12	8:H:165:LEU:N	2.34	0.43
12:L:22:SER:O	12:L:27:ILE:HD11	2.19	0.43
12:L:162:THR:HG22	12:L:162:THR:O	2.18	0.43
12:L:542:LEU:HB3	13:M:278:ARG:HD2	2.01	0.43
18:R:49:VAL:HG22	18:R:90:GLN:HG3	2.01	0.43
27:b:77:LEU:O	27:b:77:LEU:HG	2.19	0.43
8:H:77:LEU:O	8:H:81:LEU:HG	2.19	0.43
8:H:177:PRO:O	8:H:178:ALA:HB3	2.19	0.43
9:I:65:GLY:N	9:I:136:GLY:O	2.48	0.43
14:N:175:MET:O	14:N:179:MET:HG2	2.18	0.43
20:T:51:ILE:HG23	20:T:62:ILE:HD12	2.01	0.43
24:Y:141:LYS:O	24:Y:142:VAL:C	2.62	0.43
32:g:67:VAL:O	32:g:71:GLY:N	2.46	0.43
43:r:45:SER:O	43:r:51:ASN:ND2	2.47	0.43
6:F:97:ALA:HB1	6:F:111:MET:SD	2.58	0.43
10:J:26:ILE:HG23	10:J:27:TYR:N	2.34	0.43
11:K:57:MET:N	11:K:58:PRO:CD	2.81	0.43
14:N:149:LEU:HB3	14:N:154:ILE:HD11	2.00	0.43
16:P:50:ARG:NH1	52:P:501:NDP:O3X	2.42	0.43
19:S:64:LEU:HD23	19:S:64:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:94:LYS:NZ	9:I:90:PRO:O	2.46	0.42
7:G:264:SER:OG	7:G:267:THR:HG22	2.19	0.42
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.54	0.42
9:I:52:TYR:HB3	9:I:53:PRO:HD3	2.01	0.42
14:N:304:MET:SD	15:O:290:SER:OG	2.77	0.42
20:T:74:GLN:O	20:T:77:VAL:HG12	2.19	0.42
2:B:94:ASP:OD1	8:H:58:LYS:NZ	2.48	0.42
7:G:381:GLY:O	7:G:382:THR:HG23	2.19	0.42
12:L:230:HIS:N	12:L:231:PRO:CD	2.82	0.42
13:M:169:ASN:OD1	33:h:108:GLN:NE2	2.52	0.42
15:O:176:VAL:N	15:O:177:PRO:HD2	2.34	0.42
16:P:97:ARG:NE	52:P:501:NDP:H8A	2.33	0.42
12:L:432:MET:HE3	36:k:68:PHE:N	2.35	0.42
20:U:36:PHE:O	20:U:41:GLY:N	2.52	0.42
50:h:201:CDL:OB4	34:i:88:HIS:NE2	2.52	0.42
34:i:112:THR:HG23	34:i:114:GLU:HB2	2.01	0.42
37:l:29:ARG:NH2	37:l:31:GLU:OE1	2.53	0.42
37:l:39:ASP:OD2	37:l:39:ASP:N	2.48	0.42
43:r:11:ARG:HD3	43:r:19:LEU:HD12	2.01	0.42
6:F:312:CYS:O	6:F:315:VAL:HG12	2.19	0.42
7:G:613:TYR:HB3	7:G:619:VAL:HG22	2.02	0.42
10:J:25:PRO:HB2	10:J:71:THR:CG2	2.49	0.42
13:M:243:MET:HA	13:M:246:ILE:HG22	2.01	0.42
34:i:112:THR:HG23	34:i:114:GLU:CB	2.48	0.42
40:o:41:THR:HG22	40:o:43:GLN:H	1.85	0.42
3:C:169:THR:HG22	3:C:169:THR:O	2.19	0.42
4:D:175:GLU:OE1	4:D:188:ARG:NH2	2.43	0.42
6:F:351:ILE:HD11	6:F:415:VAL:HG23	2.01	0.42
9:I:67:HIS:ND1	9:I:115:MET:HE1	2.33	0.42
10:J:75:THR:HG23	11:K:88:ASP:OD1	2.18	0.42
14:N:9:ILE:O	14:N:12:THR:OG1	2.32	0.42
16:P:237:LEU:HD12	16:P:240:HIS:CD2	2.55	0.42
32:g:64:PHE:O	32:g:69:VAL:HG23	2.20	0.42
41:p:39:VAL:O	41:p:39:VAL:HG22	2.20	0.42
2:B:100:GLY:HA2	45:B:201:SF4:S4	2.60	0.42
7:G:303:VAL:HG11	7:G:603:LEU:HD11	2.01	0.42
18:R:19:ASP:O	18:R:22:ASP:N	2.47	0.42
27:b:27:LEU:HA	27:b:30:ILE:HG22	2.01	0.42
50:d:201:CDL:OA4	31:f:28:LYS:NZ	2.40	0.42
2:B:175:ARG:CZ	42:q:78:ASP:OD1	2.68	0.42
10:J:23:PRO:O	10:J:24:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:116:ILE:O	13:M:120:ILE:HG23	2.20	0.42
16:P:201:VAL:CG2	16:P:237:LEU:HD23	2.49	0.42
22:W:42:TYR:CE2	22:W:62:ARG:HD2	2.54	0.42
24:Y:38:SER:O	24:Y:42:VAL:HG23	2.20	0.42
37:l:57:ARG:NH2	37:l:74:GLU:OE2	2.44	0.42
48:F:501:FMN:N1	48:F:501:FMN:C2'	2.83	0.42
9:I:109:THR:O	42:q:129:THR:OG1	2.29	0.42
12:L:251:THR:O	12:L:252:MET:HB3	2.20	0.42
13:M:193:ASN:O	13:M:197:LEU:HD23	2.20	0.42
14:N:99:LEU:HD23	14:N:153:ILE:CD1	2.50	0.42
22:W:22:ILE:HG22	22:W:79:ARG:HG2	2.01	0.42
42:q:46:ASN:OD1	42:q:65:THR:N	2.52	0.42
8:H:24:GLU:OE2	8:H:195:ARG:NH2	2.46	0.42
11:K:93:LEU:HD22	14:N:54:GLU:HB2	2.02	0.42
12:L:3:ILE:CD1	41:p:33:THR:HG22	2.50	0.42
17:Q:33:ARG:HH22	17:Q:77:ASP:HB2	1.85	0.42
20:U:85:ASP:OD1	34:i:18:ARG:NH1	2.52	0.42
21:V:46:TYR:O	21:V:50:ILE:HG13	2.20	0.42
25:Z:142:TYR:O	25:Z:142:TYR:CG	2.73	0.42
35:j:19:ARG:O	35:j:23:ILE:HG22	2.19	0.42
36:k:19:MET:SD	36:k:20:GLU:N	2.92	0.42
40:o:14:VAL:C	40:o:108:LEU:HD23	2.45	0.42
5:E:156:ILE:HD12	5:E:161:TYR:CE2	2.55	0.42
6:F:317:MET:SD	6:F:322:LEU:HD11	2.59	0.42
7:G:54:MET:HE1	7:G:94:MET:HG2	2.02	0.42
8:H:91:MET:O	26:a:20:GLY:HA3	2.20	0.42
12:L:394:LEU:HD12	12:L:394:LEU:N	2.35	0.42
12:L:417:SER:HB2	12:L:493:ILE:HG12	2.01	0.42
20:T:22:TYR:OH	20:T:49:GLU:OE1	2.32	0.42
40:o:53:GLN:O	40:o:53:GLN:CG	2.68	0.42
42:q:44:TYR:O	42:q:65:THR:OG1	2.38	0.42
43:r:4:THR:HG22	43:r:5:ARG:N	2.35	0.42
12:L:444:ASN:O	20:U:1:SER:OG	2.38	0.41
14:N:25:ASN:HB3	14:N:28:LEU:HD23	2.01	0.41
29:d:38:GLY:O	29:d:41:THR:OG1	2.28	0.41
38:m:76:TYR:N	38:m:77:PRO:CD	2.83	0.41
39:n:83:ASP:OD1	39:n:83:ASP:N	2.53	0.41
4:D:221:ARG:HE	43:r:24:GLN:HB3	1.85	0.41
6:F:302:SER:HB2	6:F:350:LEU:HD11	2.01	0.41
6:F:318:ASP:O	6:F:322:LEU:HB2	2.19	0.41
8:H:113:VAL:CG1	8:H:136:VAL:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:69:CYS:HB3	14:N:38:LEU:HD21	2.02	0.41
19:S:72:GLN:OE1	19:S:72:GLN:N	2.53	0.41
21:V:30:THR:O	21:V:34:LEU:HG	2.21	0.41
39:n:79:TYR:O	39:n:80:ILE:HD13	2.20	0.41
12:L:92:VAL:O	12:L:96:VAL:HG23	2.20	0.41
18:R:81:THR:HG22	18:R:92:LYS:HG3	2.01	0.41
31:f:37:ARG:NH1	31:f:52:GLU:OE1	2.53	0.41
34:i:10:ARG:NH1	39:n:153:LEU:HD13	2.35	0.41
35:j:12:ARG:NH1	36:k:53:ASN:OD1	2.46	0.41
35:j:18:THR:HG22	35:j:19:ARG:N	2.35	0.41
37:l:4:THR:HG22	37:l:5:LYS:N	2.35	0.41
3:C:199:LEU:O	3:C:200:ASN:C	2.64	0.41
4:D:34:ASN:OD1	4:D:34:ASN:N	2.53	0.41
7:G:273:GLY:O	7:G:549:HIS:NE2	2.45	0.41
7:G:636:ILE:HG22	7:G:637:GLU:N	2.35	0.41
8:H:102:ILE:HD11	8:H:160:TYR:HD1	1.85	0.41
8:H:310:PHE:HB3	27:b:32:PRO:HA	2.02	0.41
12:L:419:THR:HA	12:L:422:TYR:CZ	2.56	0.41
16:P:295:THR:O	16:P:295:THR:HG23	2.21	0.41
7:G:344:CYS:HB3	7:G:510:GLY:O	2.20	0.41
12:L:258:PHE:HA	12:L:261:VAL:HG22	2.03	0.41
12:L:485:PHE:O	12:L:489:THR:OG1	2.38	0.41
37:l:30:VAL:HG12	37:l:30:VAL:O	2.21	0.41
37:l:95:VAL:HG12	37:l:96:SER:N	2.36	0.41
41:p:136:LYS:NZ	41:p:140:ASP:OD1	2.54	0.41
1:A:62:PHE:CG	8:H:140:ILE:CG2	3.03	0.41
4:D:103:PHE:HA	4:D:106:LEU:HD12	2.02	0.41
6:F:47:GLU:OE1	6:F:47:GLU:N	2.46	0.41
8:H:281:ARG:O	8:H:282:TYR:C	2.64	0.41
13:M:207:MET:O	13:M:207:MET:CG	2.68	0.41
14:N:166:ALA:HB1	14:N:288:LEU:HB2	2.02	0.41
25:Z:81:ARG:O	25:Z:85:ILE:HG12	2.21	0.41
40:o:91:HIS:O	40:o:95:VAL:HG23	2.21	0.41
1:A:2:ASN:O	1:A:5:THR:OG1	2.30	0.41
4:D:293:CYS:CB	4:D:420:THR:HG21	2.51	0.41
7:G:11:VAL:HG11	7:G:73:VAL:HG21	2.02	0.41
7:G:384:PRO:HA	7:G:387:GLU:O	2.21	0.41
7:G:604:SER:CB	7:G:611:LEU:HD13	2.51	0.41
12:L:341:MET:HG2	12:L:454:ILE:HG12	2.02	0.41
13:M:207:MET:HE3	13:M:243:MET:SD	2.61	0.41
15:O:125:GLU:O	15:O:126:ARG:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:m:95:GLY:N	38:m:96:PRO:HD2	2.36	0.41
5:E:106:THR:HB	5:E:107:PRO:HD3	2.03	0.41
5:E:204:GLU:HB3	5:E:205:PRO:HD2	2.03	0.41
6:F:56:ILE:O	6:F:60:MET:HG2	2.20	0.41
6:F:342:ASP:OD1	6:F:342:ASP:N	2.48	0.41
7:G:94:MET:HE1	7:G:116:LEU:CD1	2.50	0.41
7:G:362:TYR:O	7:G:362:TYR:CD2	2.74	0.41
9:I:41:SER:O	9:I:45:ARG:HG3	2.21	0.41
10:J:36:GLY:HA2	11:K:38:LEU:HD21	2.03	0.41
12:L:187:VAL:HG22	13:M:383:MET:CG	2.51	0.41
13:M:14:LEU:O	13:M:18:SER:OG	2.35	0.41
14:N:337:LEU:N	14:N:338:PRO:CD	2.84	0.41
15:O:101:TYR:HD1	15:O:152:TYR:HH	1.68	0.41
24:Y:3:VAL:O	24:Y:4:LYS:HB3	2.21	0.41
33:h:32:THR:HG22	33:h:32:THR:O	2.21	0.41
36:k:18:LYS:NZ	36:k:20:GLU:OE2	2.48	0.41
2:B:64:CYS:HB3	4:D:108:TYR:CB	2.50	0.41
4:D:261:ARG:O	4:D:287:ILE:HA	2.20	0.41
5:E:65:ALA:O	5:E:69:VAL:HG23	2.21	0.41
5:E:101:GLN:HB2	5:E:142:VAL:HG21	2.01	0.41
8:H:132:ALA:O	8:H:136:VAL:HG23	2.21	0.41
16:P:147:ARG:O	16:P:151:VAL:HG23	2.21	0.41
3:C:175:ARG:NE	3:C:186:GLU:OE2	2.52	0.40
7:G:460:ARG:NH2	7:G:657:LEU:HD11	2.36	0.40
7:G:604:SER:OG	7:G:611:LEU:HD13	2.20	0.40
8:H:69:SER:O	8:H:73:ILE:HG12	2.21	0.40
9:I:51:ASN:O	9:I:55:GLU:N	2.46	0.40
10:J:40:CYS:O	10:J:44:LEU:HG	2.21	0.40
12:L:384:PRO:O	12:L:389:PHE:CG	2.73	0.40
13:M:347:GLY:HA3	13:M:418:LYS:C	2.46	0.40
14:N:161:SER:OG	14:N:184:ILE:O	2.39	0.40
16:P:29:PHE:CZ	16:P:207:VAL:HG11	2.56	0.40
17:Q:32:THR:HG23	22:W:130:PRO:O	2.21	0.40
42:q:2:GLU:CG	43:r:4:THR:HG23	2.51	0.40
5:E:202:LEU:HD12	6:F:26:TYR:CE2	2.56	0.40
6:F:147:SER:O	6:F:151:VAL:HG23	2.21	0.40
7:G:286:ASN:N	7:G:290:LEU:O	2.44	0.40
12:L:369:THR:HG23	12:L:445:GLU:OE1	2.20	0.40
50:L:702:CDL:HA62	33:h:22:LEU:HD22	2.03	0.40
22:W:77:ASP:O	22:W:81:VAL:HG23	2.21	0.40
35:j:63:GLU:O	35:j:64:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:302:SER:HB2	6:F:350:LEU:CD1	2.51	0.40
11:K:1:FME:N	11:K:2:PRO:HD2	2.37	0.40
16:P:150:ALA:O	16:P:153:GLU:HG2	2.21	0.40
19:S:21:HIS:HA	19:S:55:ARG:O	2.21	0.40
39:n:10:THR:HG22	39:n:11:HIS:N	2.37	0.40
42:q:44:TYR:O	42:q:65:THR:HG21	2.20	0.40
10:J:144:MET:HE2	10:J:152:MET:HE2	2.02	0.40
12:L:24:SER:OG	12:L:25:ASN:N	2.55	0.40
12:L:30:ILE:CG2	12:L:31:ASN:N	2.84	0.40
12:L:49:LEU:HD22	41:p:32:LEU:HD21	2.02	0.40
12:L:180:ILE:HD12	13:M:397:GLY:HA2	2.04	0.40
12:L:258:PHE:O	12:L:261:VAL:HG22	2.22	0.40
13:M:257:MET:O	13:M:257:MET:HG3	2.21	0.40
13:M:441:MET:O	13:M:442:ILE:C	2.64	0.40
15:O:25:ILE:HG12	15:O:168:ALA:HB3	2.03	0.40
23:X:17:VAL:CG2	26:a:50:ARG:HH22	2.35	0.40
4:D:104:ASP:OD1	4:D:115:GLU:OE2	2.40	0.40
7:G:41:CYS:O	7:G:161:ARG:NH2	2.36	0.40
7:G:333:ASP:O	7:G:337:LYS:HG3	2.22	0.40
11:K:16:LEU:O	11:K:19:THR:OG1	2.35	0.40
12:L:517:ASN:OD1	12:L:517:ASN:C	2.64	0.40
23:X:166:PHE:O	23:X:167:PHE:C	2.64	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	86/115 (75%)	83 (96%)	3 (4%)	0	100	100
2	B	153/224 (68%)	142 (93%)	10 (6%)	1 (1%)	18	50
3	C	204/263 (78%)	193 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	412/463 (89%)	386 (94%)	26 (6%)	0	100	100
5	E	208/245 (85%)	194 (93%)	14 (7%)	0	100	100
6	F	426/464 (92%)	401 (94%)	25 (6%)	0	100	100
7	G	685/715 (96%)	649 (95%)	36 (5%)	0	100	100
8	H	304/318 (96%)	279 (92%)	25 (8%)	0	100	100
9	I	176/212 (83%)	168 (96%)	8 (4%)	0	100	100
10	J	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
11	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
12	L	604/607 (100%)	562 (93%)	42 (7%)	0	100	100
13	M	457/459 (100%)	430 (94%)	27 (6%)	0	100	100
14	N	342/345 (99%)	325 (95%)	17 (5%)	0	100	100
15	O	318/355 (90%)	293 (92%)	25 (8%)	0	100	100
16	P	282/377 (75%)	265 (94%)	17 (6%)	0	100	100
17	Q	123/175 (70%)	119 (97%)	4 (3%)	0	100	100
18	R	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
19	S	80/99 (81%)	73 (91%)	7 (9%)	0	100	100
20	T	71/156 (46%)	63 (89%)	8 (11%)	0	100	100
20	U	86/156 (55%)	82 (95%)	4 (5%)	0	100	100
21	V	110/116 (95%)	102 (93%)	8 (7%)	0	100	100
22	W	112/131 (86%)	101 (90%)	11 (10%)	0	100	100
23	X	169/172 (98%)	157 (93%)	12 (7%)	0	100	100
24	Y	138/143 (96%)	131 (95%)	7 (5%)	0	100	100
25	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
26	a	66/68 (97%)	65 (98%)	1 (2%)	0	100	100
27	b	81/83 (98%)	74 (91%)	7 (9%)	0	100	100
28	c	44/76 (58%)	43 (98%)	1 (2%)	0	100	100
29	d	117/120 (98%)	115 (98%)	2 (2%)	0	100	100
30	e	102/106 (96%)	91 (89%)	11 (11%)	0	100	100
31	f	48/57 (84%)	44 (92%)	4 (8%)	0	100	100
32	g	99/151 (66%)	96 (97%)	3 (3%)	0	100	100
33	h	135/189 (71%)	130 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	i	92/127 (72%)	81 (88%)	11 (12%)	0	100	100
35	j	61/105 (58%)	59 (97%)	2 (3%)	0	100	100
36	k	76/104 (73%)	74 (97%)	2 (3%)	0	100	100
37	l	154/186 (83%)	144 (94%)	10 (6%)	0	100	100
38	m	123/129 (95%)	117 (95%)	6 (5%)	0	100	100
39	n	174/179 (97%)	167 (96%)	7 (4%)	0	100	100
40	o	112/137 (82%)	103 (92%)	9 (8%)	0	100	100
41	p	166/176 (94%)	156 (94%)	10 (6%)	0	100	100
42	q	141/145 (97%)	132 (94%)	9 (6%)	0	100	100
43	r	92/112 (82%)	84 (91%)	8 (9%)	0	100	100
44	s	37/104 (36%)	35 (95%)	2 (5%)	0	100	100
All	All	7960/9192 (87%)	7484 (94%)	475 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	64	CYS

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	81/103 (79%)	81 (100%)	0	100	100
2	B	131/185 (71%)	130 (99%)	1 (1%)	73	80
3	C	188/227 (83%)	188 (100%)	0	100	100
4	D	362/394 (92%)	362 (100%)	0	100	100
5	E	183/205 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	579/601 (96%)	579 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	H	270/279 (97%)	270 (100%)	0	100	100
9	I	145/178 (82%)	145 (100%)	0	100	100
10	J	131/137 (96%)	131 (100%)	0	100	100
11	K	87/87 (100%)	87 (100%)	0	100	100
12	L	548/549 (100%)	548 (100%)	0	100	100
13	M	414/414 (100%)	414 (100%)	0	100	100
14	N	306/307 (100%)	306 (100%)	0	100	100
15	O	284/309 (92%)	284 (100%)	0	100	100
16	P	251/325 (77%)	251 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/94 (84%)	79 (100%)	0	100	100
19	S	73/80 (91%)	73 (100%)	0	100	100
20	T	67/135 (50%)	67 (100%)	0	100	100
20	U	81/135 (60%)	81 (100%)	0	100	100
21	V	100/102 (98%)	100 (100%)	0	100	100
22	W	108/114 (95%)	108 (100%)	0	100	100
23	X	153/154 (99%)	153 (100%)	0	100	100
24	Y	105/107 (98%)	105 (100%)	0	100	100
25	Z	120/123 (98%)	120 (100%)	0	100	100
26	a	58/58 (100%)	58 (100%)	0	100	100
27	b	72/72 (100%)	72 (100%)	0	100	100
28	c	40/67 (60%)	40 (100%)	0	100	100
29	d	106/107 (99%)	106 (100%)	0	100	100
30	e	92/94 (98%)	92 (100%)	0	100	100
31	f	46/53 (87%)	46 (100%)	0	100	100
32	g	92/129 (71%)	92 (100%)	0	100	100
33	h	122/162 (75%)	122 (100%)	0	100	100
34	i	90/118 (76%)	90 (100%)	0	100	100
35	j	58/87 (67%)	58 (100%)	0	100	100
36	k	60/78 (77%)	60 (100%)	0	100	100
37	l	141/161 (88%)	141 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
38	m	111/114 (97%)	111 (100%)	0	100	100
39	n	161/164 (98%)	161 (100%)	0	100	100
40	o	106/121 (88%)	106 (100%)	0	100	100
41	p	153/158 (97%)	153 (100%)	0	100	100
42	q	129/131 (98%)	129 (100%)	0	100	100
43	r	86/95 (90%)	86 (100%)	0	100	100
44	s	38/95 (40%)	38 (100%)	0	100	100
All	All	7062/7931 (89%)	7061 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	64	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	172	GLN
3	C	88	ASN
3	C	95	ASN
3	C	160	HIS
3	C	200	ASN
4	D	149	ASN
4	D	313	GLN
4	D	398	HIS
5	E	55	GLN
6	F	113	HIS
6	F	250	ASN
7	G	421	HIS
7	G	475	GLN
7	G	629	ASN
8	H	5	ASN
8	H	47	GLN
8	H	169	GLN
9	I	146	HIS
9	I	172	GLN
11	K	92	ASN
12	L	29	HIS

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Mol	Chain	Res	Type
12	L	56	HIS
12	L	135	ASN
12	L	230	HIS
12	L	320	ASN
12	L	514	ASN
12	L	594	ASN
13	M	175	ASN
13	M	279	GLN
13	M	374	ASN
14	N	63	GLN
14	N	125	HIS
14	N	174	GLN
14	N	204	ASN
14	N	222	ASN
15	O	180	GLN
15	O	244	ASN
16	P	37	HIS
16	P	131	HIS
17	Q	125	ASN
18	R	47	GLN
19	S	80	ASN
20	T	74	GLN
21	V	36	HIS
22	W	72	ASN
22	W	101	GLN
23	X	34	GLN
23	X	72	GLN
30	e	97	HIS
32	g	55	ASN
32	g	109	ASN
33	h	108	GLN
33	h	124	GLN
33	h	135	HIS
34	i	12	GLN
34	i	73	HIS
35	j	42	HIS
35	j	58	GLN
37	l	2	HIS
37	l	77	HIS
37	l	154	HIS
38	m	74	ASN
42	q	13	GLN

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Mol	Chain	Res	Type
42	q	31	ASN
42	q	52	ASN
42	q	113	HIS
42	q	135	HIS
43	r	12	ASN
43	r	46	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are 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	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.42	1 (20%)
12	FME	L	1	12	8,9,10	0.94	0	7,9,11	1.07	1 (14%)
43	AYA	r	1	43	6,7,8	1.28	1 (16%)	5,8,10	1.10	1 (20%)
34	SAC	i	1	34	7,8,9	1.00	0	8,9,11	0.73	0
1	FME	A	1	1	8,9,10	0.96	0	7,9,11	0.84	0
10	FME	J	1	10	8,9,10	0.93	0	7,9,11	0.94	0
13	FME	M	1	13	8,9,10	0.96	0	7,9,11	0.66	0
27	AYA	b	1	27	6,7,8	1.24	1 (16%)	5,8,10	1.40	1 (20%)
11	FME	K	1	11	8,9,10	0.92	0	7,9,11	1.14	1 (14%)
14	FME	N	1	14	8,9,10	0.90	0	7,9,11	0.93	0
8	FME	H	1	8	8,9,10	0.91	0	7,9,11	1.39	1 (14%)

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	85	4	-	3/10/13/15	-
12	FME	L	1	12	-	4/7/9/11	-
43	AYA	r	1	43	-	0/4/6/8	-
34	SAC	i	1	34	-	2/7/8/10	-
1	FME	A	1	1	-	3/7/9/11	-
10	FME	J	1	10	-	4/7/9/11	-
13	FME	M	1	13	-	0/7/9/11	-
27	AYA	b	1	27	-	1/4/6/8	-
11	FME	K	1	11	-	2/7/9/11	-
14	FME	N	1	14	-	3/7/9/11	-
8	FME	H	1	8	-	5/7/9/11	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.38	1.45	1.34
4	D	85	2MR	CZ-NH2	4.91	1.44	1.33
43	r	1	AYA	CA-N	-2.47	1.44	1.46
27	b	1	AYA	CA-N	-2.33	1.44	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	1	FME	C-CA-N	3.05	115.24	109.73
27	b	1	AYA	CB-CA-N	2.87	112.81	109.61
4	D	85	2MR	CD-NE-CZ	2.50	128.08	123.41
11	K	1	FME	C-CA-N	2.42	114.11	109.73
12	L	1	FME	C-CA-N	2.20	113.70	109.73
43	r	1	AYA	CB-CA-N	2.12	111.97	109.61

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
4	D	85	2MR	O-C-CA-CB
8	H	1	FME	O-C-CA-CB
8	H	1	FME	CA-CB-CG-SD
10	J	1	FME	CB-CA-N-CN
10	J	1	FME	C-CA-CB-CG

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Mol	Chain	Res	Type	Atoms
11	K	1	FME	C-CA-CB-CG
12	L	1	FME	O-C-CA-CB
14	N	1	FME	CB-CA-N-CN
14	N	1	FME	N-CA-CB-CG
34	i	1	SAC	C-CA-N-C1A
34	i	1	SAC	CB-CA-N-C1A
4	D	85	2MR	NE-CD-CG-CB
1	A	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
10	J	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
4	D	85	2MR	CA-CB-CG-CD
8	H	1	FME	CB-CG-SD-CE
27	b	1	AYA	C-CA-N-CT
10	J	1	FME	CB-CG-SD-CE
14	N	1	FME	C-CA-CB-CG
12	L	1	FME	CB-CG-SD-CE
12	L	1	FME	CA-CB-CG-SD
8	H	1	FME	C-CA-CB-CG
8	H	1	FME	CB-CA-N-CN
12	L	1	FME	CB-CA-N-CN

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	85	2MR	1	0
11	K	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 28 ligands modelled in this entry, 1 is monoatomic - leaving 27 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	$\#\|Z\| > 2$
52	NDP	P	501	-	49,52,52	2.26	8 (16%)	66,80,80	1.63	11 (16%)
46	PC1	I	201	-	53,53,53	0.94	4 (7%)	59,61,61	0.99	2 (3%)
49	3PE	L	701	-	50,50,50	0.85	4 (8%)	53,55,55	1.03	2 (3%)
49	3PE	H	401	-	50,50,50	0.86	4 (8%)	53,55,55	1.09	2 (3%)
47	FES	G	803	7	0,4,4	-	-	-		
54	EHZ	U	201	20	29,36,37	1.68	5 (17%)	35,44,47	1.45	4 (11%)
47	FES	E	301	5	0,4,4	-	-	-		
46	PC1	B	202	-	50,50,53	0.98	4 (8%)	56,58,61	1.00	2 (3%)
49	3PE	N	401	-	50,50,50	0.87	4 (8%)	53,55,55	1.03	2 (3%)
48	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.32	8 (16%)
50	CDL	q	201	-	68,68,99	1.05	7 (10%)	74,80,111	1.10	4 (5%)
49	3PE	f	101	-	38,38,50	0.99	4 (10%)	41,43,55	1.00	2 (4%)
49	3PE	M	501	-	50,50,50	0.87	4 (8%)	53,55,55	0.96	2 (3%)
50	CDL	d	201	-	99,99,99	0.88	7 (7%)	105,111,111	1.03	4 (3%)
45	SF4	G	801	7	0,12,12	-	-	-		
45	SF4	F	502	6	0,12,12	-	-	-		
49	3PE	i	201	-	41,41,50	0.95	4 (9%)	44,46,55	1.09	2 (4%)
54	EHZ	T	201	20	29,36,37	1.68	5 (17%)	35,44,47	1.55	5 (14%)
49	3PE	M	502	-	50,50,50	0.86	4 (8%)	53,55,55	1.08	2 (3%)
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	I	204	9	0,12,12	-	-	-		
50	CDL	h	201	-	77,77,99	0.98	7 (9%)	83,89,111	1.10	4 (4%)
45	SF4	G	802	7	0,12,12	-	-	-		
45	SF4	I	203	9	0,12,12	-	-	-		
50	CDL	L	702	-	80,80,99	0.98	8 (10%)	86,92,111	1.08	4 (4%)
49	3PE	I	202	-	50,50,50	0.86	4 (8%)	53,55,55	1.01	2 (3%)
51	ATP	O	401	-	29,33,33	1.30	4 (13%)	44,52,52	2.05	12 (27%)

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
52	NDP	P	501	-	-	10/34/77/77	0/5/5/5
46	PC1	I	201	-	-	22/57/57/57	-
49	3PE	L	701	-	-	18/54/54/54	-
49	3PE	H	401	-	-	21/54/54/54	-
47	FES	G	803	7	-	-	0/1/1/1
54	EHZ	U	201	20	-	11/42/44/45	-
47	FES	E	301	5	-	-	0/1/1/1
46	PC1	B	202	-	-	21/54/54/57	-
49	3PE	N	401	-	-	24/54/54/54	-
48	FMN	F	501	-	-	8/18/18/18	0/3/3/3
50	CDL	q	201	-	-	37/79/79/110	-
49	3PE	f	101	-	-	13/42/42/54	-
49	3PE	M	501	-	-	25/54/54/54	-
50	CDL	d	201	-	-	60/110/110/110	-
45	SF4	G	801	7	-	-	0/6/5/5
45	SF4	F	502	6	-	-	0/6/5/5
49	3PE	i	201	-	-	17/45/45/54	-
54	EHZ	T	201	20	-	16/42/44/45	-
49	3PE	M	502	-	-	18/54/54/54	-
45	SF4	B	201	2	-	-	0/6/5/5
50	CDL	h	201	-	-	41/88/88/110	-
45	SF4	I	204	9	-	-	0/6/5/5
45	SF4	G	802	7	-	-	0/6/5/5
45	SF4	I	203	9	-	-	0/6/5/5
50	CDL	L	702	-	-	41/91/91/110	-
49	3PE	I	202	-	-	15/54/54/54	-
51	ATP	O	401	-	-	7/22/38/38	0/3/3/3

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.55	1.83	1.59
54	T	201	EHZ	C15-N2	5.49	1.45	1.33
54	U	201	EHZ	C15-N2	5.42	1.45	1.33
54	U	201	EHZ	C12-N1	5.23	1.45	1.33
54	T	201	EHZ	C12-N1	5.19	1.45	1.33
51	O	401	ATP	C5-C4	4.32	1.47	1.39
52	P	501	NDP	PN-O5D	4.04	1.75	1.59
48	F	501	FMN	C4A-N5	3.50	1.37	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	O2B-C2B	-3.11	1.32	1.44
51	O	401	ATP	C5-C6	2.68	1.48	1.41
50	L	702	CDL	OA6-CA4	-2.65	1.40	1.46
50	q	201	CDL	OB6-CB4	-2.63	1.40	1.46
50	h	201	CDL	OA6-CA4	-2.62	1.40	1.46
50	d	201	CDL	OA6-CA4	-2.61	1.40	1.46
52	P	501	NDP	O4B-C4B	-2.61	1.39	1.45
49	H	401	3PE	O21-C2	-2.59	1.40	1.46
48	F	501	FMN	C10-N1	2.59	1.38	1.33
50	L	702	CDL	OA8-CA7	2.58	1.40	1.33
49	M	501	3PE	O21-C2	-2.57	1.40	1.46
49	I	202	3PE	O21-C2	-2.56	1.40	1.46
46	I	201	PC1	O21-C2	-2.55	1.40	1.46
50	L	702	CDL	OB6-CB4	-2.55	1.40	1.46
50	d	201	CDL	OA8-CA7	2.55	1.40	1.33
50	q	201	CDL	OB8-CB7	2.53	1.40	1.33
50	h	201	CDL	OA8-CA7	2.53	1.40	1.33
49	M	502	3PE	O21-C2	-2.52	1.40	1.46
46	B	202	PC1	O21-C2	-2.50	1.40	1.46
49	N	401	3PE	O21-C2	-2.50	1.40	1.46
50	L	702	CDL	OB8-CB7	2.49	1.40	1.33
50	h	201	CDL	OB8-CB7	2.48	1.40	1.33
49	L	701	3PE	O31-C31	2.47	1.40	1.33
51	O	401	ATP	C8-N7	2.47	1.36	1.31
50	d	201	CDL	OB8-CB7	2.46	1.40	1.33
49	M	501	3PE	O31-C31	2.46	1.40	1.33
49	f	101	3PE	O31-C31	2.46	1.40	1.33
49	i	201	3PE	O21-C2	-2.44	1.40	1.46
50	q	201	CDL	OA8-CA7	2.43	1.40	1.33
49	H	401	3PE	O31-C31	2.43	1.40	1.33
49	I	202	3PE	O31-C31	2.42	1.40	1.33
46	I	201	PC1	O31-C31	2.42	1.40	1.33
52	P	501	NDP	C5A-C4A	2.40	1.43	1.39
46	B	202	PC1	O31-C31	2.38	1.40	1.33
54	U	201	EHZ	C9-S1	2.37	1.81	1.76
49	f	101	3PE	O21-C2	-2.36	1.40	1.46
49	i	201	3PE	O31-C31	2.36	1.40	1.33
50	d	201	CDL	OB6-CB4	-2.36	1.40	1.46
49	M	502	3PE	O31-C31	2.34	1.40	1.33
50	q	201	CDL	OA6-CA4	-2.33	1.40	1.46
54	T	201	EHZ	C9-S1	2.32	1.81	1.76
50	q	201	CDL	OA6-CA5	2.32	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	N	401	3PE	O31-C31	2.31	1.40	1.33
49	f	101	3PE	O21-C21	2.31	1.40	1.34
50	h	201	CDL	OB6-CB4	-2.28	1.40	1.46
50	h	201	CDL	OB6-CB5	2.28	1.40	1.34
49	N	401	3PE	O31-C3	-2.27	1.40	1.45
54	U	201	EHZ	O4-C15	-2.27	1.18	1.23
54	T	201	EHZ	O4-C15	-2.23	1.19	1.23
49	L	701	3PE	O21-C2	-2.23	1.41	1.46
49	i	201	3PE	O21-C21	2.21	1.40	1.34
54	T	201	EHZ	O3-C12	-2.20	1.18	1.23
51	O	401	ATP	C5-N7	-2.20	1.34	1.39
49	M	502	3PE	O31-C3	-2.19	1.40	1.45
49	i	201	3PE	O31-C3	-2.19	1.40	1.45
50	L	702	CDL	OB6-CB5	2.18	1.40	1.34
46	B	202	PC1	O21-C21	2.17	1.40	1.34
50	d	201	CDL	OA6-CA5	2.17	1.40	1.34
49	L	701	3PE	O21-C21	2.16	1.40	1.34
52	P	501	NDP	C2A-N1A	2.15	1.37	1.33
46	B	202	PC1	O31-C3	-2.15	1.40	1.45
50	q	201	CDL	OA8-CA6	-2.14	1.40	1.45
50	d	201	CDL	OB8-CB6	-2.13	1.40	1.45
54	U	201	EHZ	O3-C12	-2.13	1.18	1.23
50	d	201	CDL	OB6-CB5	2.13	1.40	1.34
50	q	201	CDL	OB6-CB5	2.12	1.40	1.34
46	I	201	PC1	O31-C3	-2.12	1.40	1.45
49	L	701	3PE	O31-C3	-2.11	1.40	1.45
49	N	401	3PE	O21-C21	2.10	1.40	1.34
49	I	202	3PE	O31-C3	-2.10	1.40	1.45
49	M	502	3PE	O21-C21	2.10	1.40	1.34
49	H	401	3PE	O31-C3	-2.09	1.40	1.45
52	P	501	NDP	O5D-C5D	-2.09	1.36	1.44
46	I	201	PC1	O21-C21	2.09	1.40	1.34
49	M	501	3PE	O21-C21	2.09	1.40	1.34
49	f	101	3PE	O31-C3	-2.09	1.40	1.45
50	h	201	CDL	OA6-CA5	2.08	1.40	1.34
49	I	202	3PE	O21-C21	2.08	1.40	1.34
50	L	702	CDL	OA8-CA6	-2.06	1.40	1.45
50	L	702	CDL	OA6-CA5	2.05	1.40	1.34
49	H	401	3PE	O21-C21	2.05	1.40	1.34
49	M	501	3PE	O31-C3	-2.04	1.40	1.45
50	h	201	CDL	OB8-CB6	-2.03	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.03	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	C2B-C1B	2.00	1.58	1.53

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	PN-O3-PA	-7.22	108.06	132.83
51	O	401	ATP	C5-C4-N3	-6.06	118.84	126.75
54	T	201	EHZ	C8-C9-S1	5.36	120.27	113.63
54	U	201	EHZ	C8-C9-S1	5.18	120.03	113.63
51	O	401	ATP	N3-C4-N9	4.68	134.80	127.08
50	d	201	CDL	OB6-CB5-C51	4.18	120.50	111.50
50	L	702	CDL	OB6-CB5-C51	4.12	120.38	111.50
49	i	201	3PE	O21-C21-C22	4.09	120.31	111.50
49	M	502	3PE	O21-C21-C22	4.08	120.30	111.50
50	h	201	CDL	OA6-CA5-C11	4.08	120.30	111.50
51	O	401	ATP	C2-N3-C4	4.01	121.22	111.75
46	B	202	PC1	O21-C21-C22	4.00	120.13	111.50
50	q	201	CDL	OB6-CB5-C51	4.00	120.12	111.50
49	H	401	3PE	O21-C21-C22	3.92	119.94	111.50
50	L	702	CDL	OA6-CA5-C11	3.89	119.89	111.50
50	d	201	CDL	OA6-CA5-C11	3.84	119.78	111.50
49	L	701	3PE	O21-C21-C22	3.83	119.76	111.50
49	N	401	3PE	O21-C21-C22	3.77	119.64	111.50
49	I	202	3PE	O21-C21-C22	3.71	119.51	111.50
46	I	201	PC1	O21-C21-C22	3.71	119.49	111.50
51	O	401	ATP	PB-O3B-PG	-3.71	120.11	132.83
49	f	101	3PE	O21-C21-C22	3.69	119.46	111.50
49	M	501	3PE	O21-C21-C22	3.68	119.42	111.50
50	q	201	CDL	OA6-CA5-C11	3.66	119.39	111.50
51	O	401	ATP	N3-C2-N1	-3.61	122.95	128.60
50	h	201	CDL	OB6-CB5-C51	3.57	119.19	111.50
48	F	501	FMN	C4-N3-C2	-3.50	119.17	125.64
51	O	401	ATP	PA-O3A-PB	-3.41	121.12	132.83
51	O	401	ATP	C4-C5-N7	-3.41	106.47	110.62
52	P	501	NDP	O2B-P2B-O1X	-3.21	96.99	109.39
52	P	501	NDP	PA-O5B-C5B	-3.08	103.64	121.68
51	O	401	ATP	C5-N7-C8	2.99	107.75	103.51
48	F	501	FMN	C4A-C10-N1	-2.98	117.81	124.73
48	F	501	FMN	C4A-C4-N3	2.88	120.51	113.19
50	h	201	CDL	OA8-CA7-C31	2.84	120.83	111.91
50	d	201	CDL	OB8-CB7-C71	2.84	120.81	111.91
51	O	401	ATP	C4-N9-C8	2.83	108.80	105.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	PN-O5D-C5D	-2.77	105.42	121.68
48	F	501	FMN	C4A-C10-N10	2.77	120.53	116.48
49	M	502	3PE	O31-C31-C32	2.67	120.27	111.91
46	I	201	PC1	O31-C31-C32	2.64	120.19	111.91
49	L	701	3PE	O31-C31-C32	2.62	120.14	111.91
49	i	201	3PE	O31-C31-C32	2.62	120.12	111.91
49	H	401	3PE	O31-C31-C32	2.61	120.10	111.91
48	F	501	FMN	O4-C4-C4A	-2.60	119.70	126.60
52	P	501	NDP	O3X-P2B-O2X	2.55	117.39	107.64
49	N	401	3PE	O31-C31-C32	2.53	119.84	111.91
50	q	201	CDL	OB8-CB7-C71	2.51	119.79	111.91
50	q	201	CDL	OA8-CA7-C31	2.48	119.69	111.91
49	I	202	3PE	O31-C31-C32	2.46	119.64	111.91
50	d	201	CDL	OA8-CA7-C31	2.46	119.63	111.91
50	h	201	CDL	OB8-CB7-C71	2.43	119.54	111.91
50	L	702	CDL	OA8-CA7-C31	2.43	119.53	111.91
49	f	101	3PE	O31-C31-C32	2.41	119.48	111.91
51	O	401	ATP	C6-C5-N7	2.41	136.50	132.02
51	O	401	ATP	N9-C8-N7	-2.40	110.63	113.91
46	B	202	PC1	O31-C31-C32	2.40	119.43	111.91
49	M	501	3PE	O31-C31-C32	2.39	119.42	111.91
50	L	702	CDL	OB8-CB7-C71	2.39	119.41	111.91
48	F	501	FMN	C10-N1-C2	2.35	121.60	116.90
54	T	201	EHZ	C13-C12-N1	2.34	120.37	116.42
48	F	501	FMN	C4-C4A-C10	2.34	120.72	116.79
52	P	501	NDP	C2A-N1A-C6A	-2.32	114.78	118.77
54	T	201	EHZ	C7-C8-C9	-2.30	108.64	113.89
54	U	201	EHZ	C14-C13-C12	-2.29	108.55	112.36
52	P	501	NDP	O2N-PN-O1N	2.28	123.51	112.24
52	P	501	NDP	N3A-C4A-N9A	2.28	130.84	127.08
54	U	201	EHZ	C10-S1-C9	2.27	108.95	101.87
54	T	201	EHZ	O2-C9-S1	-2.22	119.73	122.61
48	F	501	FMN	C10-C4A-N5	-2.12	120.35	124.86
52	P	501	NDP	O5D-PN-O1N	-2.12	100.79	109.07
54	U	201	EHZ	C13-C12-N1	2.11	119.98	116.42
52	P	501	NDP	C5A-C4A-N3A	-2.06	124.06	126.75
54	T	201	EHZ	C5-C6-C7	-2.06	108.94	114.85
51	O	401	ATP	C2-N1-C6	2.05	122.28	118.77
52	P	501	NDP	C5B-C4B-C3B	-2.02	107.59	115.18

There are no chirality outliers.

All (425) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	O22-C21-O21-C2
46	B	202	PC1	C22-C21-O21-C2
46	I	201	PC1	C11-O13-P-O14
46	I	201	PC1	C1-O11-P-O12
48	F	501	FMN	C2'-C1'-N10-C10
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C3'-C4'-C5'-O5'
48	F	501	FMN	O4'-C4'-C5'-O5'
48	F	501	FMN	C5'-O5'-P-O2P
48	F	501	FMN	C5'-O5'-P-O3P
49	H	401	3PE	C11-O13-P-O14
49	H	401	3PE	O13-C11-C12-N
49	H	401	3PE	O22-C21-O21-C2
49	I	202	3PE	O13-C11-C12-N
49	L	701	3PE	C11-O13-P-O12
49	L	701	3PE	C11-O13-P-O14
49	L	701	3PE	C22-C21-O21-C2
49	M	501	3PE	C1-O11-P-O12
49	M	501	3PE	C1-O11-P-O13
49	M	501	3PE	C1-O11-P-O14
49	N	401	3PE	C11-O13-P-O11
49	N	401	3PE	C11-O13-P-O12
49	N	401	3PE	C11-O13-P-O14
49	N	401	3PE	O13-C11-C12-N
49	N	401	3PE	O21-C2-C3-O31
49	i	201	3PE	O13-C11-C12-N
49	i	201	3PE	C22-C21-O21-C2
50	L	702	CDL	CA2-OA2-PA1-OA3
50	L	702	CDL	CA3-OA5-PA1-OA4
50	L	702	CDL	OB7-CB5-OB6-CB4
50	d	201	CDL	CB2-C1-CA2-OA2
50	d	201	CDL	C1-CA2-OA2-PA1
50	d	201	CDL	CA2-OA2-PA1-OA3
50	d	201	CDL	CA2-OA2-PA1-OA4
50	d	201	CDL	CB2-OB2-PB2-OB3
50	d	201	CDL	CB2-OB2-PB2-OB4
50	d	201	CDL	C51-CB5-OB6-CB4
50	h	201	CDL	CA3-OA5-PA1-OA3
50	h	201	CDL	CA3-OA5-PA1-OA4
50	h	201	CDL	CB2-OB2-PB2-OB4
50	h	201	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
50	q	201	CDL	CB3-OB5-PB2-OB3
50	q	201	CDL	C51-CB5-OB6-CB4
51	O	401	ATP	C5'-O5'-PA-O1A
51	O	401	ATP	C5'-O5'-PA-O2A
52	P	501	NDP	C5B-O5B-PA-O1A
52	P	501	NDP	C5B-O5B-PA-O3
52	P	501	NDP	C2N-C3N-C7N-N7N
54	T	201	EHZ	C6-C7-C8-C9
54	T	201	EHZ	S1-C10-C11-N1
54	T	201	EHZ	C12-C13-C14-N2
54	T	201	EHZ	N2-C15-C16-O5
54	T	201	EHZ	O4-C15-C16-O5
54	T	201	EHZ	C16-C17-C20-O6
54	U	201	EHZ	O1-C7-C8-C9
54	U	201	EHZ	C6-C7-C8-C9
46	I	201	PC1	O32-C31-O31-C3
50	d	201	CDL	OB9-CB7-OB8-CB6
50	d	201	CDL	C71-CB7-OB8-CB6
50	h	201	CDL	OA9-CA7-OA8-CA6
49	L	701	3PE	O22-C21-O21-C2
49	i	201	3PE	O22-C21-O21-C2
50	d	201	CDL	OB7-CB5-OB6-CB4
50	q	201	CDL	OB7-CB5-OB6-CB4
46	B	202	PC1	C32-C31-O31-C3
46	I	201	PC1	C32-C31-O31-C3
50	h	201	CDL	C31-CA7-OA8-CA6
49	H	401	3PE	C22-C21-O21-C2
50	L	702	CDL	C51-CB5-OB6-CB4
49	M	502	3PE	C32-C31-O31-C3
46	B	202	PC1	O32-C31-O31-C3
50	d	201	CDL	O1-C1-CA2-OA2
49	N	401	3PE	C32-C31-O31-C3
49	N	401	3PE	O32-C31-O31-C3
52	P	501	NDP	O4B-C4B-C5B-O5B
52	P	501	NDP	O4D-C4D-C5D-O5D
54	T	201	EHZ	C21-C22-C23-C24
49	M	502	3PE	O32-C31-O31-C3
50	q	201	CDL	CA2-C1-CB2-OB2
49	H	401	3PE	C32-C31-O31-C3
52	P	501	NDP	O4D-C1D-N1N-C6N
50	q	201	CDL	O1-C1-CB2-OB2
49	M	501	3PE	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
46	I	201	PC1	C22-C21-O21-C2
49	M	502	3PE	C22-C21-O21-C2
46	B	202	PC1	C21-C22-C23-C24
50	q	201	CDL	CA5-C11-C12-C13
50	L	702	CDL	CB5-C51-C52-C53
49	M	501	3PE	C32-C31-O31-C3
50	d	201	CDL	CB7-C71-C72-C73
46	I	201	PC1	O22-C21-O21-C2
49	H	401	3PE	O32-C31-O31-C3
49	f	101	3PE	C31-C32-C33-C34
49	M	501	3PE	O32-C31-O31-C3
50	L	702	CDL	C11-CA5-OA6-CA4
46	I	201	PC1	C1-O11-P-O13
49	H	401	3PE	C11-O13-P-O11
49	I	202	3PE	C11-O13-P-O11
49	L	701	3PE	C11-O13-P-O11
49	M	501	3PE	C11-O13-P-O11
50	L	702	CDL	CA3-OA5-PA1-OA2
50	d	201	CDL	CA2-OA2-PA1-OA5
50	d	201	CDL	CB2-OB2-PB2-OB5
50	h	201	CDL	CA3-OA5-PA1-OA2
50	q	201	CDL	C31-CA7-OA8-CA6
49	M	502	3PE	O22-C21-O21-C2
50	L	702	CDL	OA7-CA5-OA6-CA4
49	M	502	3PE	C35-C36-C37-C38
49	M	502	3PE	C21-C22-C23-C24
50	q	201	CDL	C40-C41-C42-C43
50	h	201	CDL	C11-CA5-OA6-CA4
46	B	202	PC1	C36-C37-C38-C39
49	f	101	3PE	C3A-C3B-C3C-C3D
50	L	702	CDL	C12-C13-C14-C15
50	d	201	CDL	C33-C34-C35-C36
50	d	201	CDL	C40-C41-C42-C43
50	h	201	CDL	C74-C75-C76-C77
50	q	201	CDL	C38-C39-C40-C41
54	T	201	EHZ	C18-C17-C20-O6
54	T	201	EHZ	C19-C17-C20-O6
49	L	701	3PE	C36-C37-C38-C39
49	f	101	3PE	C32-C33-C34-C35
49	L	701	3PE	C3-C2-O21-C21
50	h	201	CDL	OA7-CA5-OA6-CA4
49	I	202	3PE	C38-C39-C3A-C3B

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Mol	Chain	Res	Type	Atoms
50	d	201	CDL	C57-C58-C59-C60
50	h	201	CDL	C32-C33-C34-C35
50	q	201	CDL	C12-C13-C14-C15
46	I	201	PC1	C25-C26-C27-C28
50	d	201	CDL	C16-C17-C18-C19
49	M	502	3PE	C3E-C3F-C3G-C3H
46	B	202	PC1	C3A-C3B-C3C-C3D
49	I	202	3PE	C3D-C3E-C3F-C3G
50	d	201	CDL	C71-C72-C73-C74
50	d	201	CDL	C79-C80-C81-C82
49	H	401	3PE	C37-C38-C39-C3A
50	L	702	CDL	CB7-C71-C72-C73
46	B	202	PC1	C39-C3A-C3B-C3C
49	M	501	3PE	C2B-C2C-C2D-C2E
49	N	401	3PE	C39-C3A-C3B-C3C
50	h	201	CDL	C18-C19-C20-C21
46	B	202	PC1	C26-C27-C28-C29
46	B	202	PC1	C28-C29-C2A-C2B
49	N	401	3PE	C22-C23-C24-C25
49	f	101	3PE	C22-C23-C24-C25
50	d	201	CDL	C15-C16-C17-C18
50	q	201	CDL	C34-C35-C36-C37
49	I	202	3PE	C34-C35-C36-C37
50	d	201	CDL	C73-C74-C75-C76
49	f	101	3PE	O13-C11-C12-N
50	L	702	CDL	CA7-C31-C32-C33
46	B	202	PC1	C38-C39-C3A-C3B
49	M	501	3PE	C38-C39-C3A-C3B
49	M	501	3PE	C3A-C3B-C3C-C3D
50	h	201	CDL	C56-C57-C58-C59
49	N	401	3PE	C31-C32-C33-C34
50	q	201	CDL	OA9-CA7-OA8-CA6
54	T	201	EHZ	C13-C14-N2-C15
50	q	201	CDL	C43-C44-C45-C46
50	L	702	CDL	CB3-CB4-CB6-OB8
50	d	201	CDL	C14-C15-C16-C17
49	M	502	3PE	C28-C29-C2A-C2B
50	q	201	CDL	C53-C54-C55-C56
50	h	201	CDL	C51-CB5-OB6-CB4
49	H	401	3PE	C2E-C2F-C2G-C2H
49	f	101	3PE	C38-C39-C3A-C3B
46	I	201	PC1	C37-C38-C39-C3A

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Mol	Chain	Res	Type	Atoms
49	H	401	3PE	C3E-C3F-C3G-C3H
50	d	201	CDL	C62-C63-C64-C65
54	U	201	EHZ	C21-C22-C23-C24
50	L	702	CDL	O1-C1-CB2-OB2
52	P	501	NDP	C3B-C4B-C5B-O5B
50	L	702	CDL	CB2-C1-CA2-OA2
50	h	201	CDL	OB7-CB5-OB6-CB4
49	M	501	3PE	C33-C34-C35-C36
49	M	501	3PE	C39-C3A-C3B-C3C
50	h	201	CDL	CA4-CA3-OA5-PA1
46	B	202	PC1	C25-C26-C27-C28
50	d	201	CDL	C59-C60-C61-C62
49	M	502	3PE	C3C-C3D-C3E-C3F
46	B	202	PC1	C2C-C2D-C2E-C2F
49	N	401	3PE	C36-C37-C38-C39
49	L	701	3PE	C28-C29-C2A-C2B
49	I	202	3PE	C22-C21-O21-C2
50	q	201	CDL	C11-CA5-OA6-CA4
50	q	201	CDL	OB5-CB3-CB4-OB6
50	d	201	CDL	C23-C24-C25-C26
49	L	701	3PE	C37-C38-C39-C3A
50	q	201	CDL	O1-C1-CA2-OA2
49	I	202	3PE	O22-C21-O21-C2
50	L	702	CDL	C52-C53-C54-C55
50	d	201	CDL	C34-C35-C36-C37
50	d	201	CDL	C58-C59-C60-C61
51	O	401	ATP	O4'-C4'-C5'-O5'
49	i	201	3PE	C2A-C2B-C2C-C2D
50	L	702	CDL	C19-C20-C21-C22
49	N	401	3PE	C26-C27-C28-C29
46	B	202	PC1	C29-C2A-C2B-C2C
50	q	201	CDL	OA7-CA5-OA6-CA4
50	d	201	CDL	C21-C22-C23-C24
50	L	702	CDL	CA2-OA2-PA1-OA5
50	q	201	CDL	CA3-OA5-PA1-OA2
50	q	201	CDL	C37-C38-C39-C40
49	i	201	3PE	C24-C25-C26-C27
49	I	202	3PE	C21-C22-C23-C24
49	H	401	3PE	C22-C23-C24-C25
50	L	702	CDL	CA2-C1-CB2-OB2
49	H	401	3PE	C28-C29-C2A-C2B
50	d	201	CDL	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
49	H	401	3PE	C1-C2-C3-O31
49	L	701	3PE	C22-C23-C24-C25
49	M	501	3PE	C1-C2-C3-O31
49	N	401	3PE	C1-C2-C3-O31
49	i	201	3PE	C1-C2-C3-O31
46	B	202	PC1	C2F-C2G-C2H-C2I
49	H	401	3PE	C3A-C3B-C3C-C3D
50	L	702	CDL	C84-C85-C86-C87
50	q	201	CDL	C72-C73-C74-C75
49	M	502	3PE	C38-C39-C3A-C3B
49	M	501	3PE	C22-C21-O21-C2
52	P	501	NDP	C3D-C4D-C5D-O5D
54	U	201	EHZ	C5-C6-C7-O1
50	d	201	CDL	C37-C38-C39-C40
49	L	701	3PE	C2F-C2G-C2H-C2I
49	f	101	3PE	C3E-C3F-C3G-C3H
50	q	201	CDL	C14-C15-C16-C17
50	d	201	CDL	C18-C19-C20-C21
50	h	201	CDL	C71-C72-C73-C74
49	N	401	3PE	C3B-C3C-C3D-C3E
50	d	201	CDL	C77-C78-C79-C80
48	F	501	FMN	C5'-O5'-P-O1P
49	i	201	3PE	C26-C27-C28-C29
50	d	201	CDL	C17-C18-C19-C20
50	q	201	CDL	OA5-CA3-CA4-OA6
50	h	201	CDL	C11-C12-C13-C14
50	d	201	CDL	C51-C52-C53-C54
50	d	201	CDL	C84-C85-C86-C87
54	U	201	EHZ	C2-C3-C4-C5
49	M	502	3PE	C26-C27-C28-C29
50	h	201	CDL	C36-C37-C38-C39
49	N	401	3PE	C22-C21-O21-C2
49	M	501	3PE	C36-C37-C38-C39
50	q	201	CDL	OB5-CB3-CB4-CB6
49	I	202	3PE	C3F-C3G-C3H-C3I
49	i	201	3PE	C22-C23-C24-C25
50	d	201	CDL	CB5-C51-C52-C53
49	N	401	3PE	C33-C34-C35-C36
49	N	401	3PE	C3F-C3G-C3H-C3I
50	h	201	CDL	C51-C52-C53-C54
49	f	101	3PE	C1-C2-C3-O31
50	d	201	CDL	CA3-CA4-CA6-OA8

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Mol	Chain	Res	Type	Atoms
49	H	401	3PE	C35-C36-C37-C38
46	I	201	PC1	C11-O13-P-O11
50	h	201	CDL	CB2-OB2-PB2-OB5
50	q	201	CDL	CB3-OB5-PB2-OB2
46	I	201	PC1	C32-C33-C34-C35
46	B	202	PC1	O11-C1-C2-O21
50	h	201	CDL	OB5-CB3-CB4-OB6
50	L	702	CDL	C34-C35-C36-C37
49	I	202	3PE	C2F-C2G-C2H-C2I
49	H	401	3PE	O21-C2-C3-O31
50	d	201	CDL	OA6-CA4-CA6-OA8
50	d	201	CDL	OB6-CB4-CB6-OB8
49	M	502	3PE	C39-C3A-C3B-C3C
50	d	201	CDL	C11-CA5-OA6-CA4
49	M	502	3PE	C3D-C3E-C3F-C3G
49	M	501	3PE	O22-C21-O21-C2
49	M	502	3PE	C2B-C2C-C2D-C2E
54	T	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	O2-C9-S1-C10
49	N	401	3PE	O22-C21-O21-C2
50	d	201	CDL	OA7-CA5-OA6-CA4
49	i	201	3PE	C36-C37-C38-C39
46	B	202	PC1	O11-C1-C2-C3
49	N	401	3PE	O11-C1-C2-C3
50	L	702	CDL	O1-C1-CA2-OA2
54	U	201	EHZ	C2-C1-C21-C22
49	H	401	3PE	C24-C25-C26-C27
49	L	701	3PE	C3A-C3B-C3C-C3D
54	U	201	EHZ	C19-C17-C20-O6
49	i	201	3PE	C3-C2-O21-C21
50	d	201	CDL	CB3-CB4-OB6-CB5
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
50	d	201	CDL	C11-C12-C13-C14
50	L	702	CDL	CA3-CA4-CA6-OA8
49	M	501	3PE	C35-C36-C37-C38
54	T	201	EHZ	O1-C7-C8-C9
50	L	702	CDL	OB6-CB4-CB6-OB8
50	h	201	CDL	C34-C35-C36-C37
46	I	201	PC1	C39-C3A-C3B-C3C
51	O	401	ATP	PG-O3B-PB-O1B
50	d	201	CDL	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
50	d	201	CDL	CB3-OB5-PB2-OB2
50	h	201	CDL	CB3-OB5-PB2-OB2
50	q	201	CDL	CB2-OB2-PB2-OB5
49	M	501	3PE	C27-C28-C29-C2A
49	M	502	3PE	C2F-C2G-C2H-C2I
50	h	201	CDL	C14-C15-C16-C17
46	I	201	PC1	C1-O11-P-O14
49	H	401	3PE	C1-O11-P-O12
49	I	202	3PE	C11-O13-P-O12
49	M	501	3PE	C11-O13-P-O12
49	M	501	3PE	C11-O13-P-O14
49	N	401	3PE	C1-O11-P-O14
50	L	702	CDL	CA2-OA2-PA1-OA4
50	d	201	CDL	CB3-OB5-PB2-OB3
50	h	201	CDL	CB2-OB2-PB2-OB3
52	P	501	NDP	C5B-O5B-PA-O2A
50	d	201	CDL	C74-C75-C76-C77
50	L	702	CDL	C54-C55-C56-C57
49	i	201	3PE	C32-C33-C34-C35
49	M	501	3PE	C12-C11-O13-P
49	M	502	3PE	C12-C11-O13-P
49	N	401	3PE	C12-C11-O13-P
49	i	201	3PE	C12-C11-O13-P
46	B	202	PC1	C31-C32-C33-C34
50	q	201	CDL	C71-C72-C73-C74
50	L	702	CDL	C71-CB7-OB8-CB6
49	f	101	3PE	O11-C1-C2-O21
46	B	202	PC1	C2B-C2C-C2D-C2E
46	I	201	PC1	O13-C11-C12-N
49	i	201	3PE	O21-C2-C3-O31
49	L	701	3PE	C2B-C2C-C2D-C2E
50	L	702	CDL	C23-C24-C25-C26
49	H	401	3PE	C25-C26-C27-C28
50	L	702	CDL	OB9-CB7-OB8-CB6
54	U	201	EHZ	C18-C17-C20-O6
49	f	101	3PE	O11-C1-C2-C3
50	q	201	CDL	OA5-CA3-CA4-CA6
50	d	201	CDL	C80-C81-C82-C83
49	M	501	3PE	C31-C32-C33-C34
49	I	202	3PE	C32-C33-C34-C35
50	L	702	CDL	C22-C23-C24-C25
49	N	401	3PE	O11-C1-C2-O21

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Mol	Chain	Res	Type	Atoms
49	i	201	3PE	C2B-C2C-C2D-C2E
50	h	201	CDL	C17-C18-C19-C20
50	q	201	CDL	C51-C52-C53-C54
50	d	201	CDL	CB3-CB4-CB6-OB8
50	h	201	CDL	CA3-CA4-CA6-OA8
50	q	201	CDL	C31-C32-C33-C34
49	L	701	3PE	C33-C34-C35-C36
50	q	201	CDL	C42-C43-C44-C45
49	N	401	3PE	C35-C36-C37-C38
51	O	401	ATP	PG-O3B-PB-O2B
52	P	501	NDP	PN-O3-PA-O2A
46	I	201	PC1	C34-C35-C36-C37
49	M	501	3PE	C3D-C3E-C3F-C3G
54	T	201	EHZ	C1-C2-C3-C4
46	I	201	PC1	C27-C28-C29-C2A
49	M	502	3PE	C2D-C2E-C2F-C2G
49	f	101	3PE	C37-C38-C39-C3A
49	i	201	3PE	C27-C28-C29-C2A
50	d	201	CDL	CA5-C11-C12-C13
49	L	701	3PE	C34-C35-C36-C37
46	I	201	PC1	O21-C2-C3-O31
50	h	201	CDL	C19-C20-C21-C22
50	L	702	CDL	C32-C33-C34-C35
50	L	702	CDL	C77-C78-C79-C80
49	L	701	3PE	C2A-C2B-C2C-C2D
54	U	201	EHZ	C7-C8-C9-O2
50	h	201	CDL	CA3-CA4-OA6-CA5
50	h	201	CDL	CA6-CA4-OA6-CA5
50	h	201	CDL	CB6-CB4-OB6-CB5
50	q	201	CDL	CA3-CA4-OA6-CA5
50	d	201	CDL	C52-C53-C54-C55
49	I	202	3PE	C24-C25-C26-C27
49	I	202	3PE	C2E-C2F-C2G-C2H
50	L	702	CDL	C13-C14-C15-C16
51	O	401	ATP	C3'-C4'-C5'-O5'
49	I	202	3PE	C29-C2A-C2B-C2C
54	T	201	EHZ	C11-C10-S1-C9
50	q	201	CDL	C35-C36-C37-C38
49	f	101	3PE	O21-C2-C3-O31
50	L	702	CDL	OA6-CA4-CA6-OA8
50	L	702	CDL	C78-C79-C80-C81
50	L	702	CDL	C82-C83-C84-C85

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Mol	Chain	Res	Type	Atoms
46	I	201	PC1	C1-C2-C3-O31
50	q	201	CDL	CA3-CA4-CA6-OA8
49	M	502	3PE	C2E-C2F-C2G-C2H
50	h	201	CDL	OB5-CB3-CB4-CB6
46	B	202	PC1	C24-C25-C26-C27
49	H	401	3PE	C32-C33-C34-C35
50	d	201	CDL	OA9-CA7-OA8-CA6
46	I	201	PC1	C24-C25-C26-C27
54	T	201	EHZ	C3-C4-C5-C6
50	h	201	CDL	C13-C14-C15-C16
50	d	201	CDL	C61-C62-C63-C64
50	L	702	CDL	C52-C51-CB5-OB6
50	h	201	CDL	CB3-CB4-OB6-CB5
50	q	201	CDL	CA6-CA4-OA6-CA5
50	h	201	CDL	C72-C73-C74-C75
49	M	501	3PE	C26-C27-C28-C29
50	h	201	CDL	C52-C51-CB5-OB6
49	H	401	3PE	C34-C35-C36-C37
49	N	401	3PE	C25-C26-C27-C28
46	I	201	PC1	O11-C1-C2-O21
50	h	201	CDL	C22-C23-C24-C25
50	q	201	CDL	C32-C33-C34-C35
51	O	401	ATP	C5'-O5'-PA-O3A
50	d	201	CDL	C31-CA7-OA8-CA6
50	L	702	CDL	C12-C11-CA5-OA6
49	L	701	3PE	C3F-C3G-C3H-C3I
50	L	702	CDL	C52-C51-CB5-OB7
49	M	501	3PE	C3C-C3D-C3E-C3F
46	I	201	PC1	C36-C37-C38-C39
49	i	201	3PE	C11-O13-P-O14
50	L	702	CDL	CB2-OB2-PB2-OB3
50	d	201	CDL	CB3-OB5-PB2-OB4
50	L	702	CDL	C74-C75-C76-C77
50	h	201	CDL	C52-C51-CB5-OB7
50	L	702	CDL	C80-C81-C82-C83
49	f	101	3PE	C35-C36-C37-C38
49	L	701	3PE	C2C-C2D-C2E-C2F
50	d	201	CDL	C42-C43-C44-C45
46	I	201	PC1	C12-C11-O13-P
50	d	201	CDL	C41-C42-C43-C44
50	h	201	CDL	C1-CB2-OB2-PB2
50	h	201	CDL	CA7-C31-C32-C33

Continued on next page...

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Mol	Chain	Res	Type	Atoms
49	i	201	3PE	C33-C34-C35-C36
50	d	201	CDL	C72-C71-CB7-OB8
46	B	202	PC1	O31-C31-C32-C33
50	d	201	CDL	C32-C31-CA7-OA8

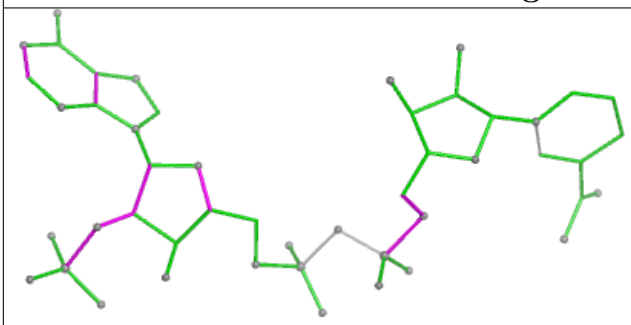
There are no ring outliers.

15 monomers are involved in 23 short contacts:

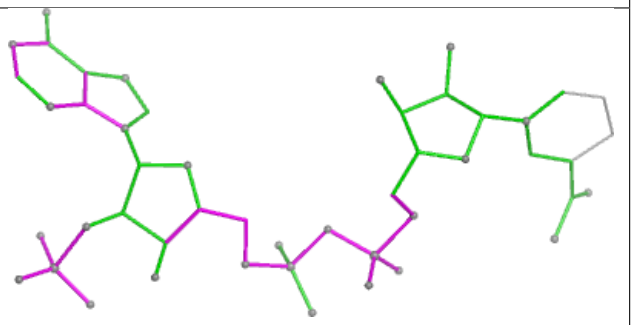
Mol	Chain	Res	Type	Clashes	Symm-Clashes
52	P	501	NDP	6	0
46	I	201	PC1	1	0
46	B	202	PC1	1	0
48	F	501	FMN	2	0
50	q	201	CDL	1	0
50	d	201	CDL	1	0
45	G	801	SF4	1	0
45	F	502	SF4	1	0
49	i	201	3PE	1	0
54	T	201	EHZ	1	0
49	M	502	3PE	1	0
45	B	201	SF4	1	0
50	h	201	CDL	1	0
50	L	702	CDL	2	0
51	O	401	ATP	2	0

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

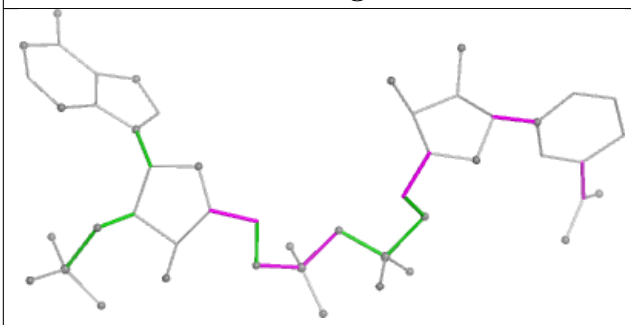
Ligand NDP P 501



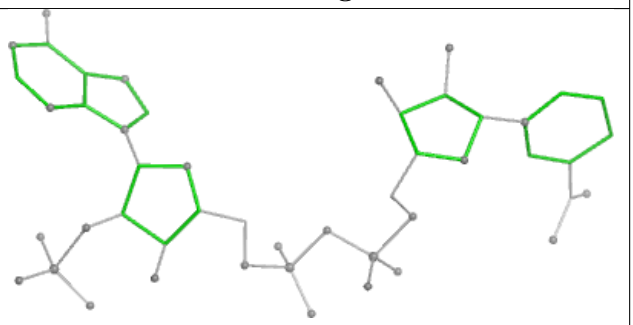
Bond lengths



Bond angles

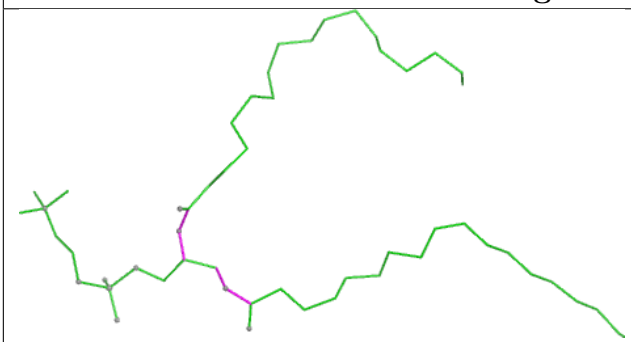


Torsions

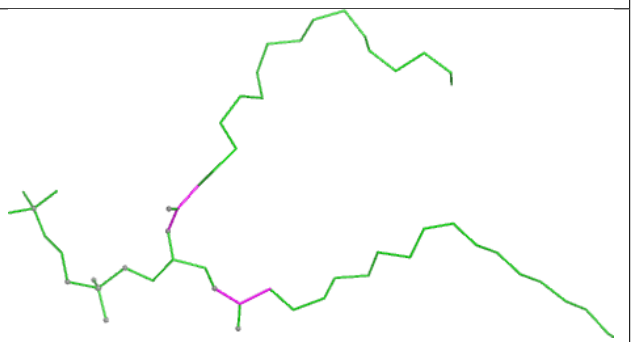


Rings

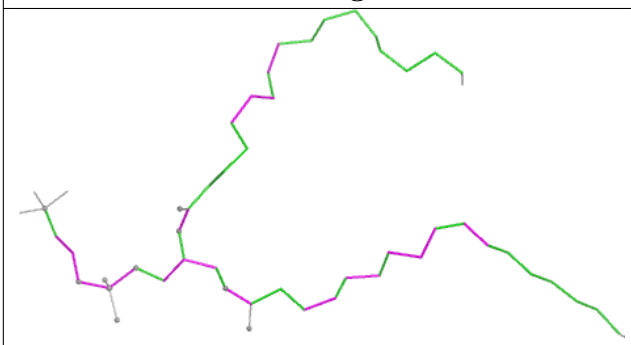
Ligand PC1 I 201



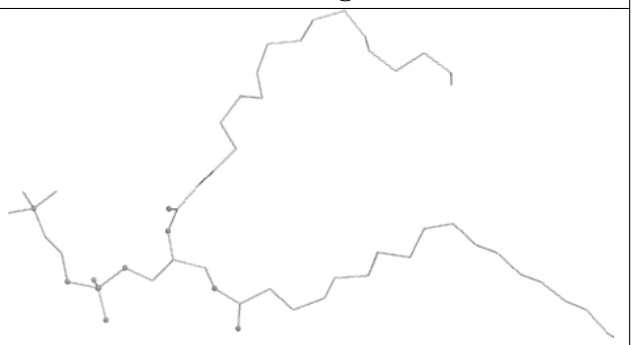
Bond lengths



Bond angles

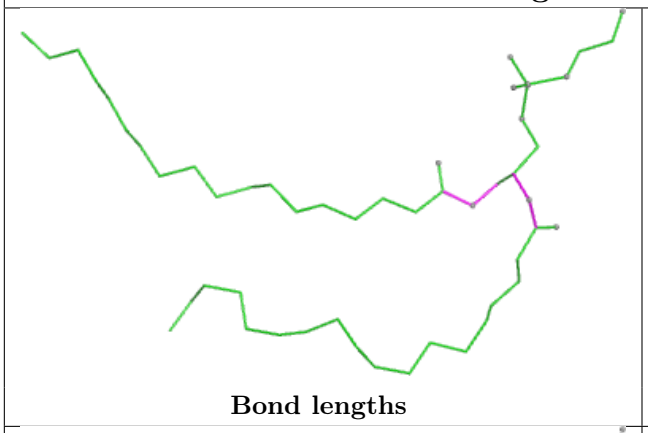


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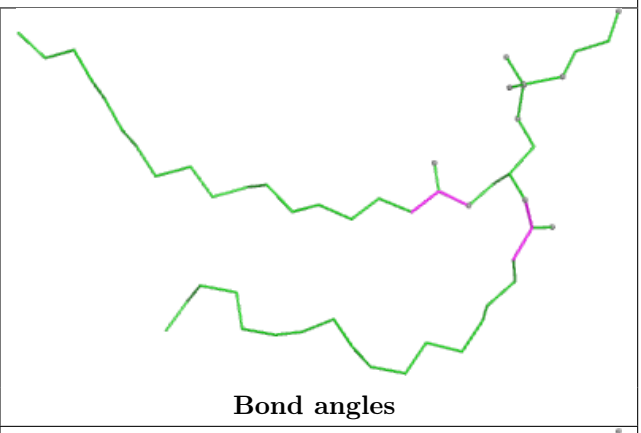


Rings

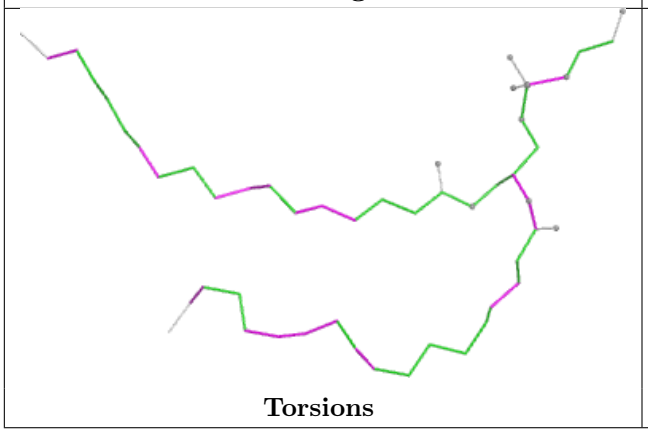
Ligand 3PE L 701



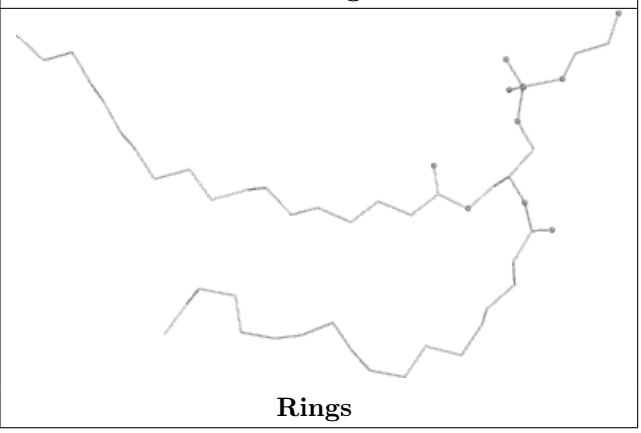
Bond lengths



Bond angles

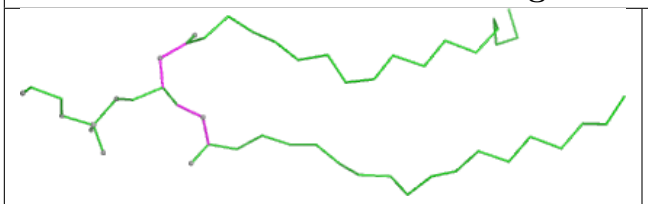


Torsions



Rings

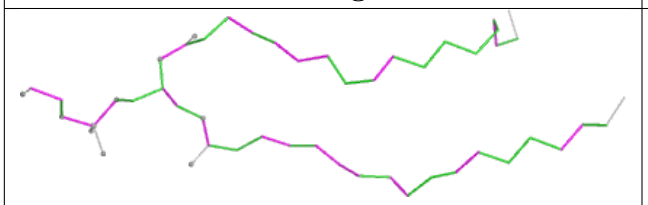
Ligand 3PE H 401



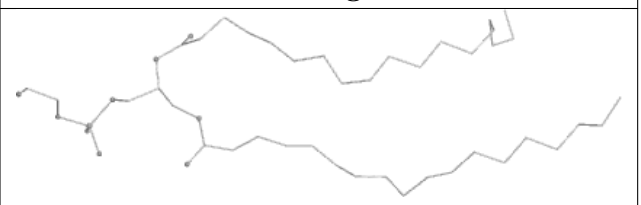
Bond lengths



Bond angles

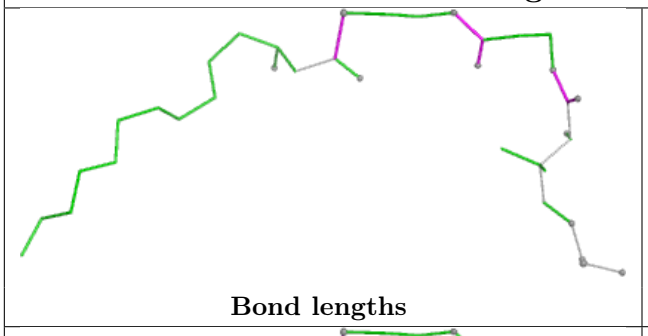


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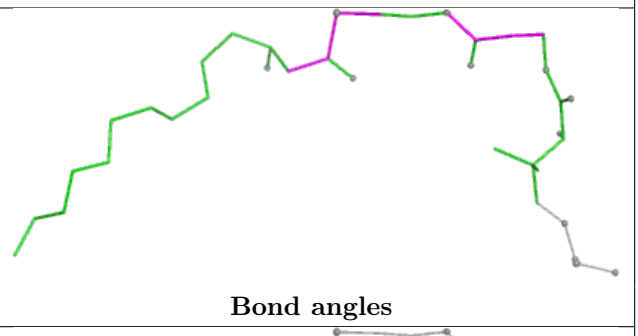


Rings

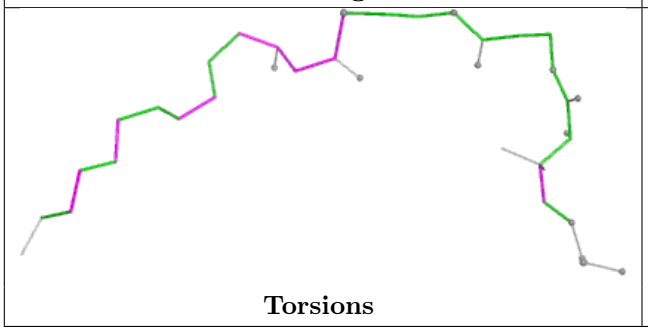
Ligand EHZ U 201



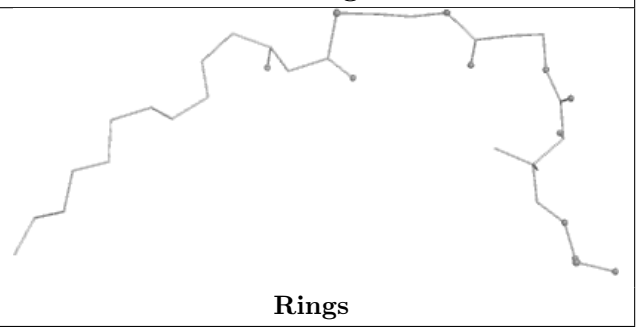
Bond lengths



Bond angles

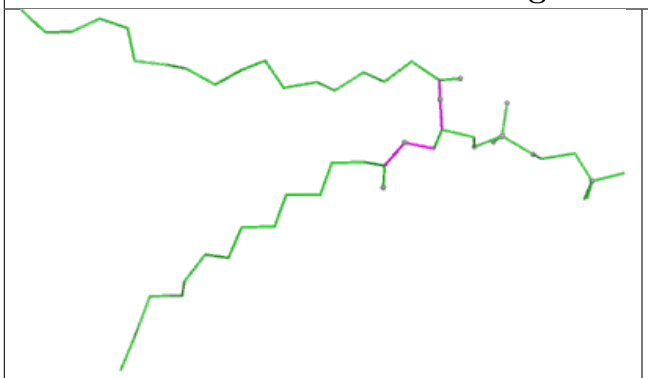


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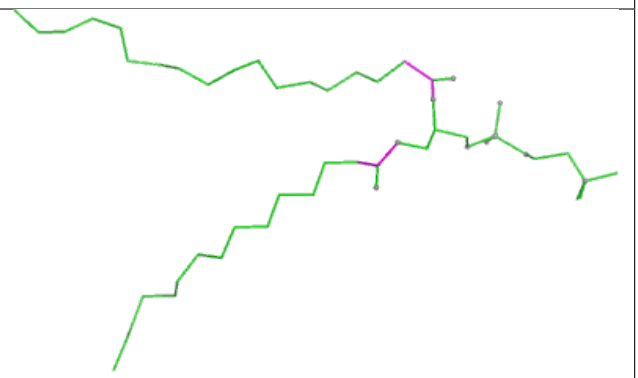


Rings

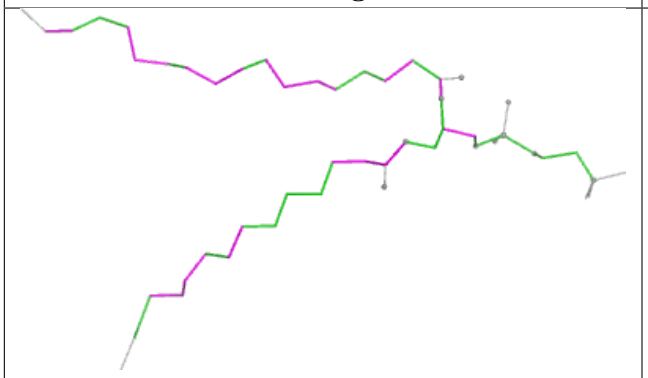
Ligand PC1 B 202



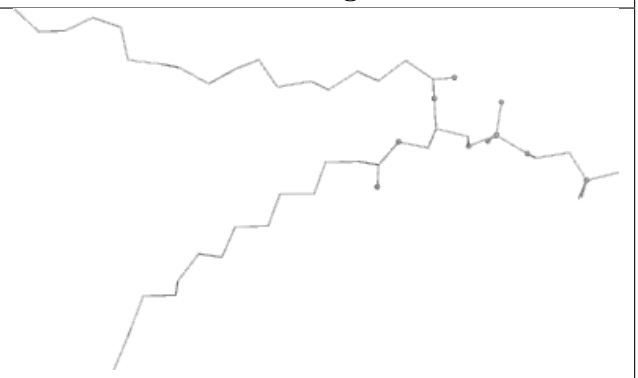
Bond lengths



Bond angles

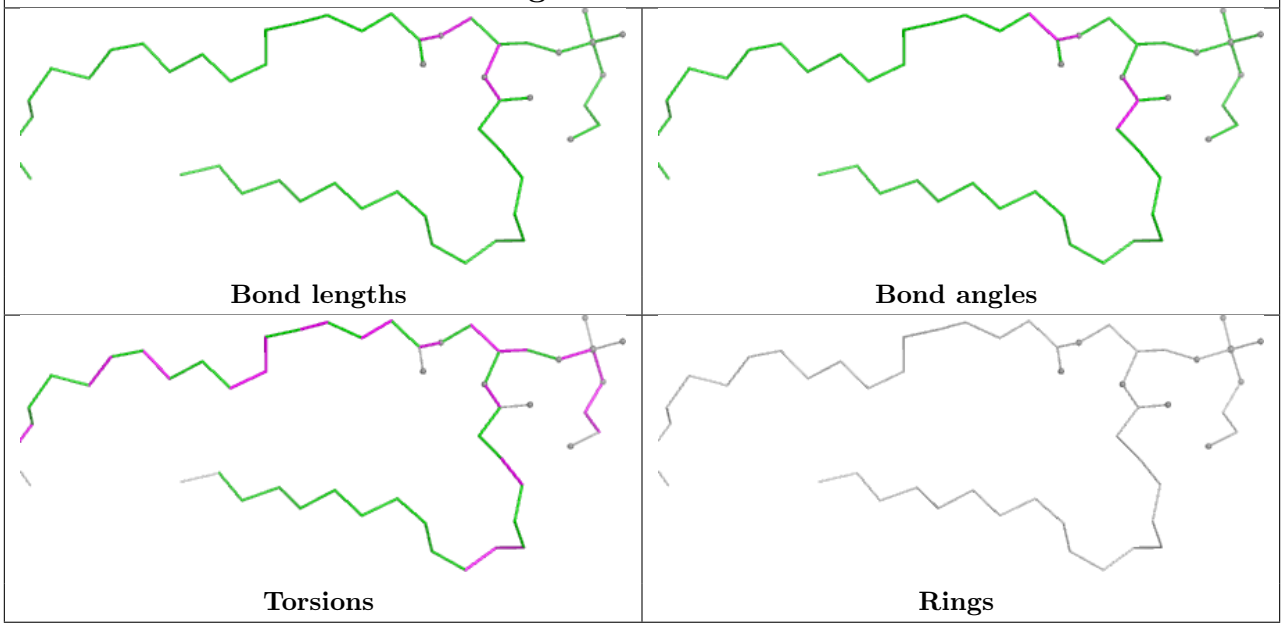


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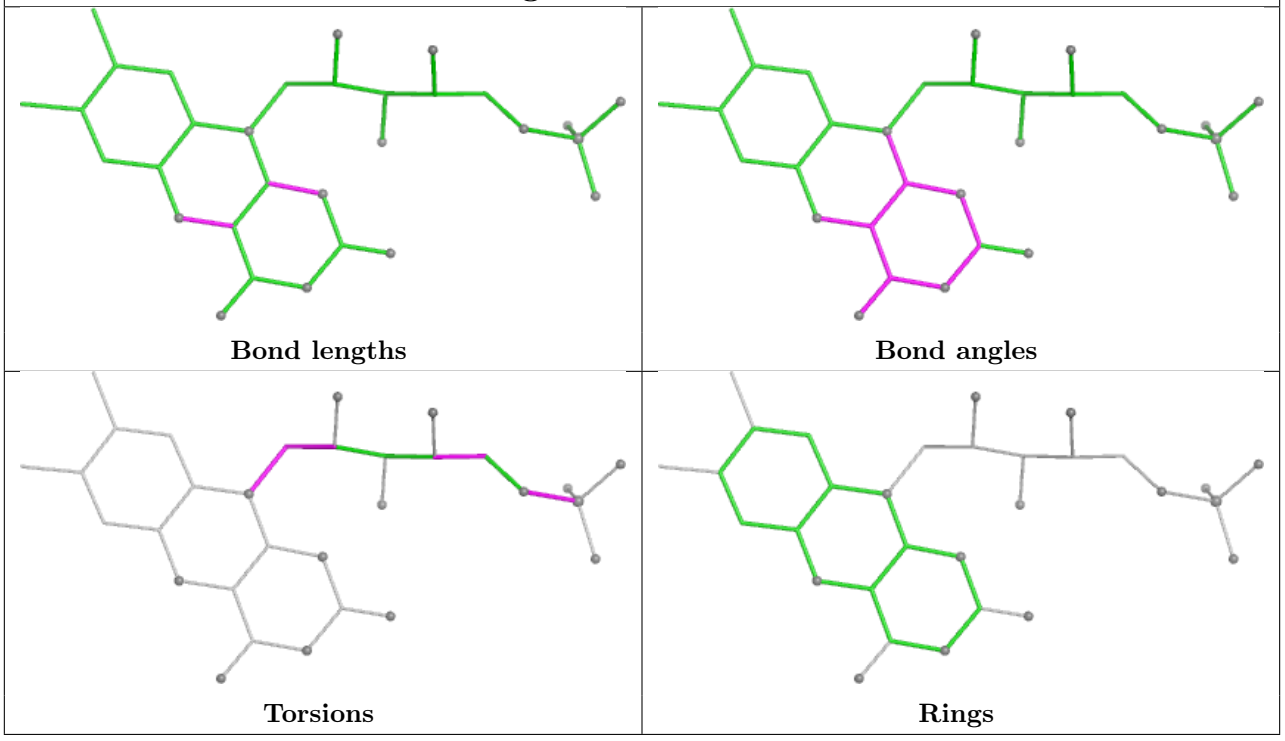


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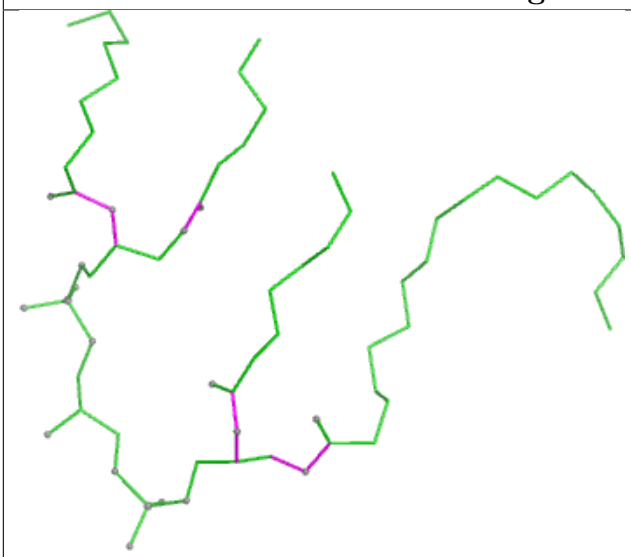
Ligand 3PE N 401



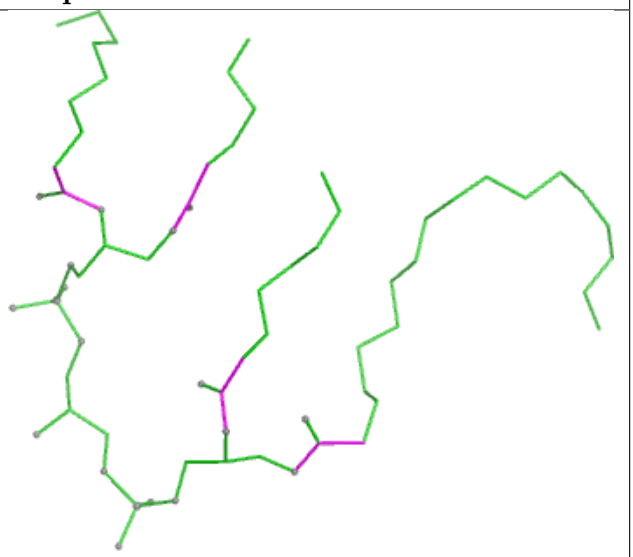
Ligand FMN F 501



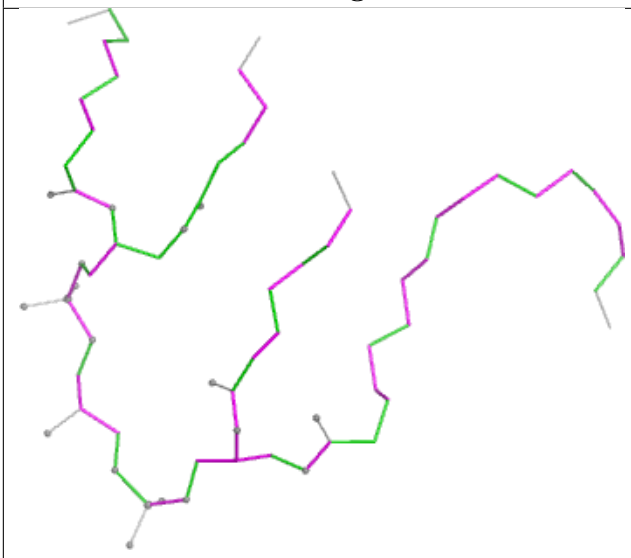
Ligand CDL q 201



Bond lengths



Bond angles

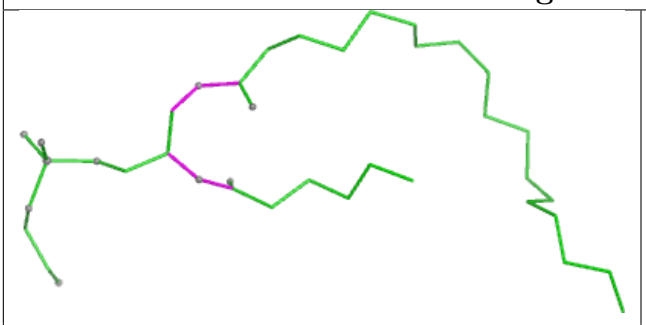


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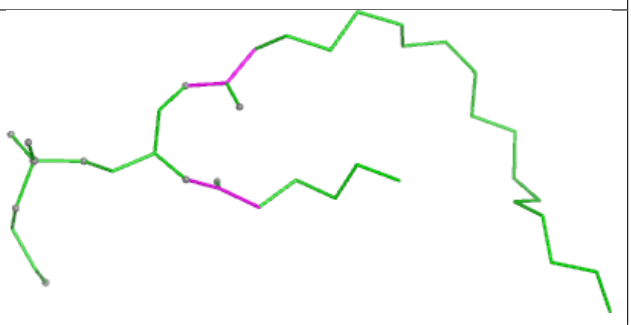


Rings

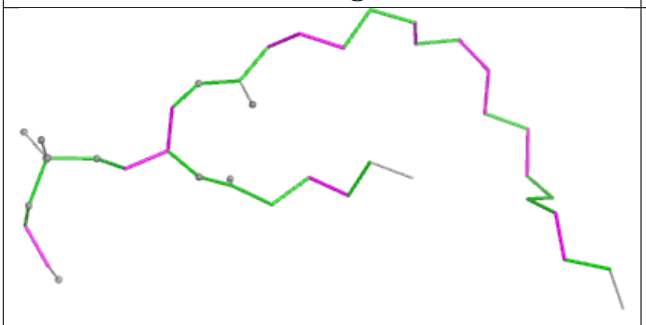
Ligand 3PE f 101



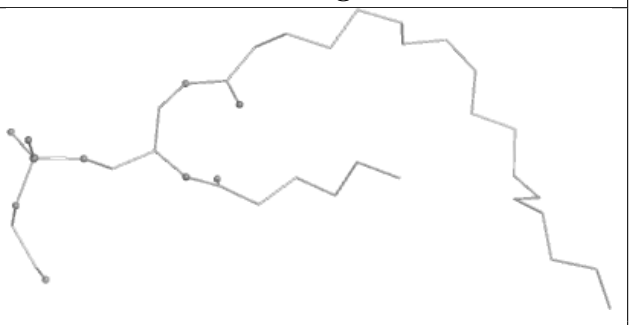
Bond lengths



Bond angles

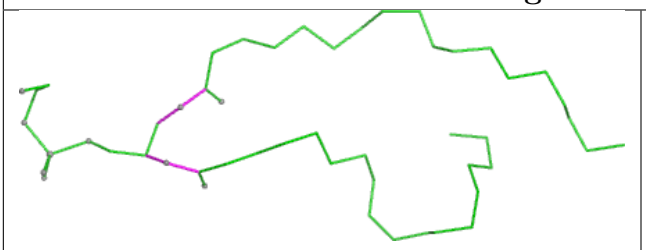


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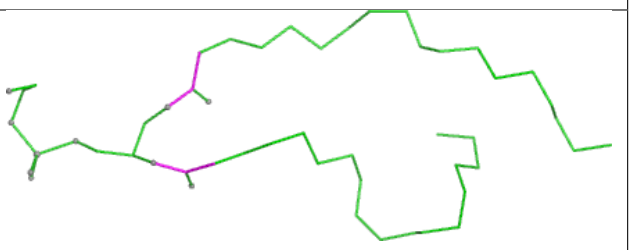


Rings

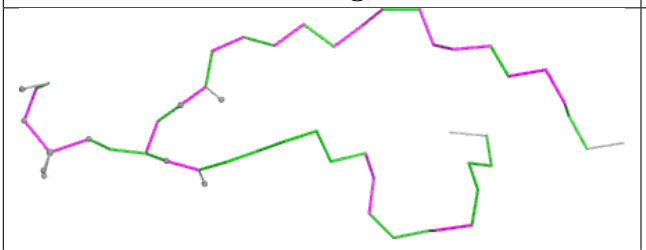
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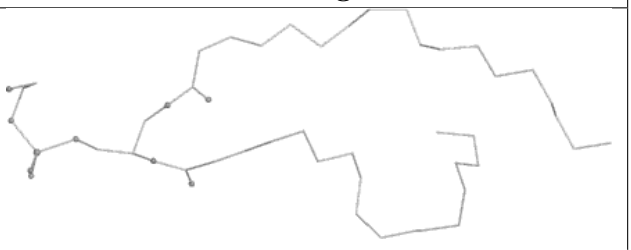
Bond lengths



Bond angles

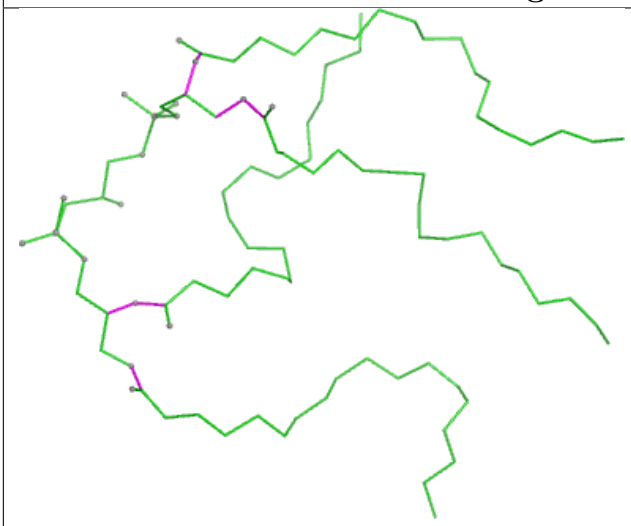


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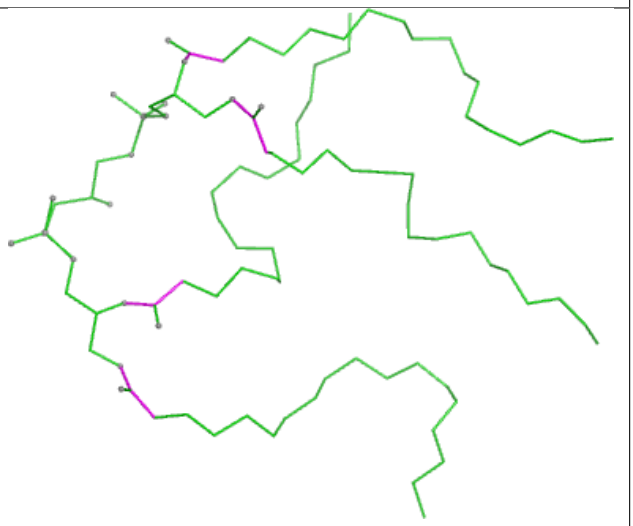


Rings

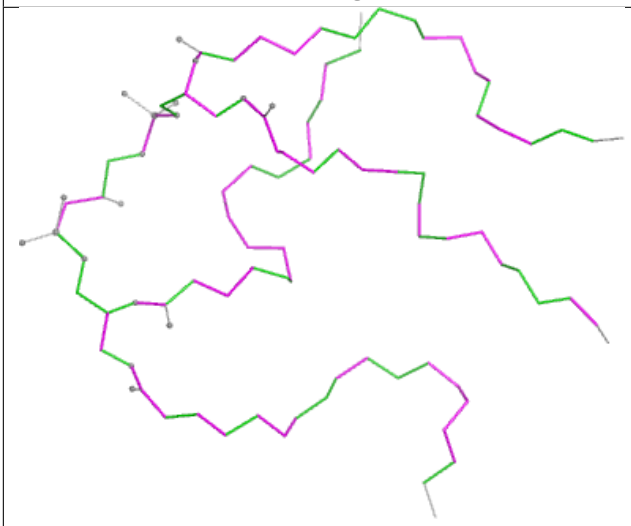
Ligand CDL d 201



Bond lengths



Bond angles

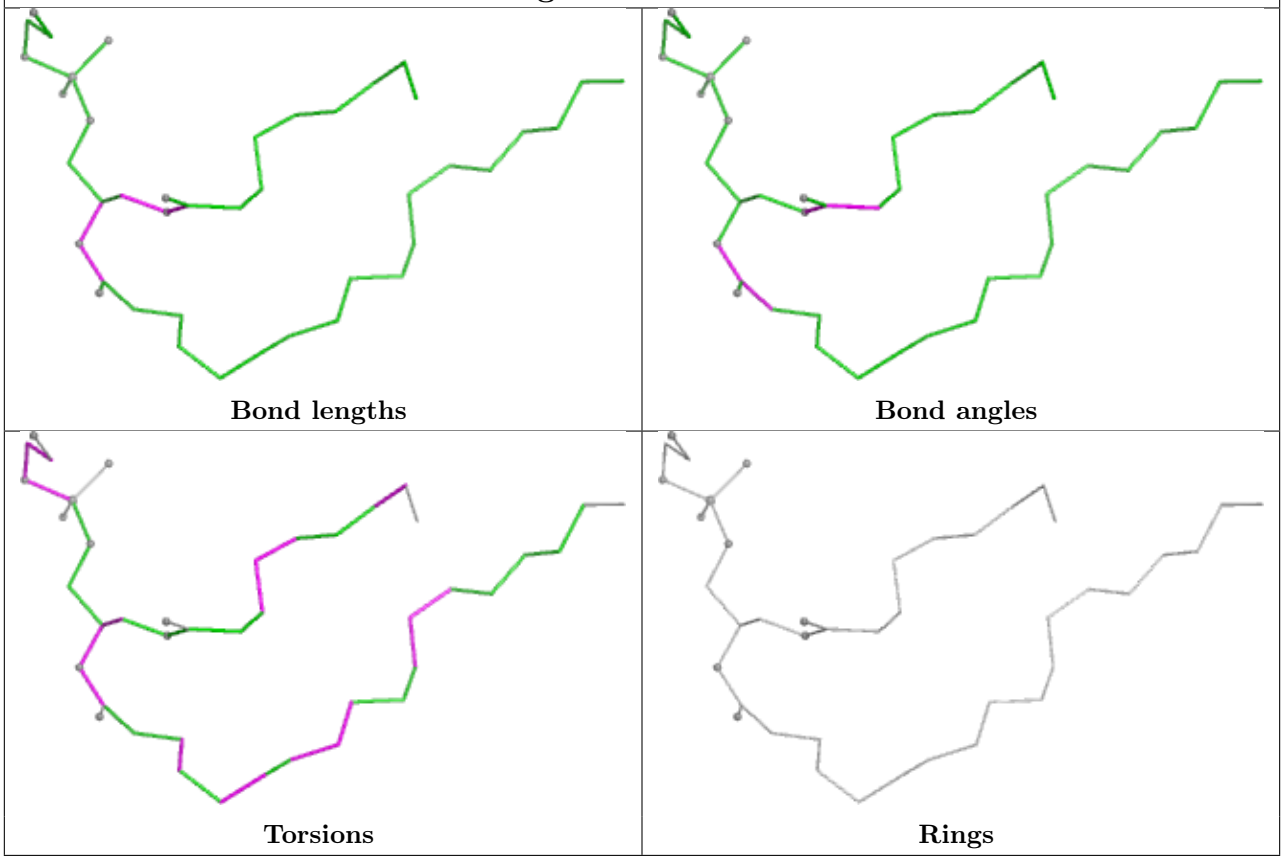


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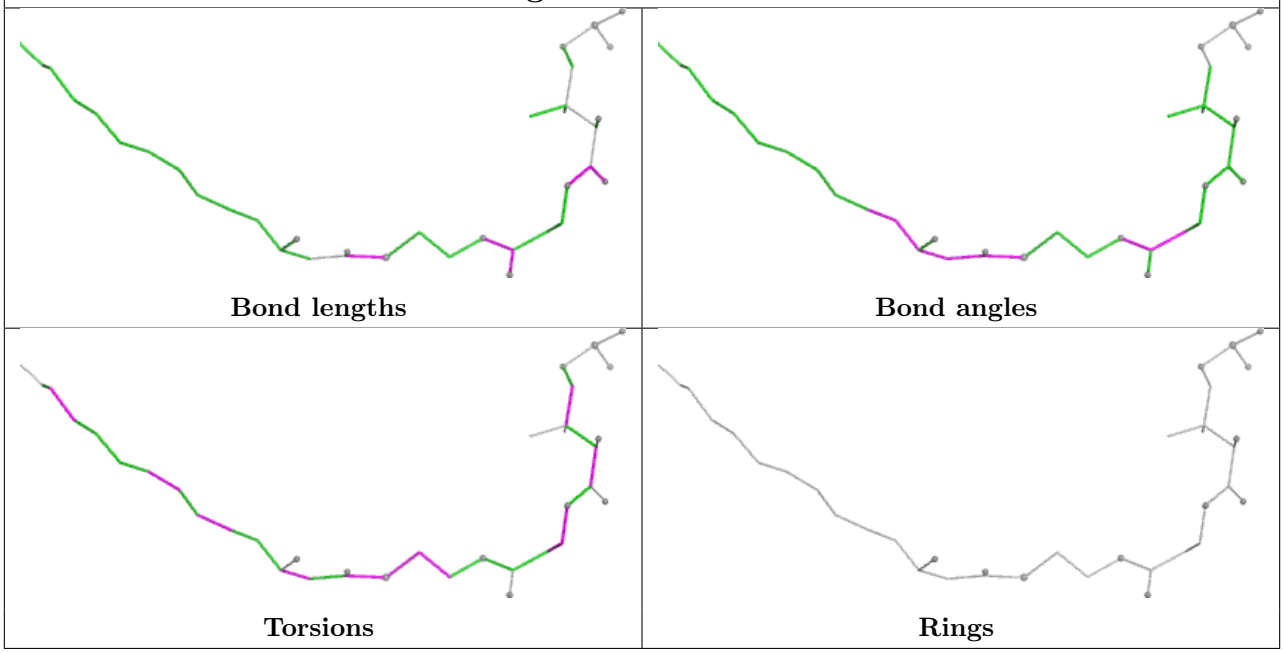


Rings

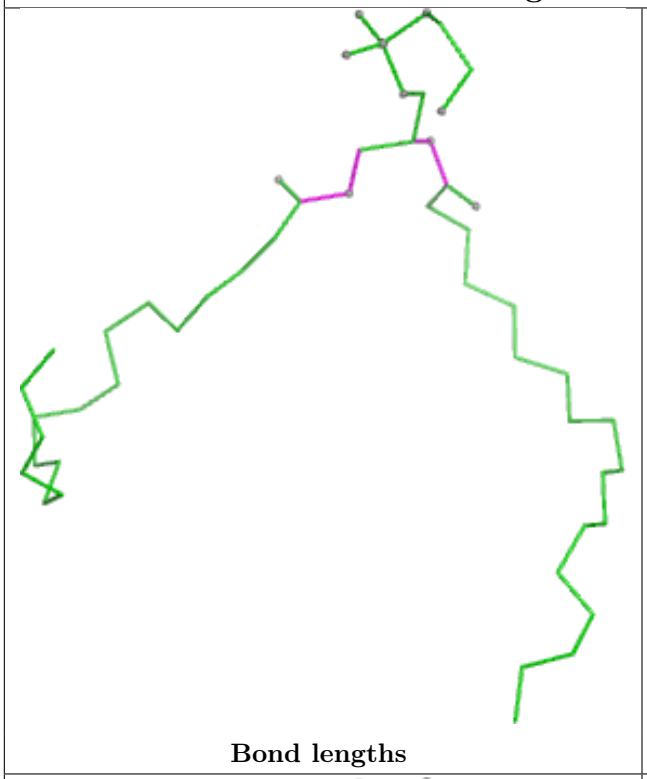
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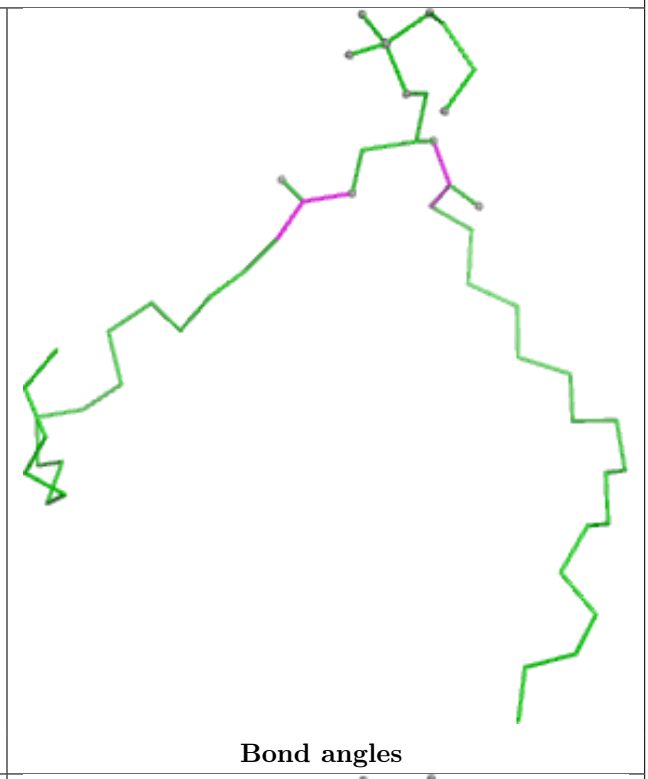
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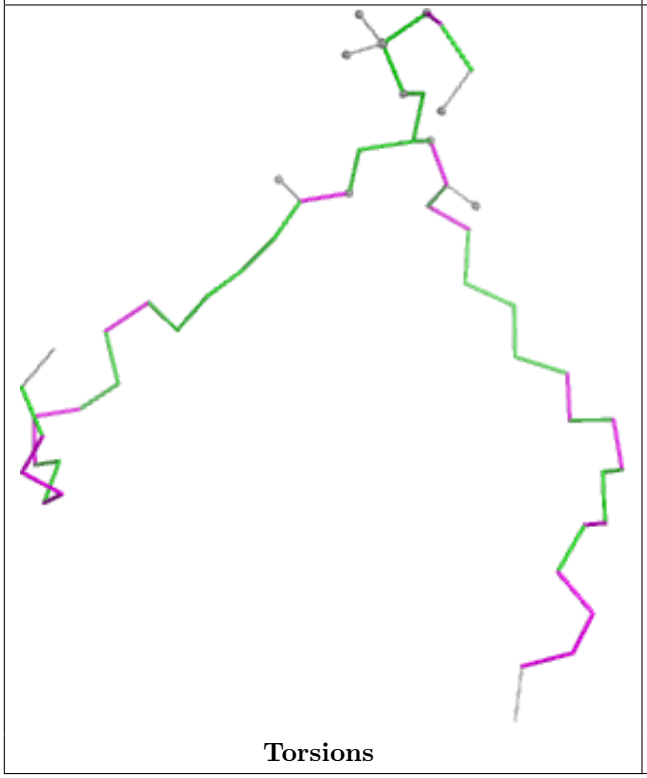
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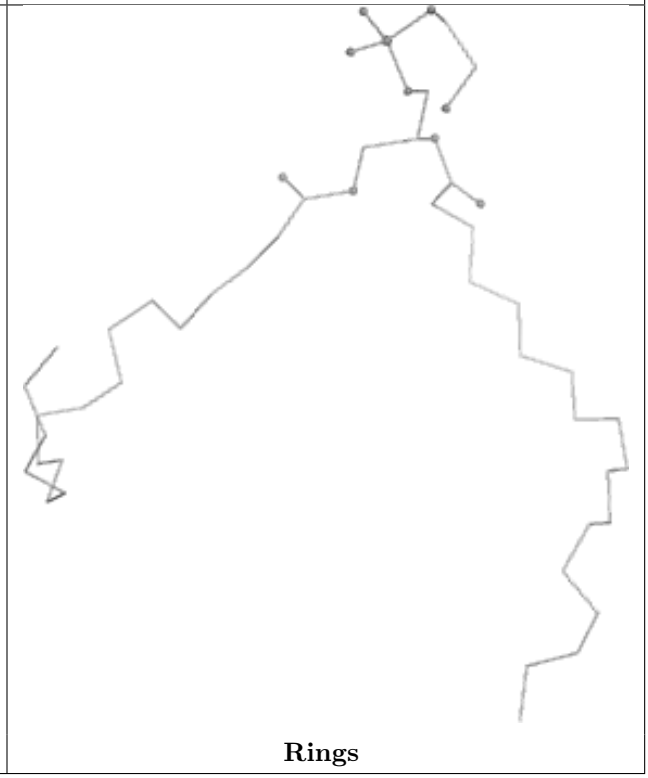
Bond lengths



Bond angles



Torsions

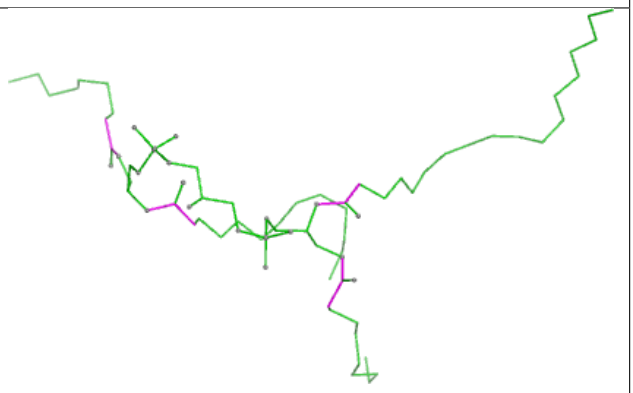


Rings

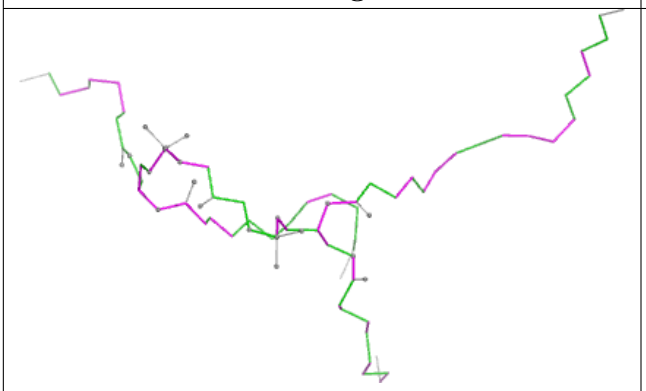
Ligand CDL h 201



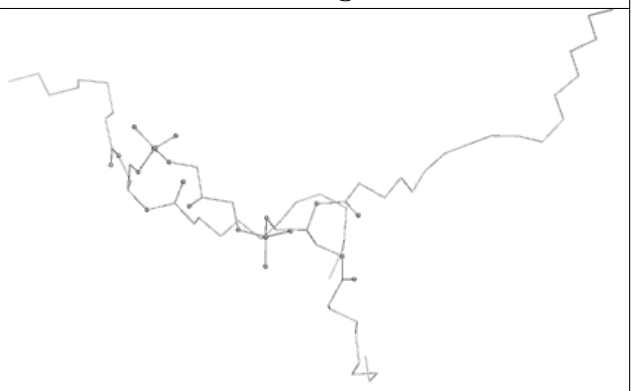
Bond lengths



Bond angles

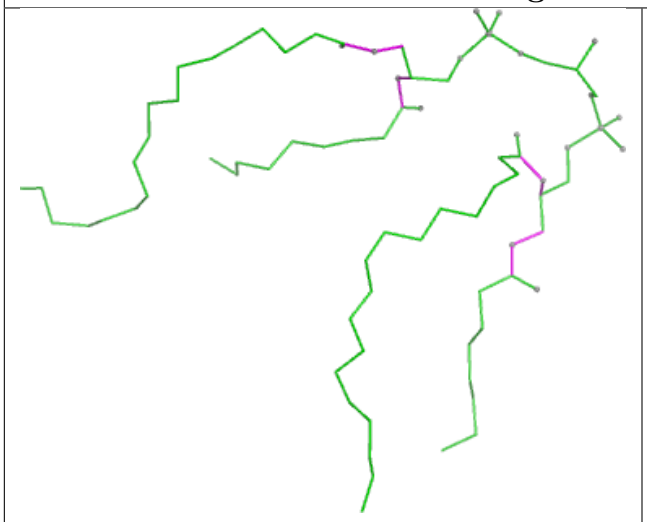


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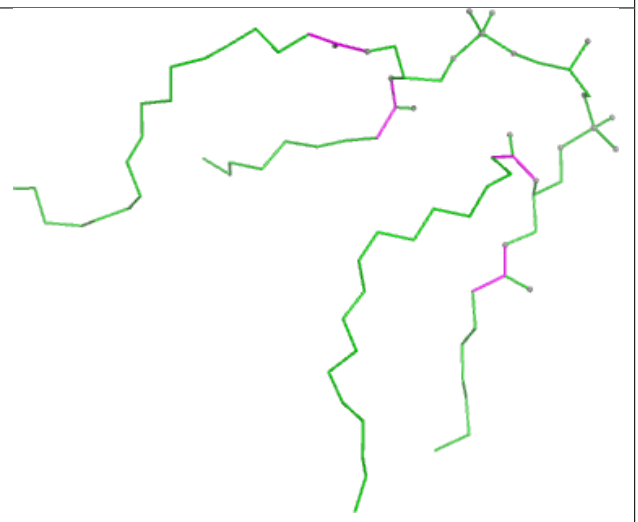


Rings

Ligand CDL L 702



Bond lengths



Bond angles

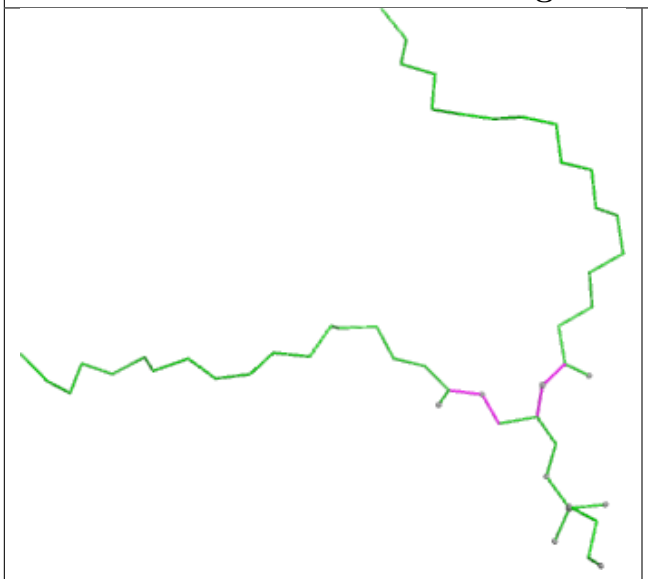


Torsions



Rings

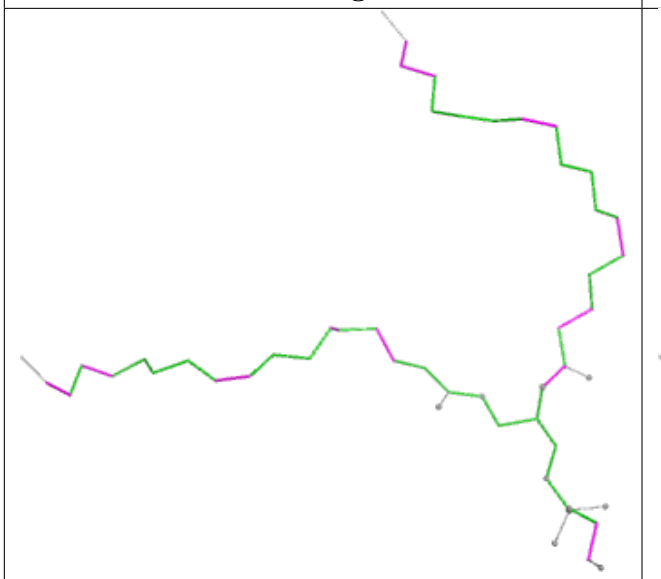
Ligand 3PE I 202



Bond lengths



Bond angles

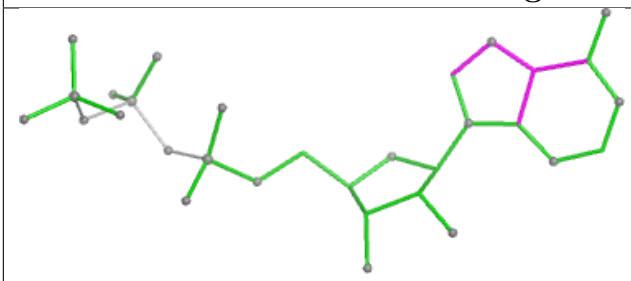


Torsions

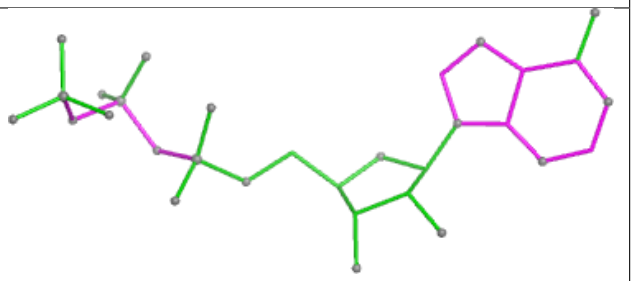


Rings

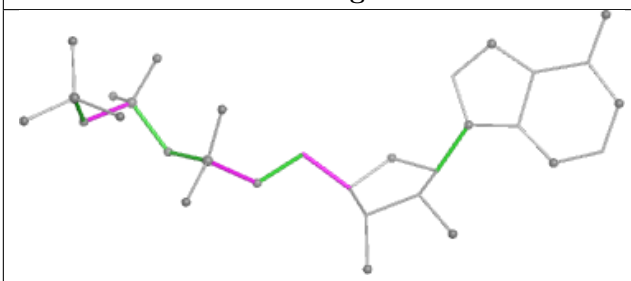
Ligand ATP O 401



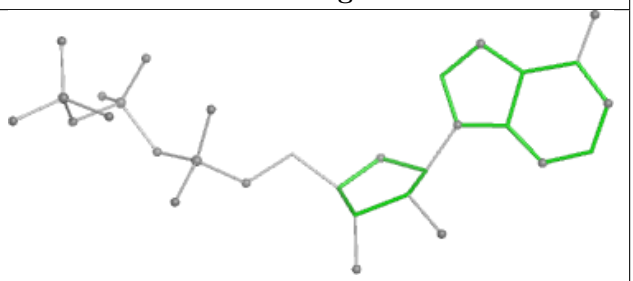
Bond lengths



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.

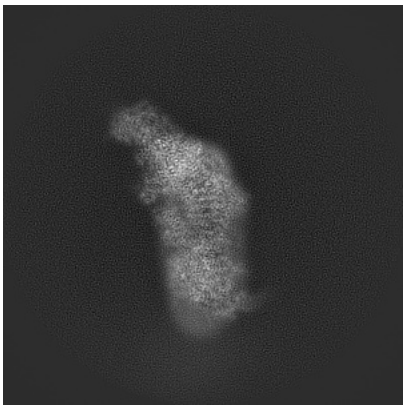
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11810. These allow visual inspection of the internal detail of the map and identification of artifacts.

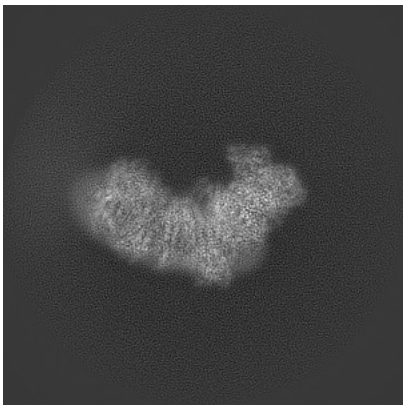
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

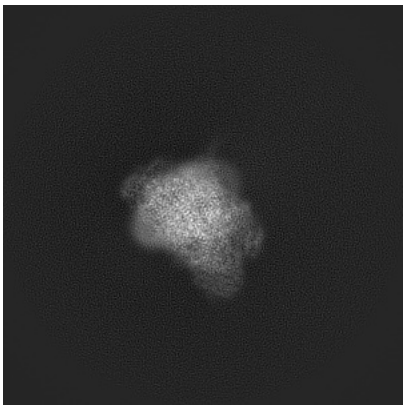
6.1.1 Primary map



X

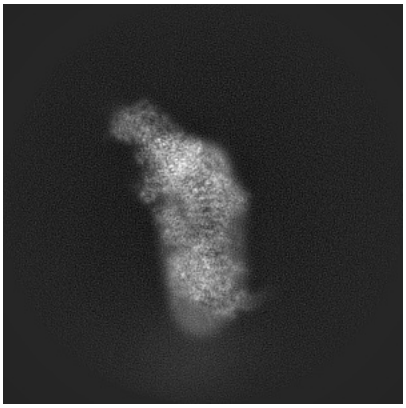


Y

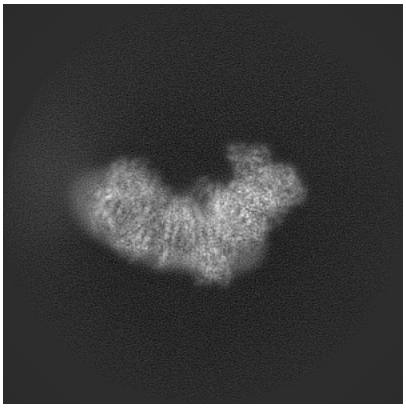


Z

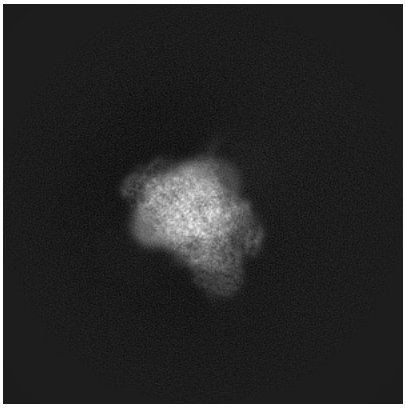
6.1.2 Raw map



X



Y

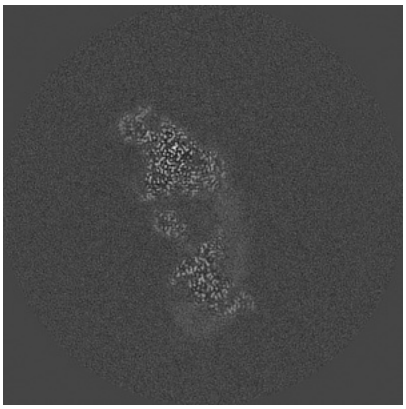


Z

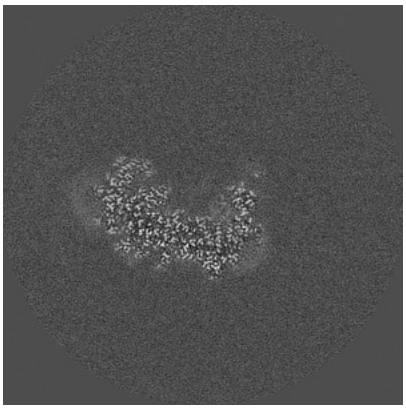
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

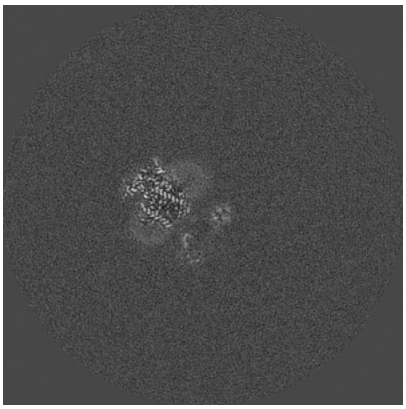
6.2.1 Primary map



X Index: 180

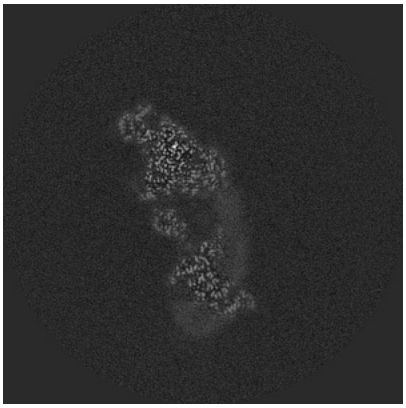


Y Index: 180

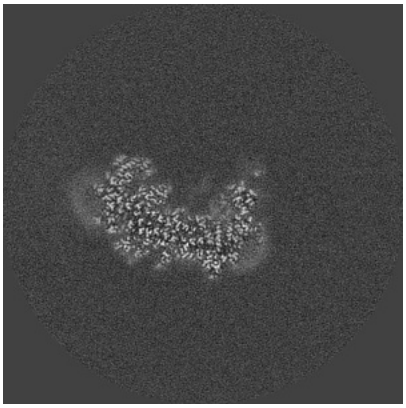


Z Index: 180

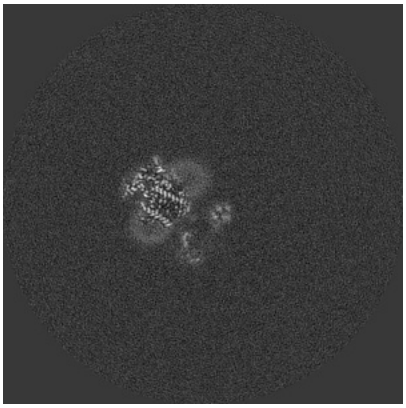
6.2.2 Raw map



X Index: 180



Y Index: 180

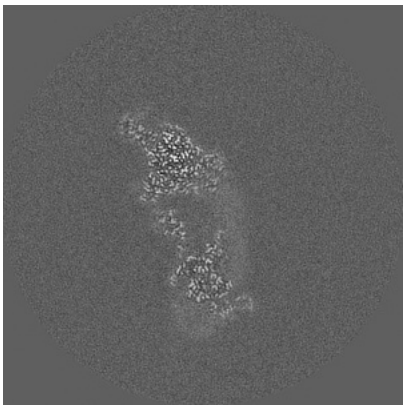


Z Index: 180

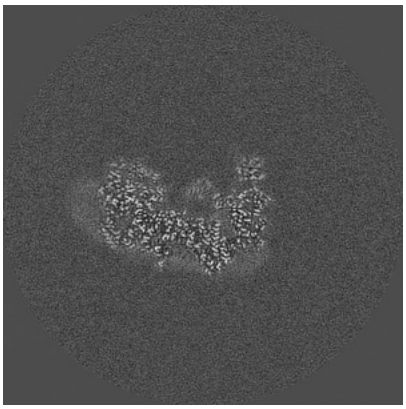
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

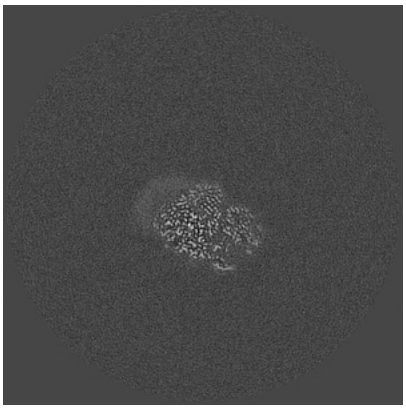
6.3.1 Primary map



X Index: 178

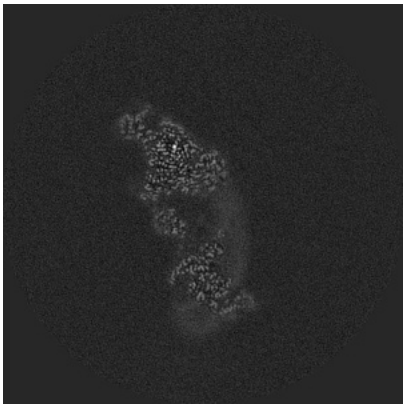


Y Index: 173

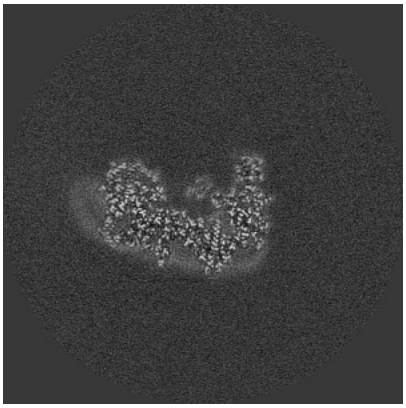


Z Index: 219

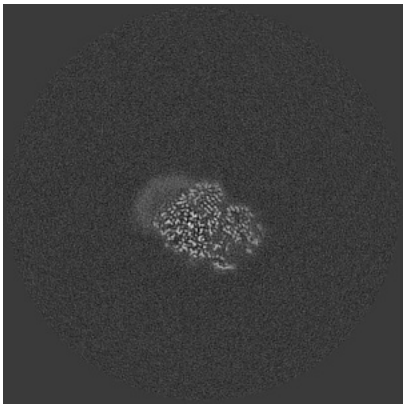
6.3.2 Raw map



X Index: 179



Y Index: 172

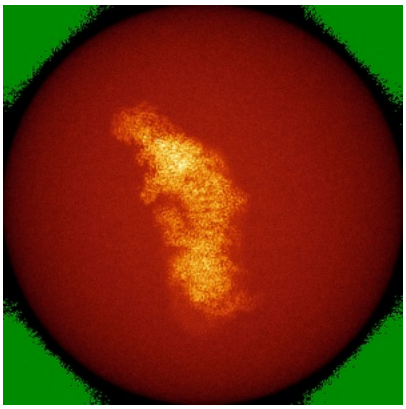


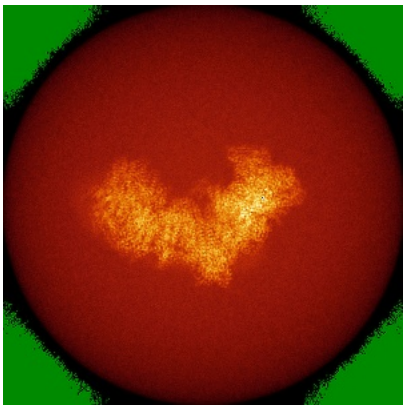
Z Index: 219

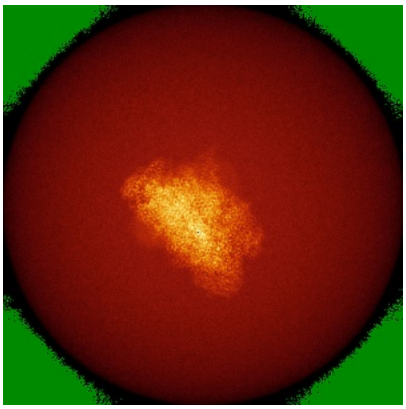
The images above show the largest variance slices of the map in three orthogonal directions.

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

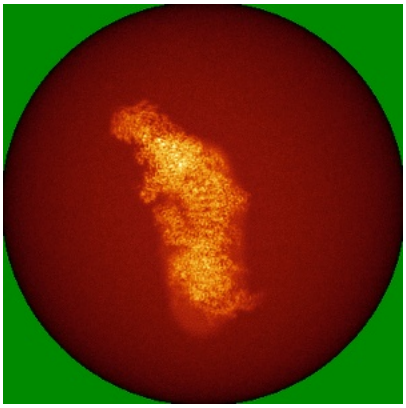
6.4.1 Primary map

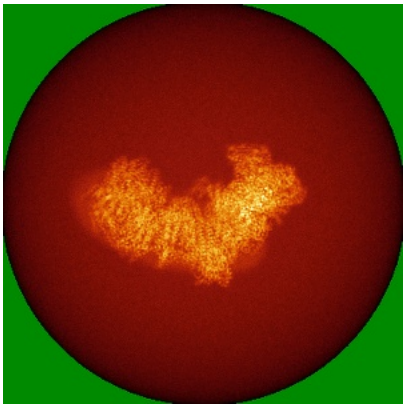

X

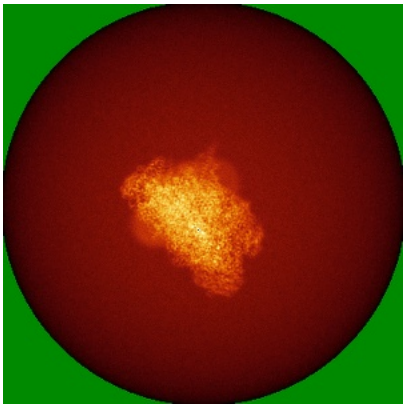

Y


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



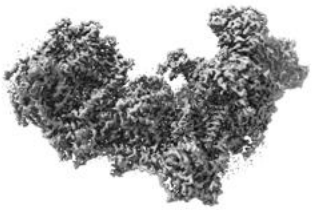
Z

The images above show the 3D surface view of the map at the recommended contour level 0.0355. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

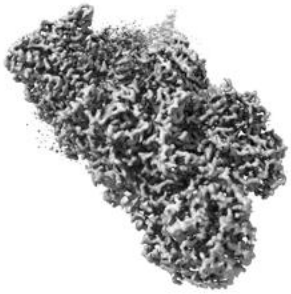
6.5.2 Raw map



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.

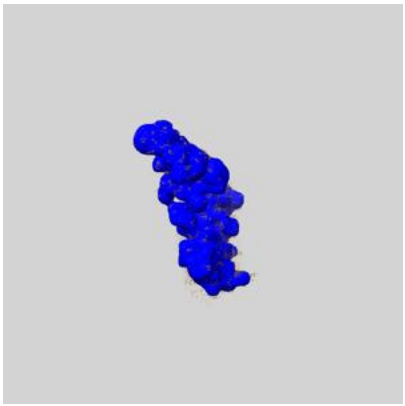
6.6 Mask visualisation

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

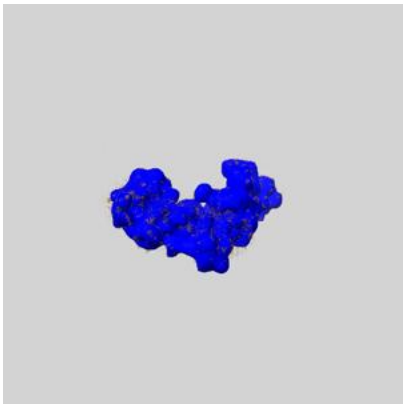
A mask typically either:

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

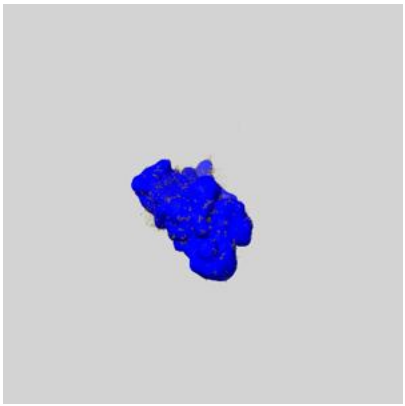
6.6.1 emd_11810_msk_1.map



X



Y

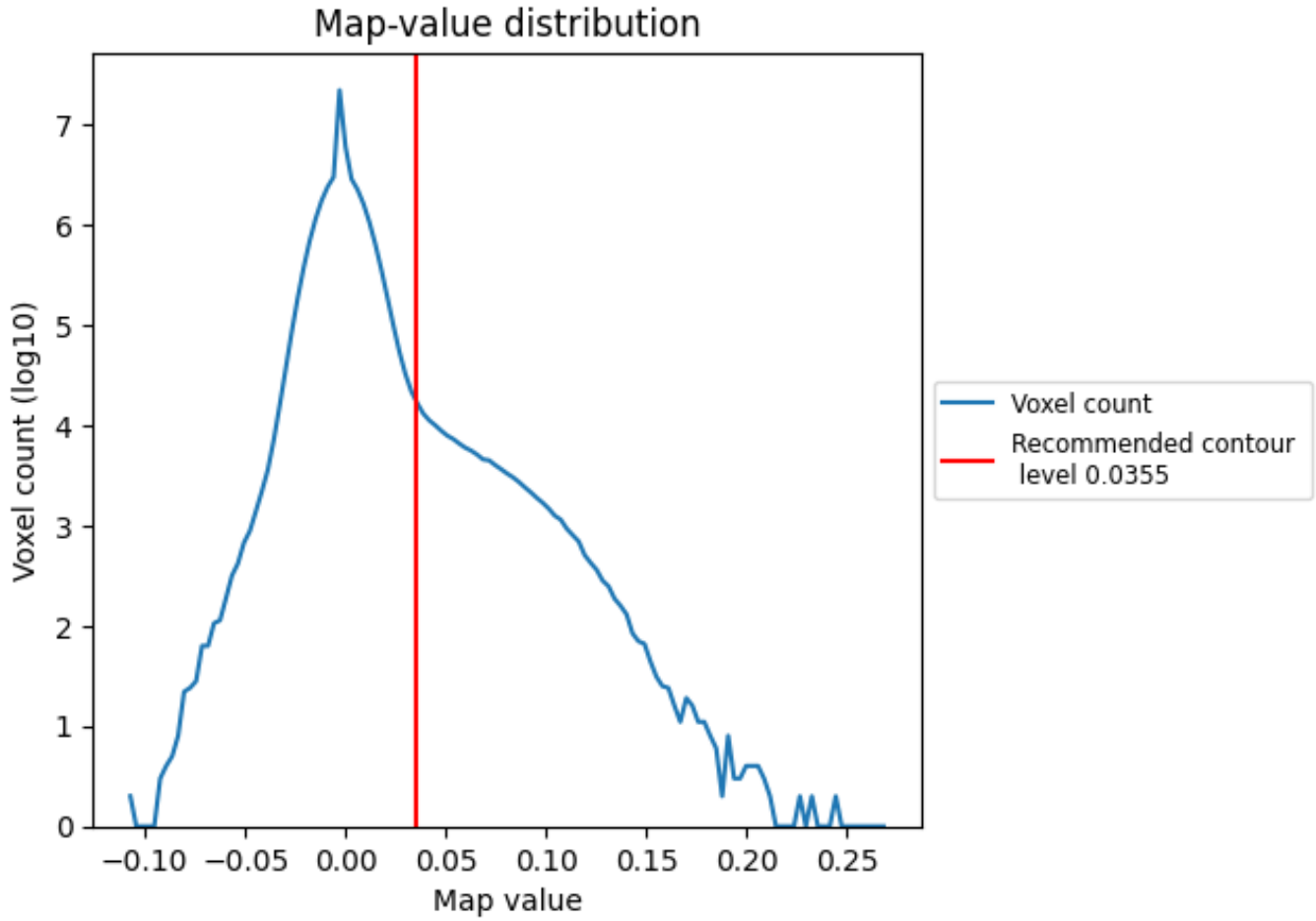


Z

7 Map analysis

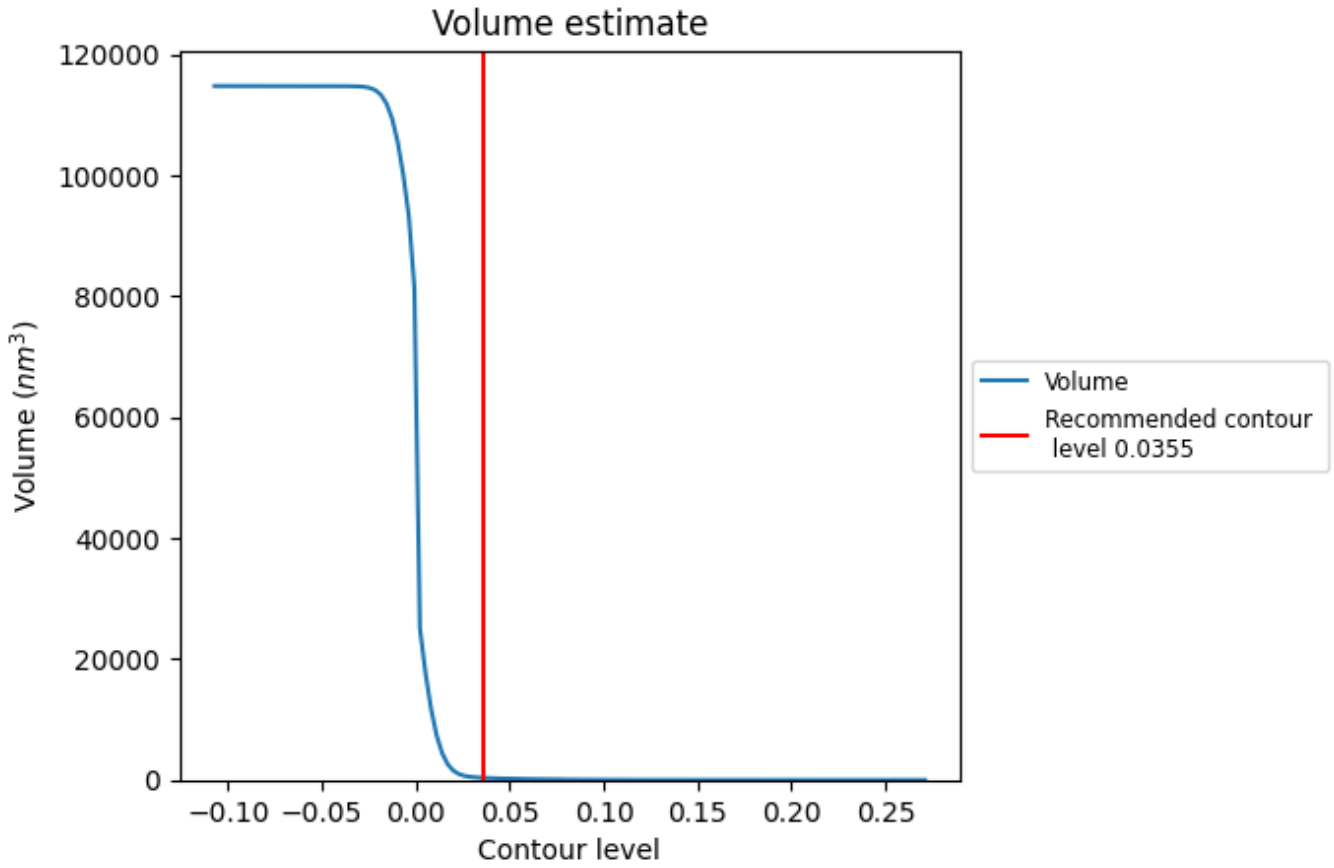
This section contains the results of statistical analysis of the map.

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.

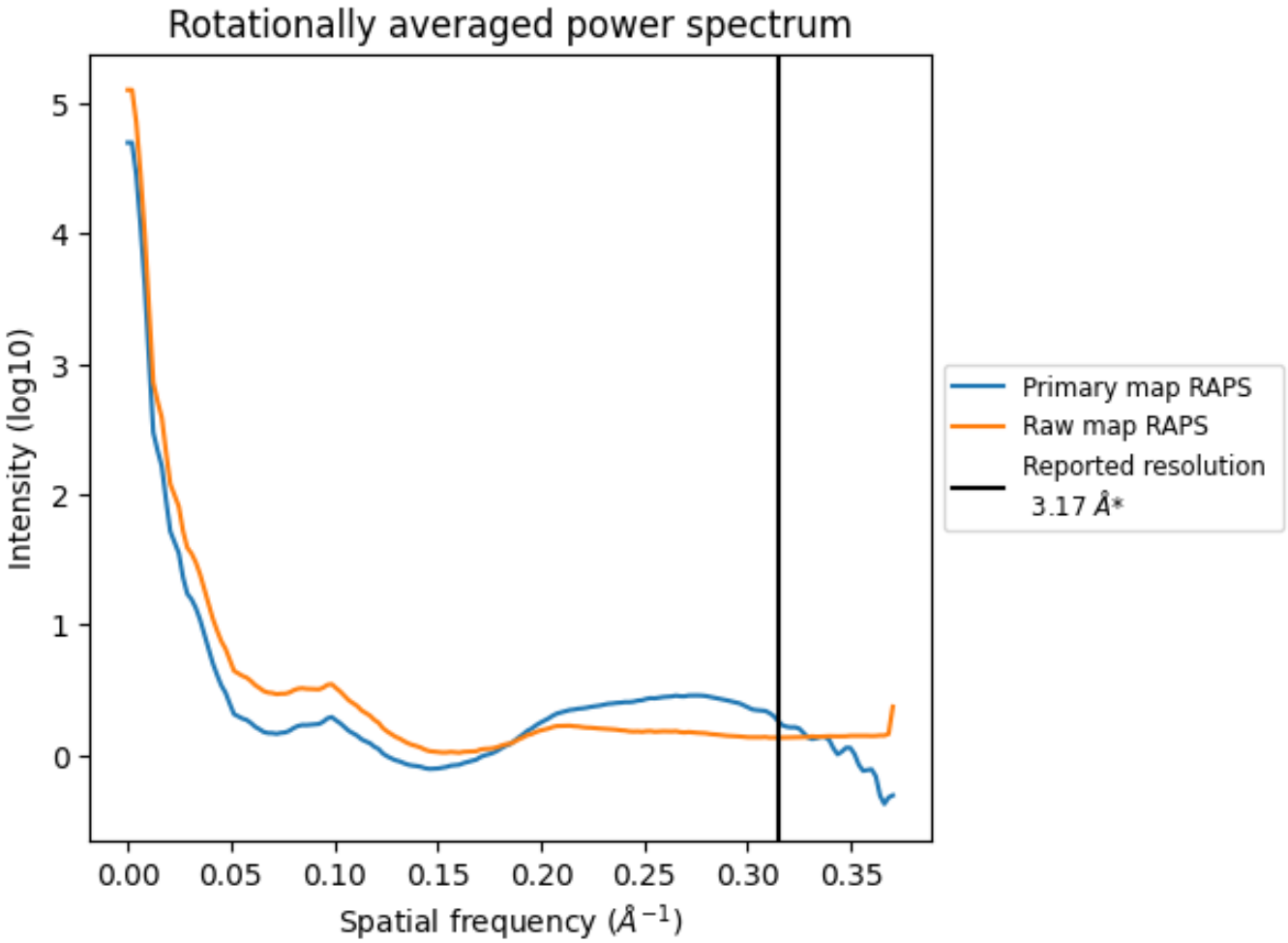
7.2 Volume estimate



The volume at the recommended contour level is 352 nm^3; this corresponds to an approximate mass of 318 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)

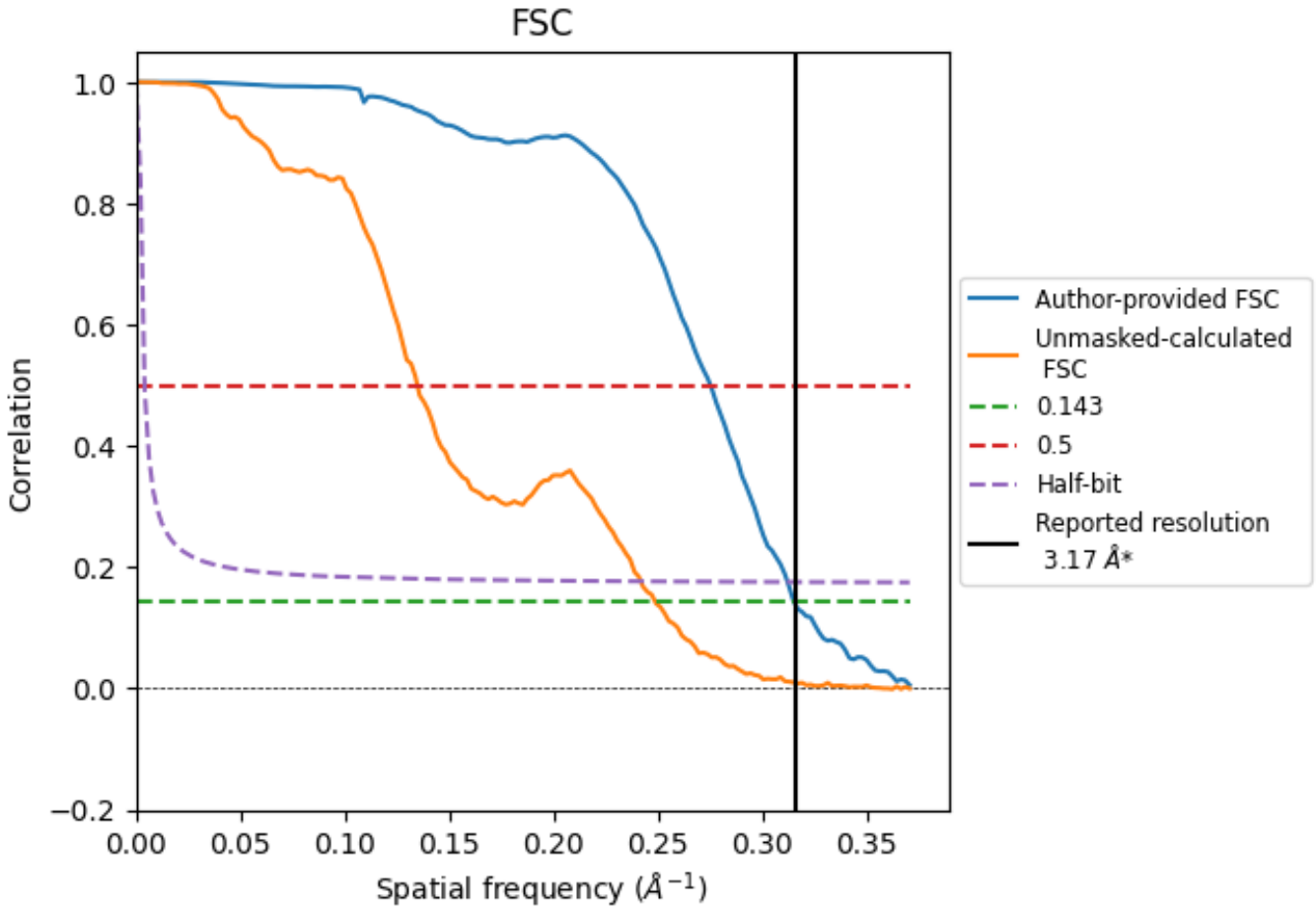


*Reported resolution corresponds to spatial frequency of 0.315 Å^{-1}

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 0.315 Å^{-1}

8.2 Resolution estimates (i)

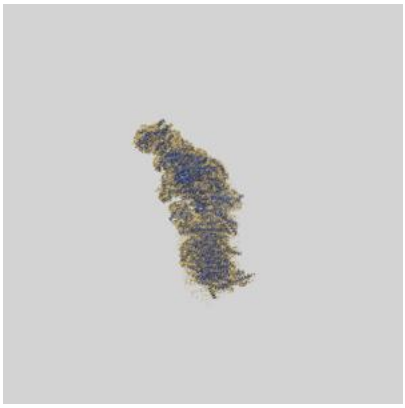
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.17	-	-
Author-provided FSC curve	3.17	3.64	3.21
Unmasked-calculated*	4.02	7.42	4.14

*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 4.02 differs from the reported value 3.17 by more than 10 %

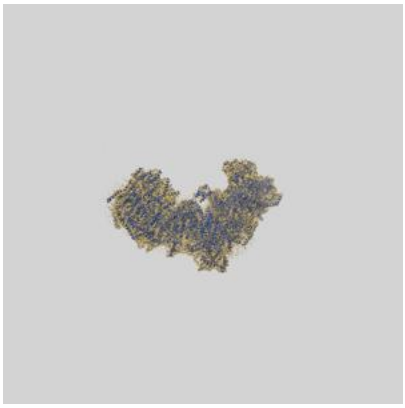
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11810 and PDB model 7AK5. Per-residue inclusion information can be found in section 3 on page 18.

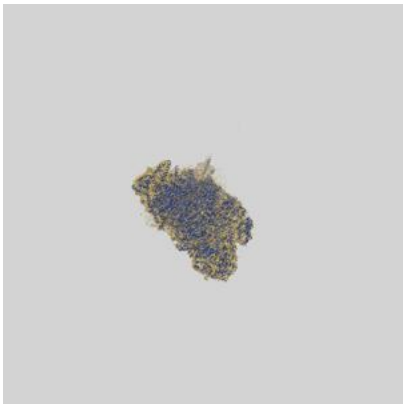
9.1 Map-model overlay



X



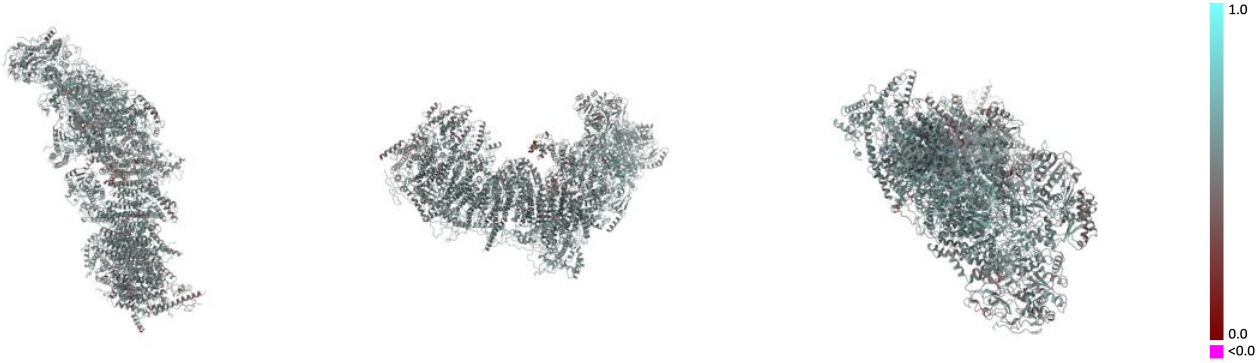
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0355 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.

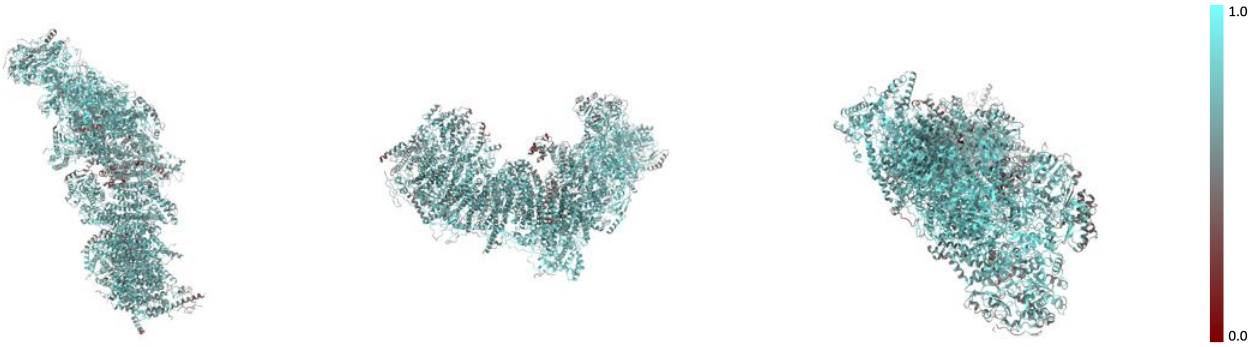
9.2 Q-score mapped to coordinate model (i)



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.

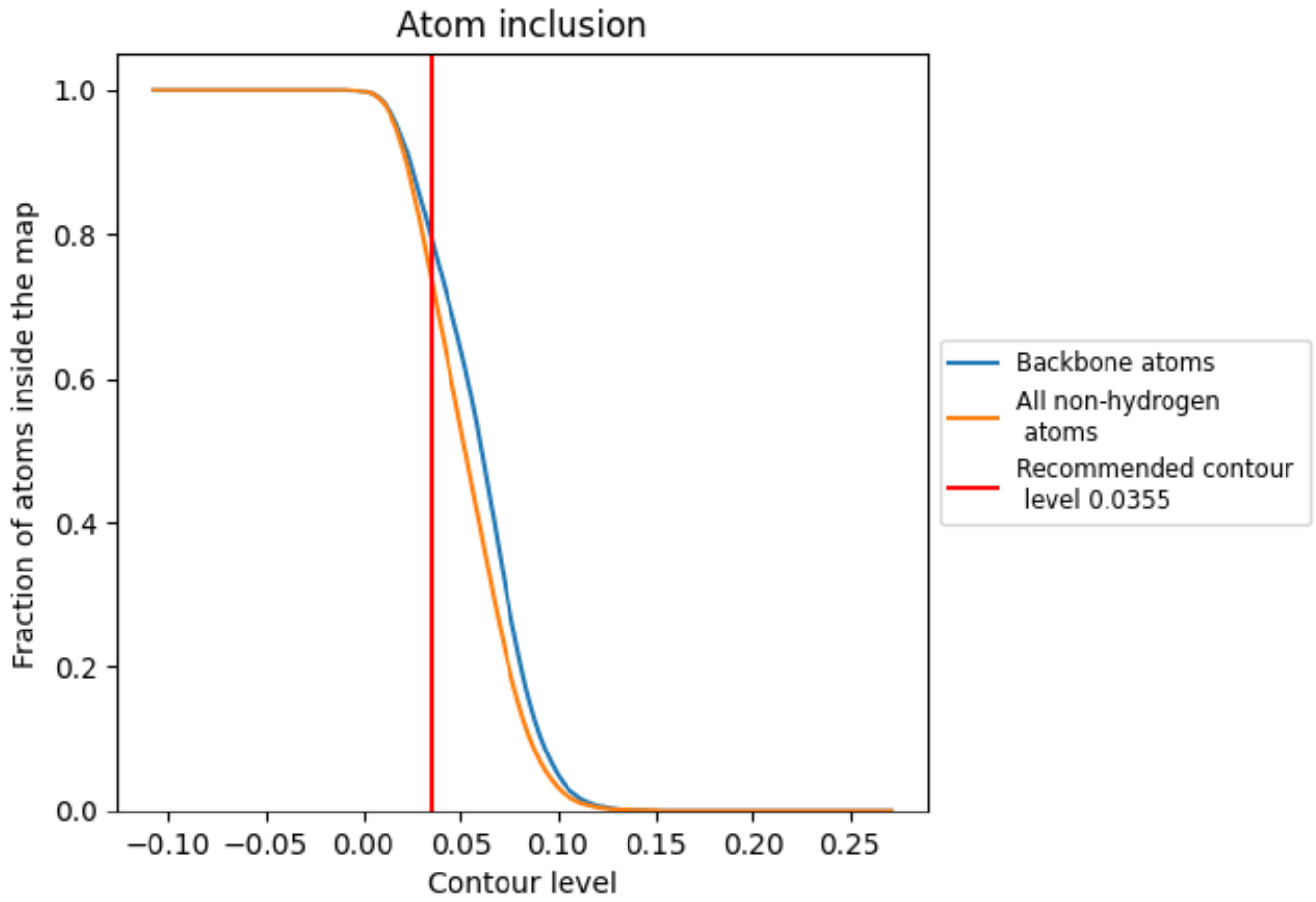
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0355).

9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.0355) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7320	0.5420
A	0.7310	0.5410
B	0.8160	0.5700
C	0.8220	0.5850
D	0.8190	0.5800
E	0.6660	0.5120
F	0.7070	0.5260
G	0.7420	0.5450
H	0.7700	0.5520
I	0.8180	0.5820
J	0.6670	0.5220
K	0.7780	0.5560
L	0.7300	0.5360
M	0.7900	0.5650
N	0.8010	0.5660
O	0.7320	0.5430
P	0.6990	0.5190
Q	0.7640	0.5600
R	0.7700	0.5720
S	0.5860	0.4850
T	0.3860	0.3940
U	0.6150	0.4920
V	0.6780	0.5190
W	0.6900	0.5260
X	0.7430	0.5490
Y	0.6860	0.5240
Z	0.7450	0.5480
a	0.8100	0.5600
b	0.7080	0.5220
c	0.6620	0.5130
d	0.7340	0.5520
e	0.7480	0.5520
f	0.6760	0.5200
g	0.7320	0.5410
h	0.7450	0.5580



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.6510	0.5040
j	0.6280	0.5000
k	0.5970	0.4830
l	0.7150	0.5420
m	0.7040	0.5280
n	0.6860	0.5330
o	0.5750	0.4700
p	0.7050	0.5290
q	0.7920	0.5700
r	0.7520	0.5560
s	0.6720	0.5200