Full wwPDB EM Validation Report ⓘ

Aug 27, 2026 – 02:32 am BST

PDB ID	:	7AK6 / pdb_00007ak6
EMDB ID	:	EMD-11811
Title	:	Cryo-EM structure of ND6-P25L mutant respiratory complex I from Mus musculus at 3.8 A
Authors	:	Yin, Z.; Bridges, H.R.; Grba, D.; Hirst, J.
Deposited on	:	2020-09-29
Resolution	:	3.82 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:

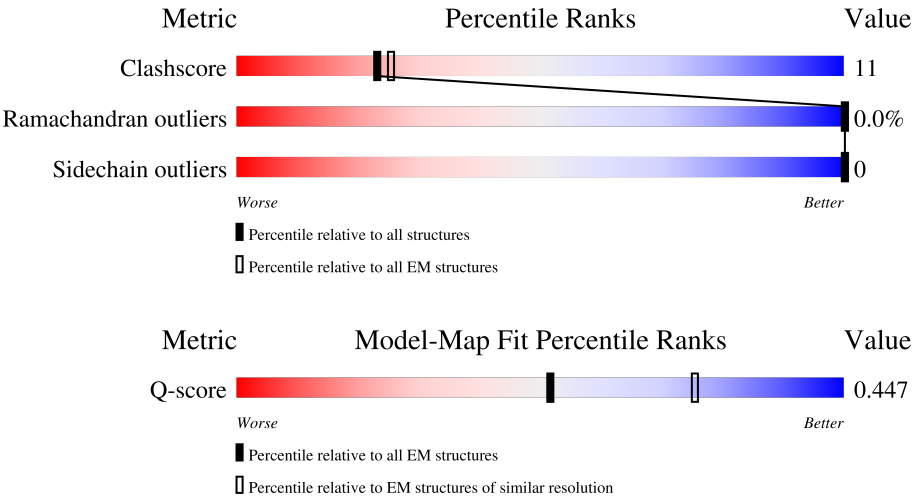
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.82 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	9152 (3.32 - 4.32)

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	52% 52% 28% · 19%
2	B	224	16% 52% 17% 31%
3	C	263	19% 52% 27% 21%
4	D	463	25% 65% 24% 10%

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Mol	Chain	Length	Quality of chain
5	E	248	55% 63% 22% 15%
6	F	464	56% 70% 22% 8%
7	G	727	41% 71% 23% 6%
8	H	318	45% 65% 31%
9	I	212	16% 54% 30% 16%
10	J	172	68% 72% 28%
11	K	98	50% 70% 29%
12	L	607	61% 68% 32%
13	M	459	36% 65% 35%
14	N	345	32% 68% 31%
15	O	355	50% 67% 23% 10%
16	P	377	47% 54% 22% 24%
17	Q	175	26% 53% 18% 29%
18	R	116	34% 65% 16% 19%
19	S	99	73% 59% 24% 17%
20	T	156	44% 30% 16% 54%
20	U	156	48% 41% 15% 44%
21	V	116	62% 74% 22%
22	W	131	53% 67% 20% 13%
23	X	172	59% 69% 30%
24	Y	143	85% 87% 11%
25	Z	144	43% 78% 18%
26	a	68	46% 74% 26%
27	b	84	60% 88% 10%
28	c	76	43% 53% 8% 39%

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Mol	Chain	Length	Quality of chain
29	d	120	49% 85% 14%
30	e	106	42% 79% 19%
31	f	57	63% 81% 9% 11%
32	g	151	40% 51% 17% 32%
33	h	189	30% 59% 14% 28%
34	i	128	55% 59% 15% 26%
35	j	105	55% 49% 10% 41%
36	k	104	67% 56% 18% 26%
37	l	186	54% 68% 16% 16%
38	m	129	69% 78% 19%
39	n	179	68% 79% 20%
40	o	137	72% 65% 18% 17%
41	p	176	56% 77% 18% 5%
42	q	145	48% 78% 21%
43	r	112	48% 59% 27% 14%
44	s	104	32% 29% 9% 62%

2 Entry composition (i)

There are 54 unique types of molecules in this entry. The entry contains 65323 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	93	761	527	105	124	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	207	1721	1111	296	311	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	417	3369	2155	576	614	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	686	Total	C	N	O	S	0	0
			5281	3313	917	1010	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	305	Total	C	N	O	S	0	0
			2441	1642	367	411	21		

- 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
			1278	858	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	319	Total	C	N	O	S	0	0
			2599	1668	430	491	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	288	Total	C	N	O	S	0	0
			2281	1453	412	409	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	72	Total	C	N	O	S	0	0
			584	376	86	117	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	82	Total	C	N	O	S	0	0
			643	422	104	113	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	51	Total	C	N	O	S	0	0
			433	278	78	75	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	102	Total	C	N	O	S	0	0
			858	555	137	162	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	95	Total	C	N	O	S	0	0
			802	524	138	137	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	62	Total	C	N	O	S	0	0
			537	355	88	93	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	77	Total	C	N	O	S	0	0
			626	414	106	104	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		

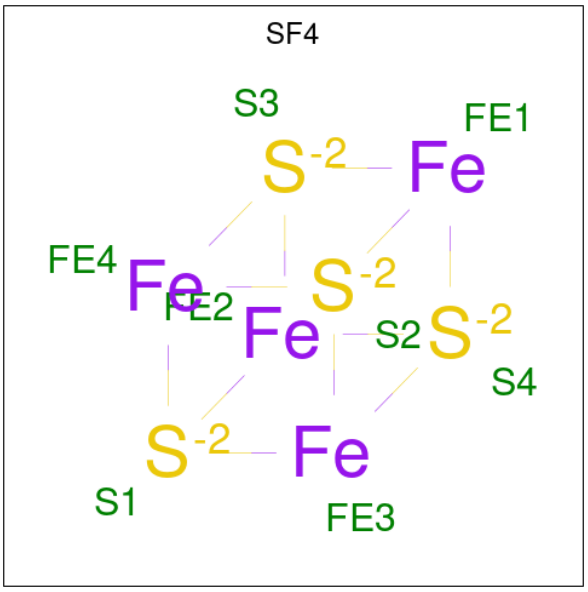
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

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.

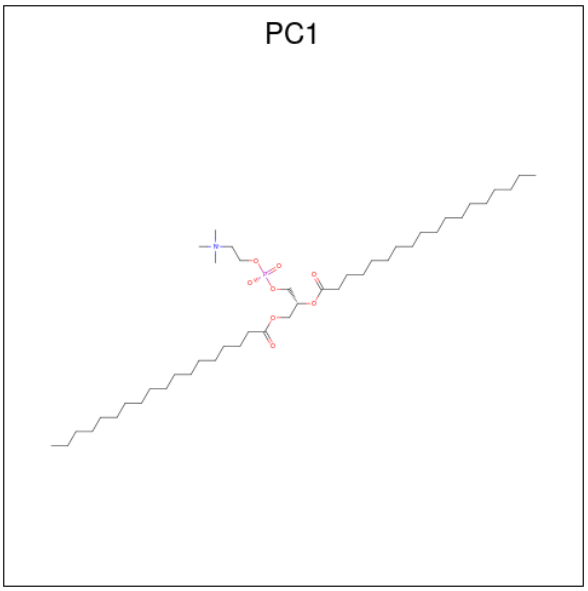
Mol	Chain	Residues	Atoms				AltConf	Trace
44	s	39	Total	C	N	O	0	0
			329	207	59	63		

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



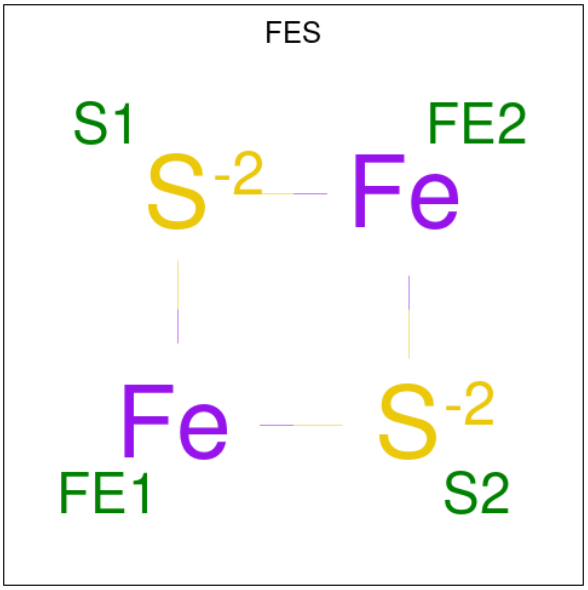
Mol	Chain	Residues	Atoms			AltConf
45	B	1	Total	Fe	S	0
			8	4	4	
45	F	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	G	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	
45	I	1	Total	Fe	S	0
			8	4	4	

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



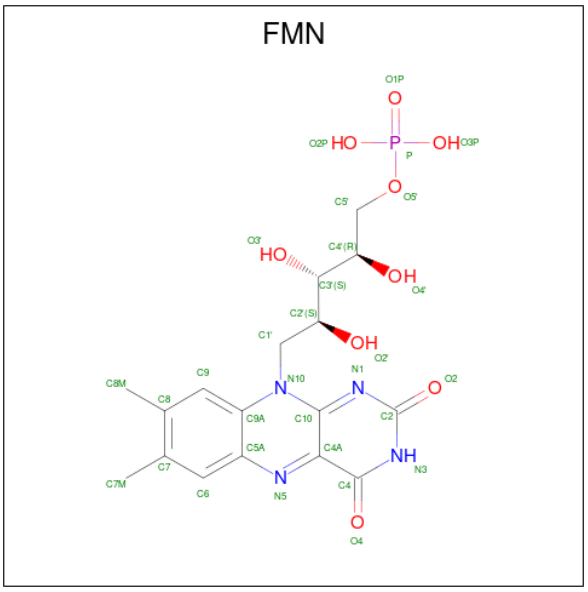
Mol	Chain	Residues	Atoms					AltConf
46	B	1	Total	C	N	O	P	0
			26	16	1	8	1	

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



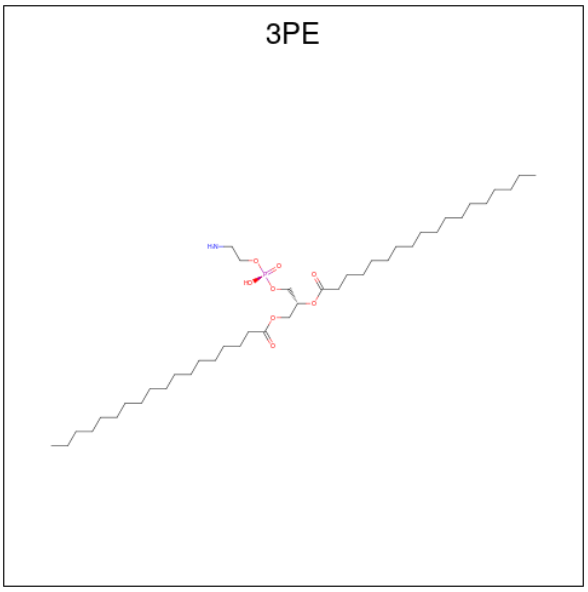
Mol	Chain	Residues	Atoms				AltConf
47	E	1	Total	Fe	S		0
			4	2	2		
47	G	1	Total	Fe	S		0
			4	2	2		

- 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
			42	32	1	8	1	
49	J	1	Total	C	N	O	P	0
			38	28	1	8	1	

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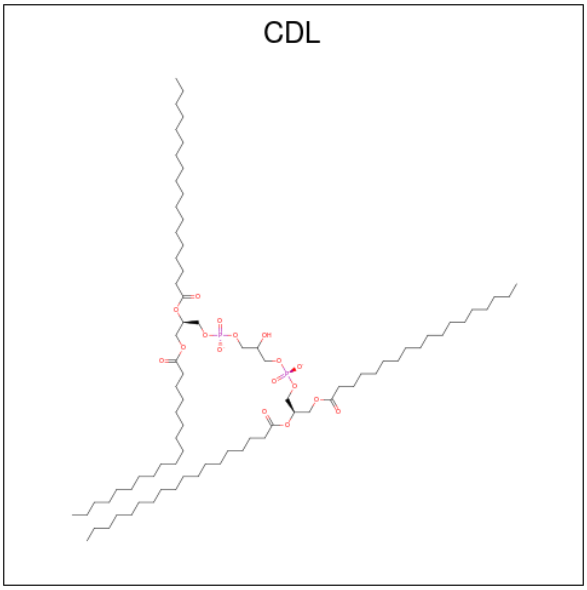
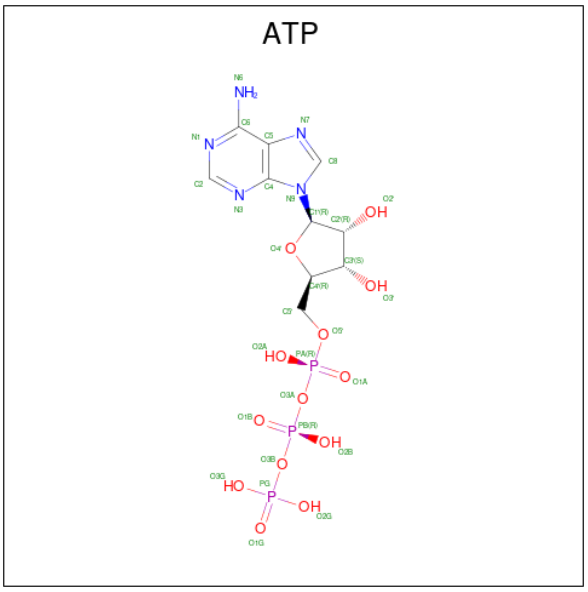
Mol	Chain	Residues	Atoms					AltConf
49	L	1	Total	C	N	O	P	0
			45	35	1	8	1	
49	M	1	Total	C	N	O	P	0
			38	28	1	8	1	

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



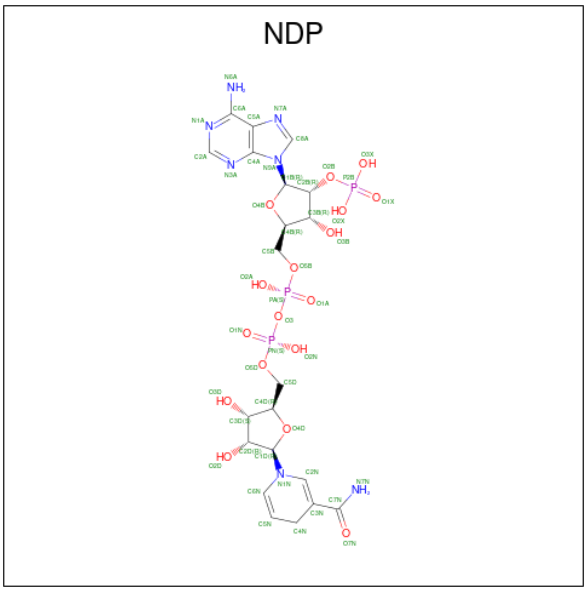
Mol	Chain	Residues	Atoms				AltConf
50	L	1	Total	C	O	P	0
			54	35	17	2	
50	d	1	Total	C	O	P	0
			50	31	17	2	

- 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: $C_{21}H_{30}N_7O_{17}P_3$).

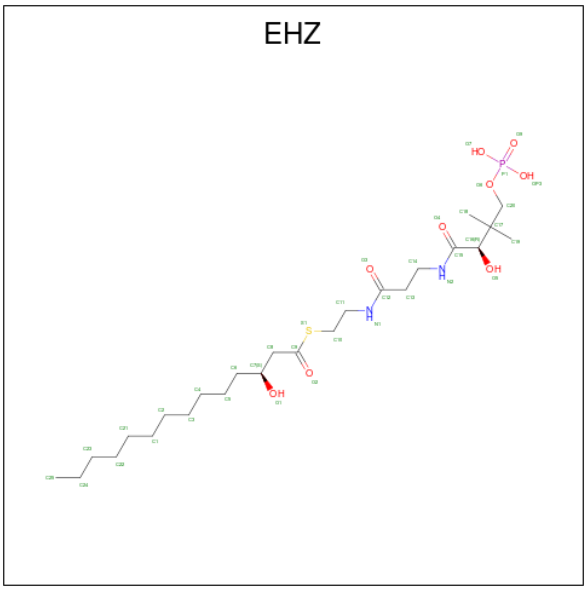


Mol	Chain	Residues	Atoms					AltConf
52	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

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

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

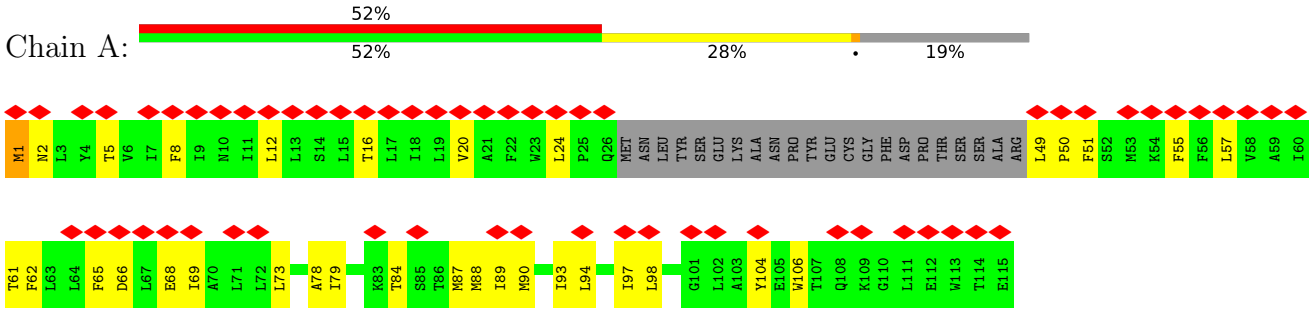


Mol	Chain	Residues	Atoms					AltConf
54	T	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
54	U	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

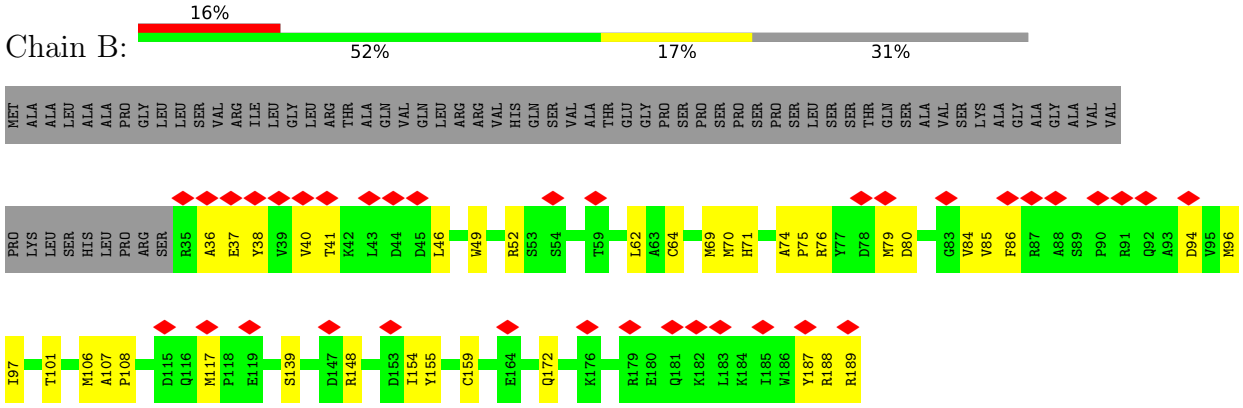
3 Residue-property plots (i)

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

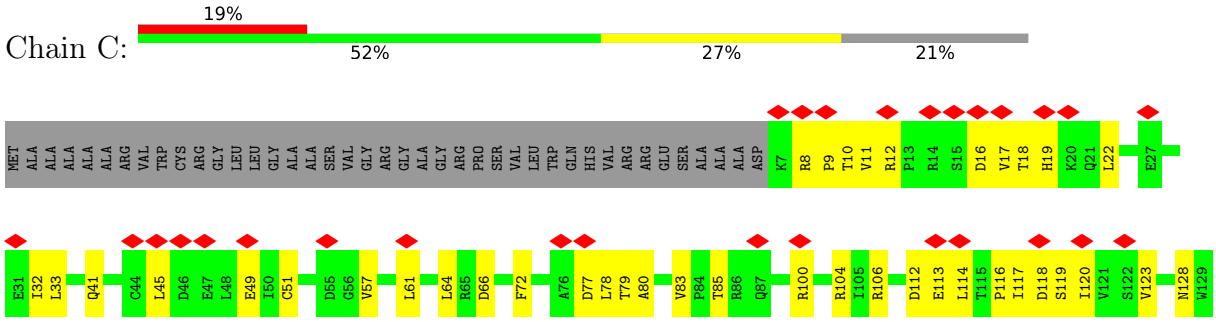
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

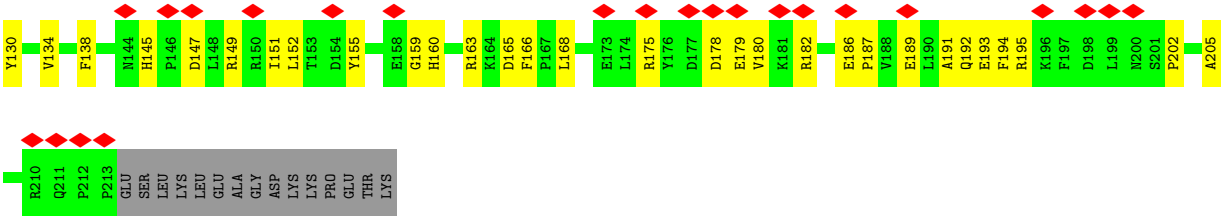


• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



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

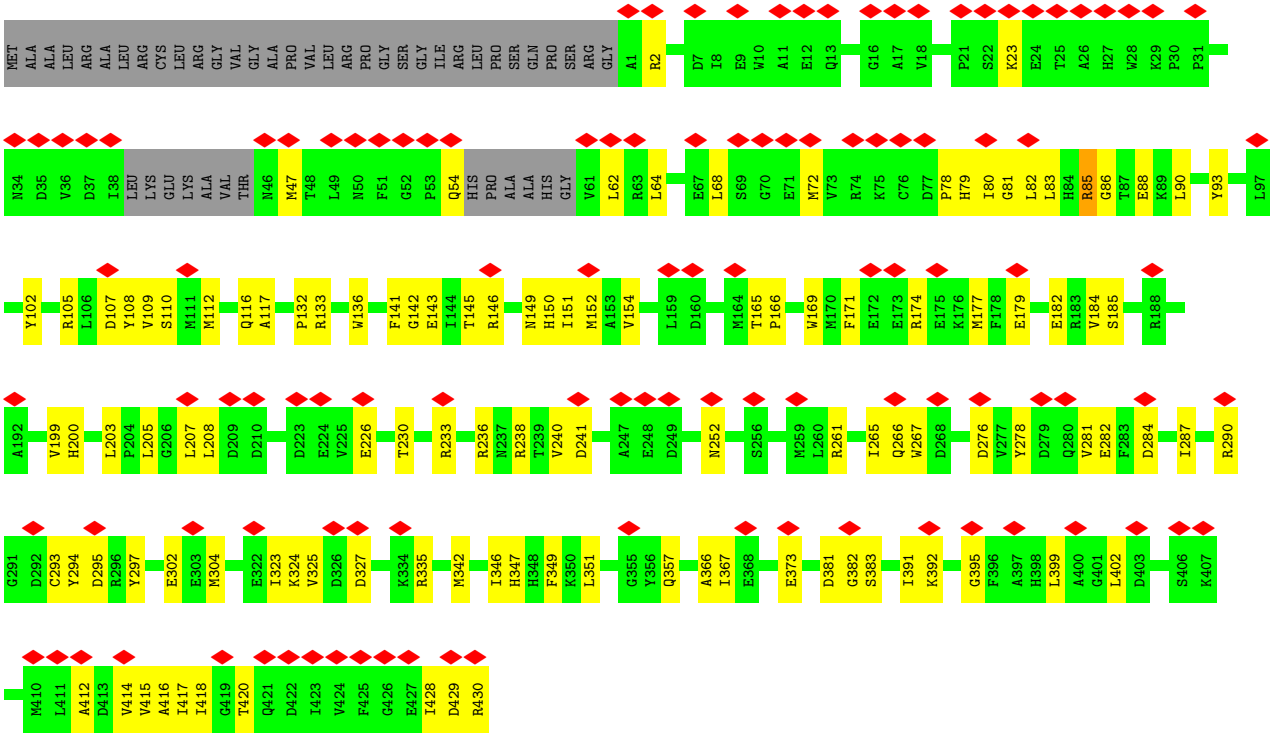




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain D:

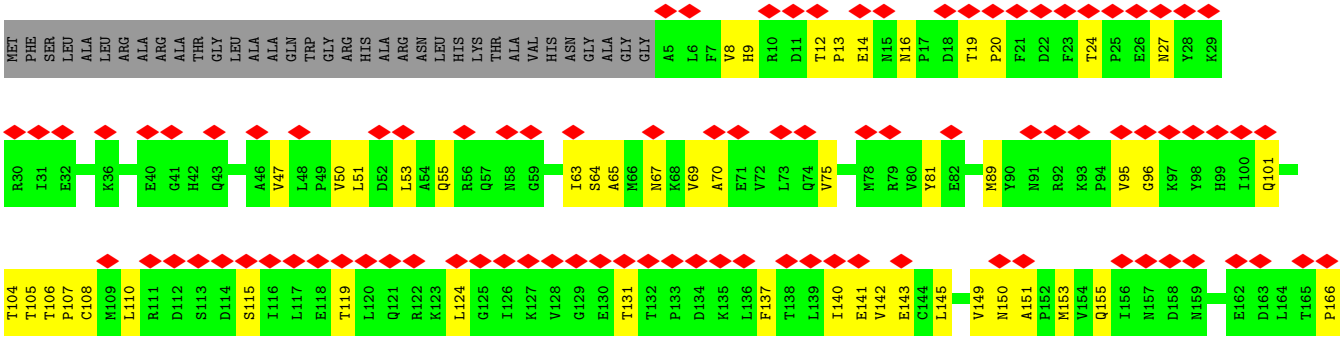


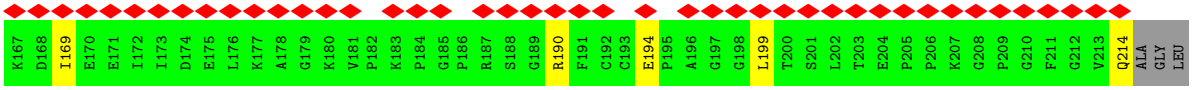


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



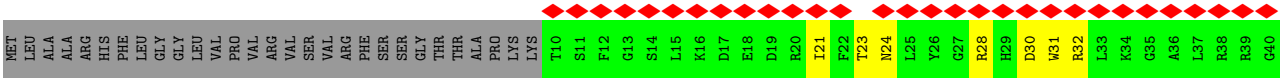


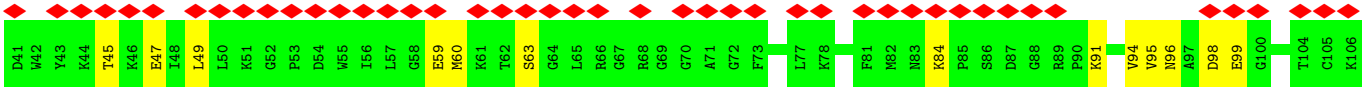


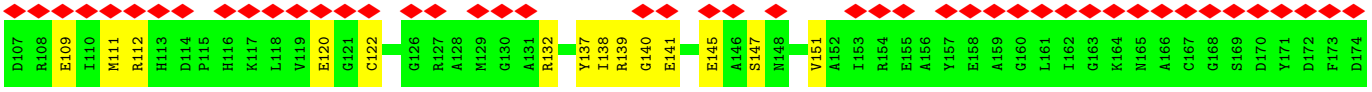
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

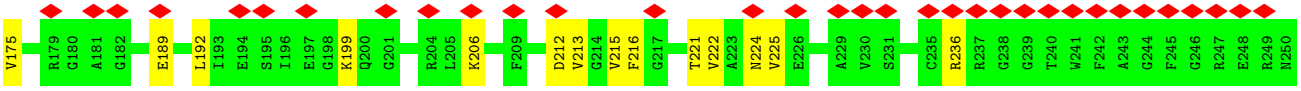
Chain F:

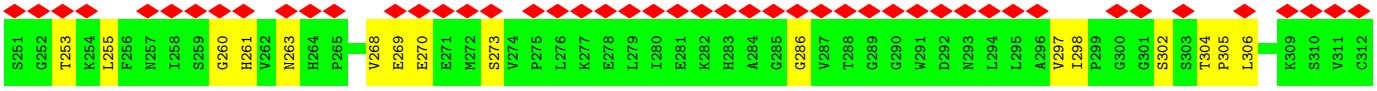


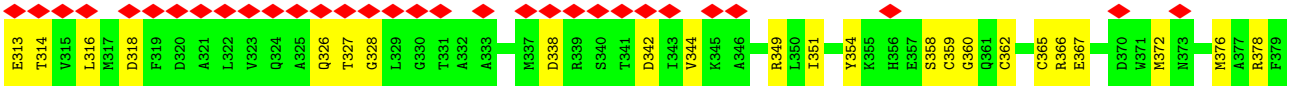


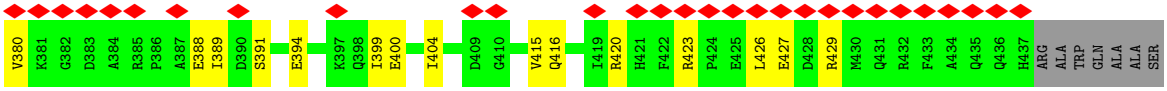








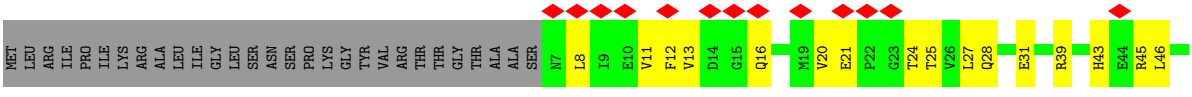




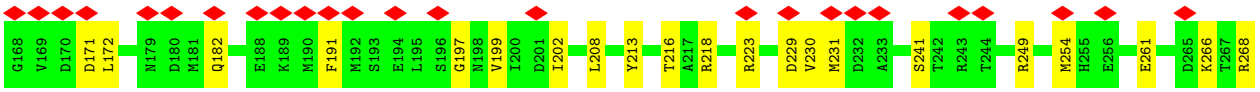
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

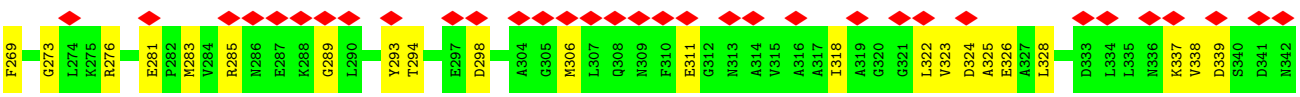
Chain G:

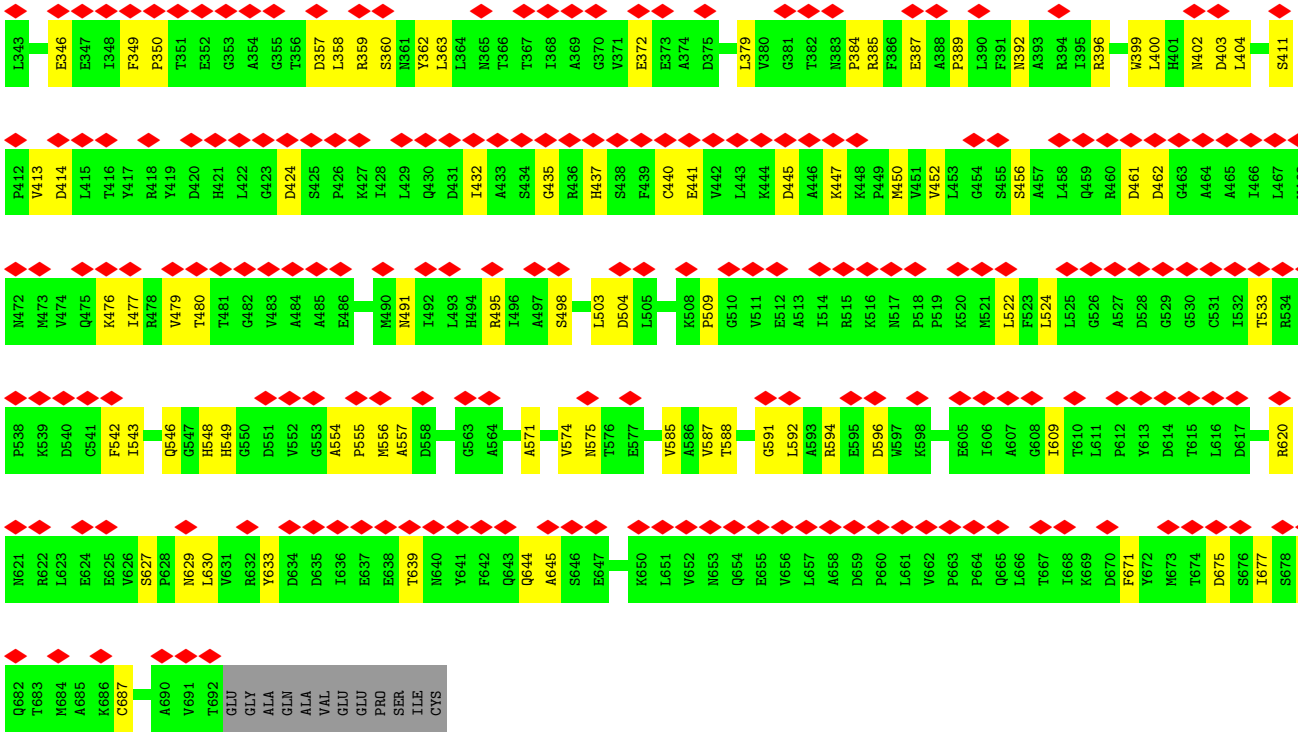








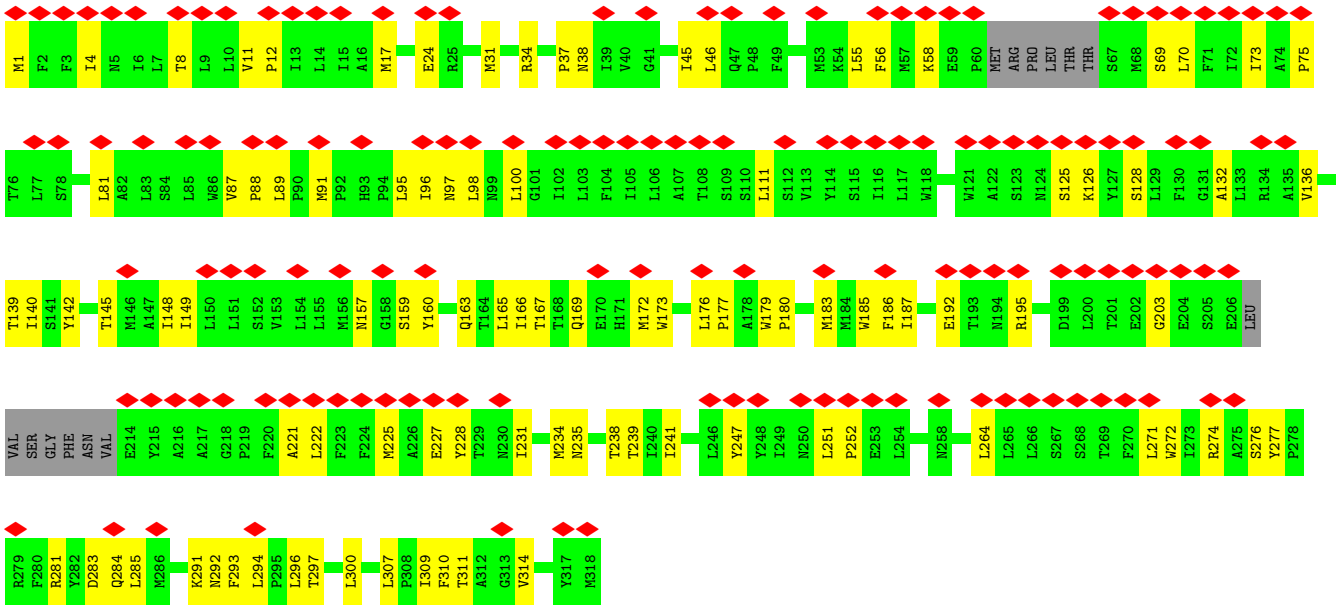




• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:

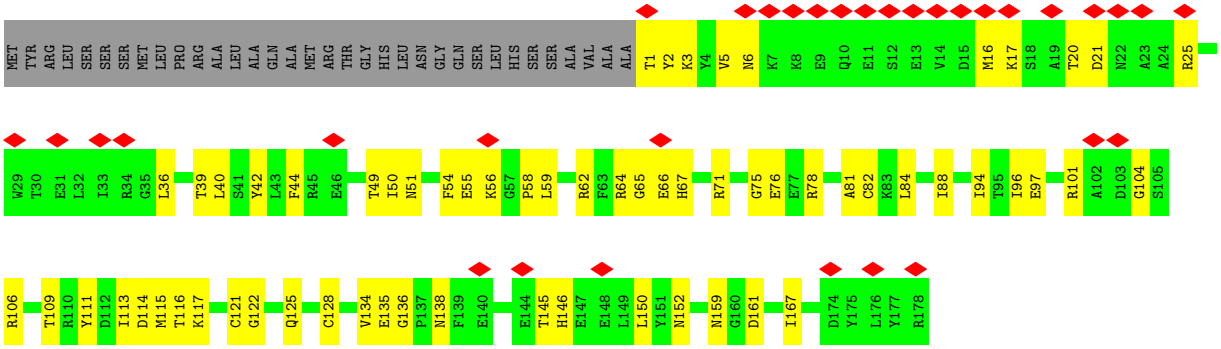




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:

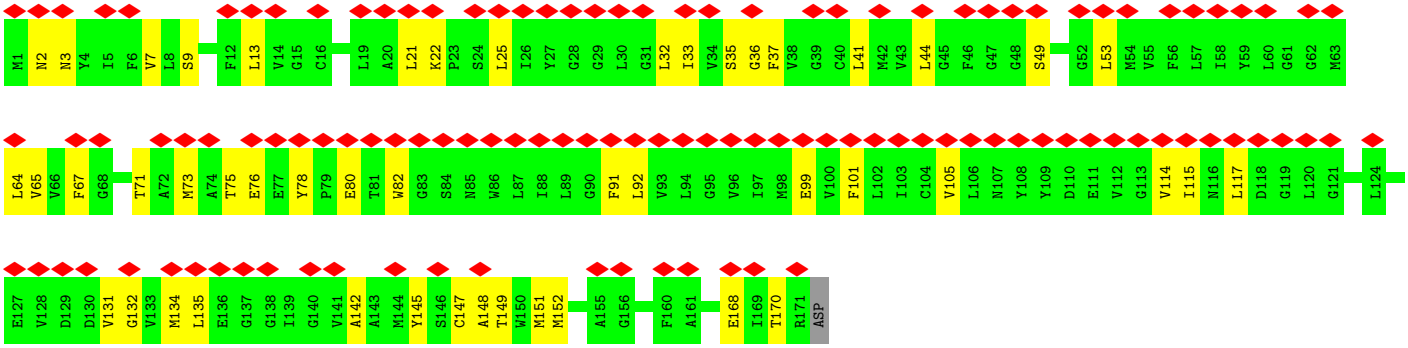




• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J:

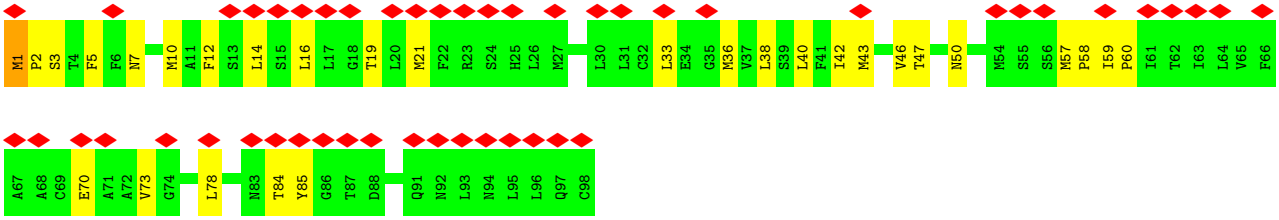




• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K:

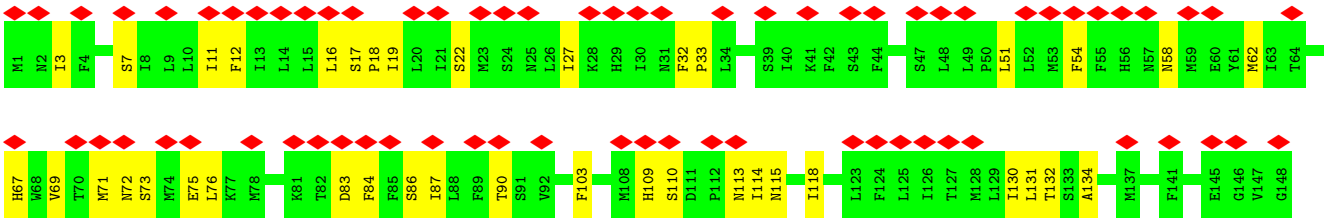


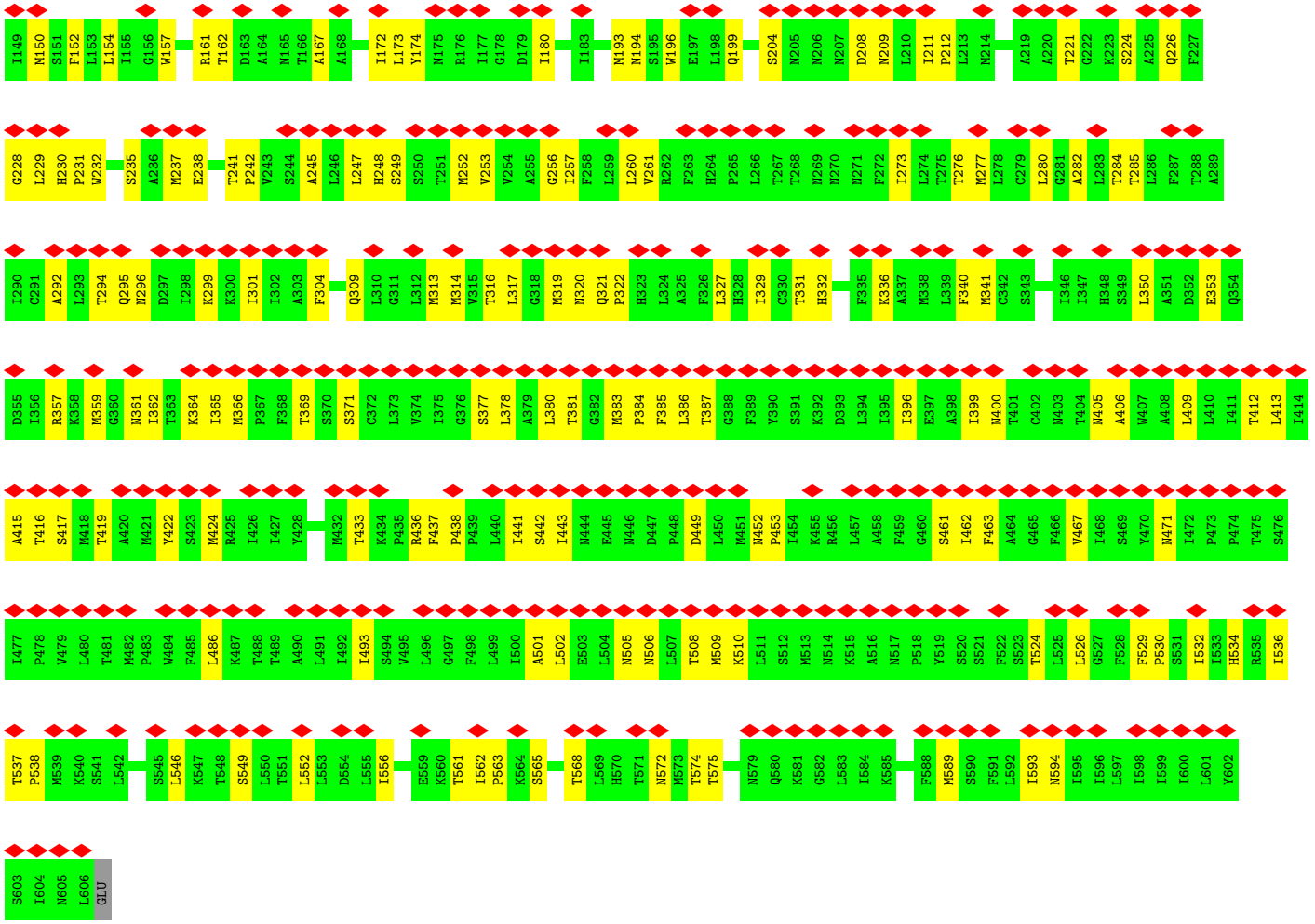


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L:



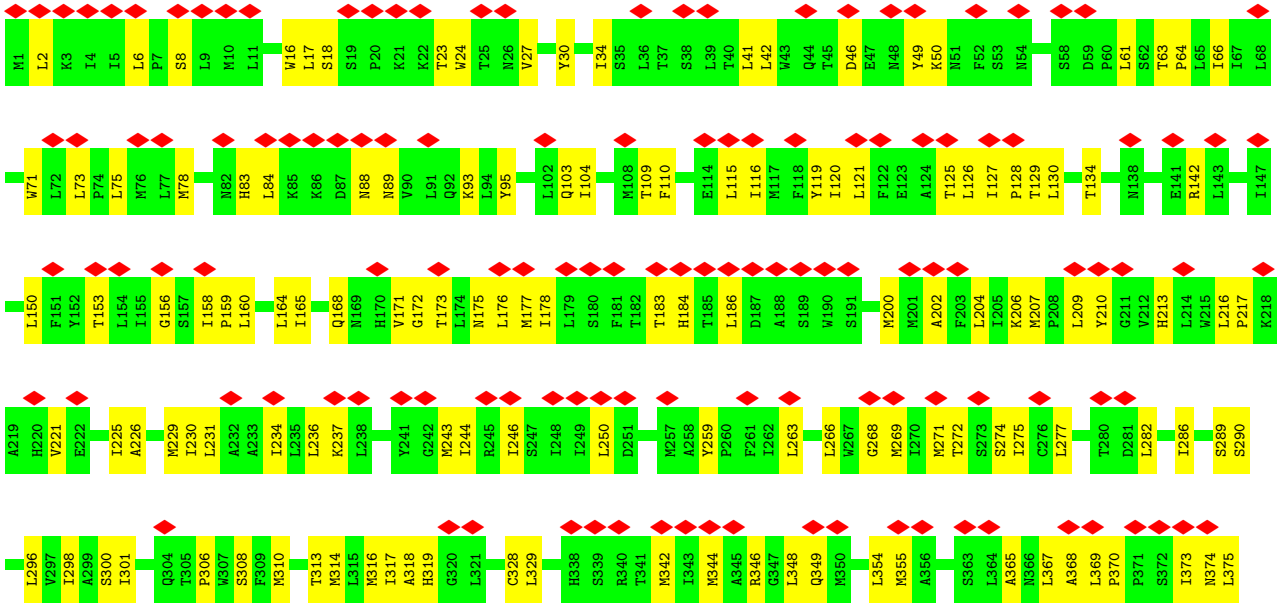


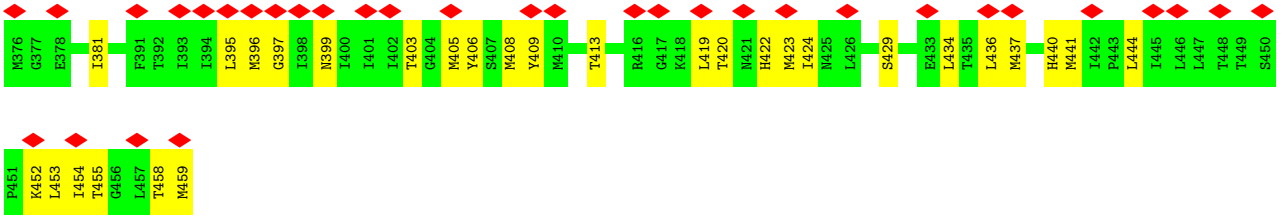


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M:



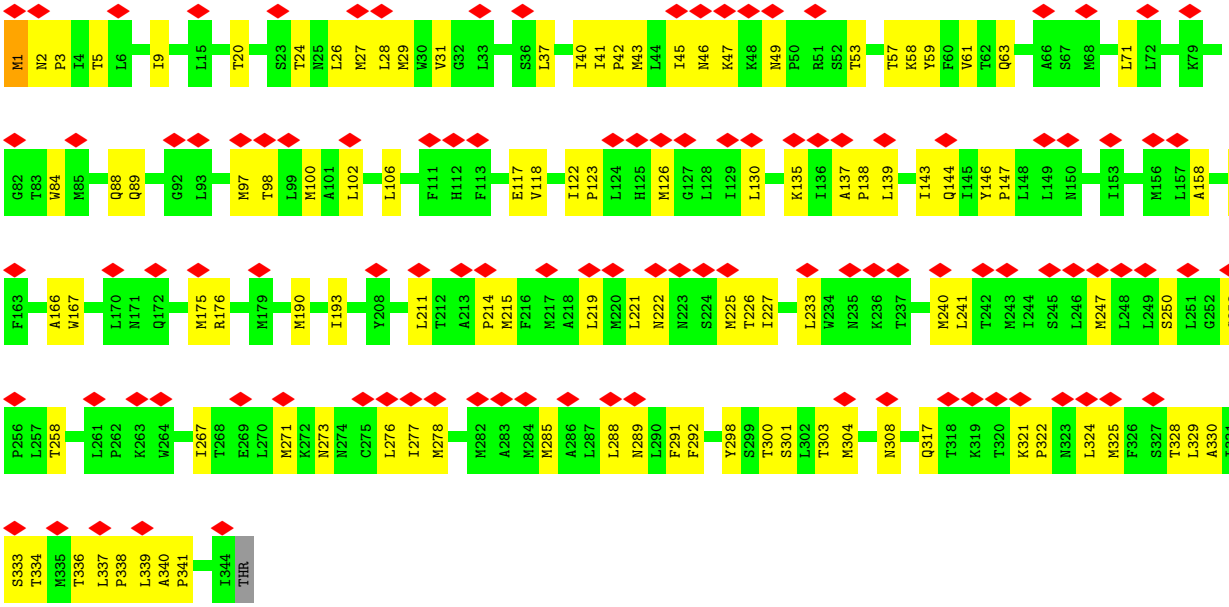




• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N:

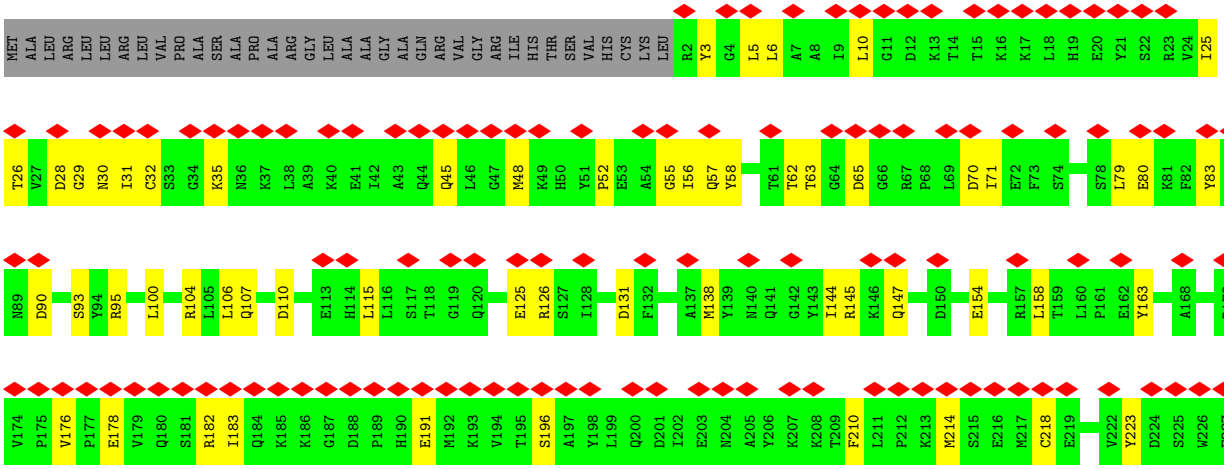


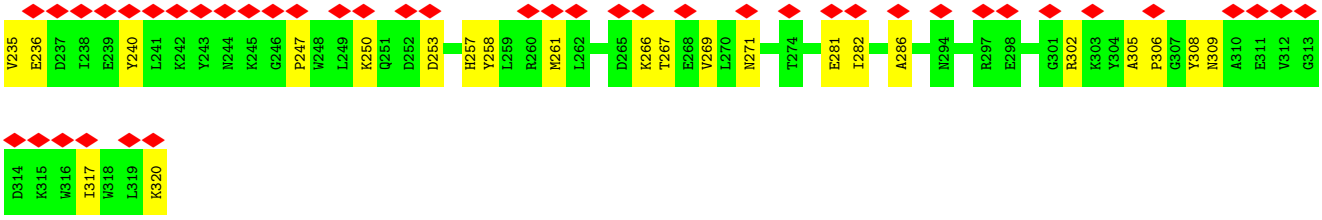


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O:

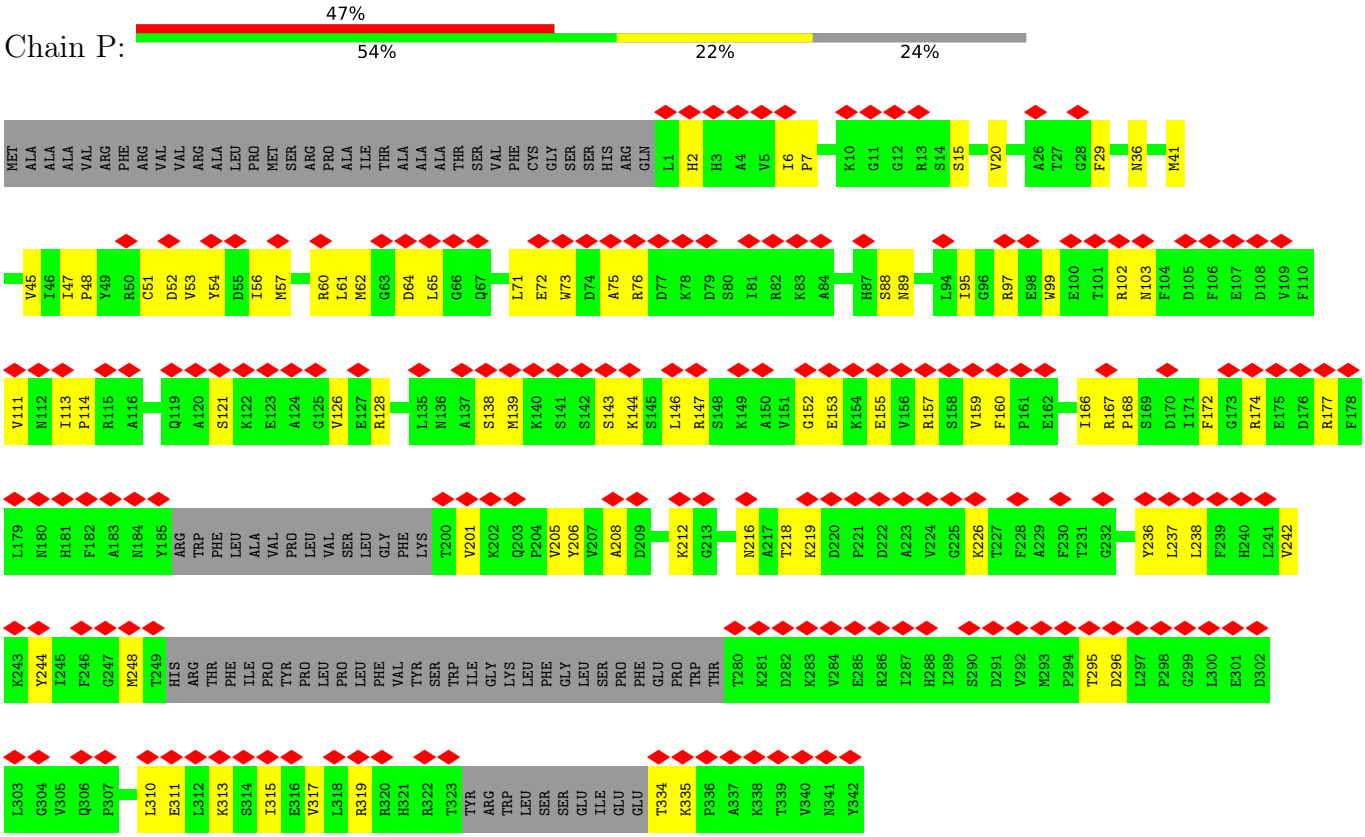






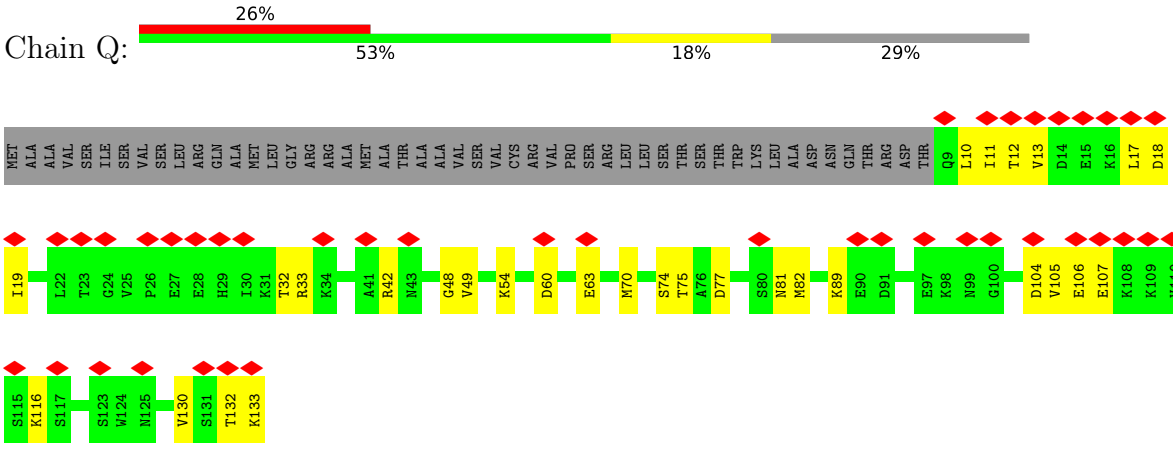
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:



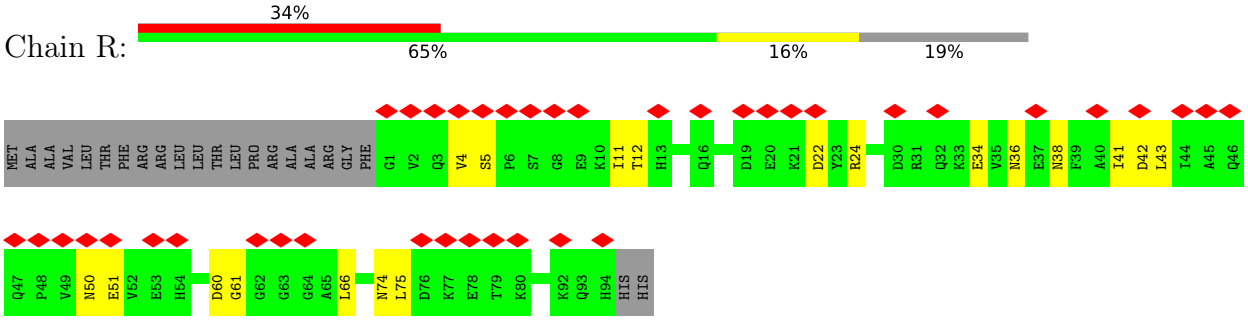
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain Q:



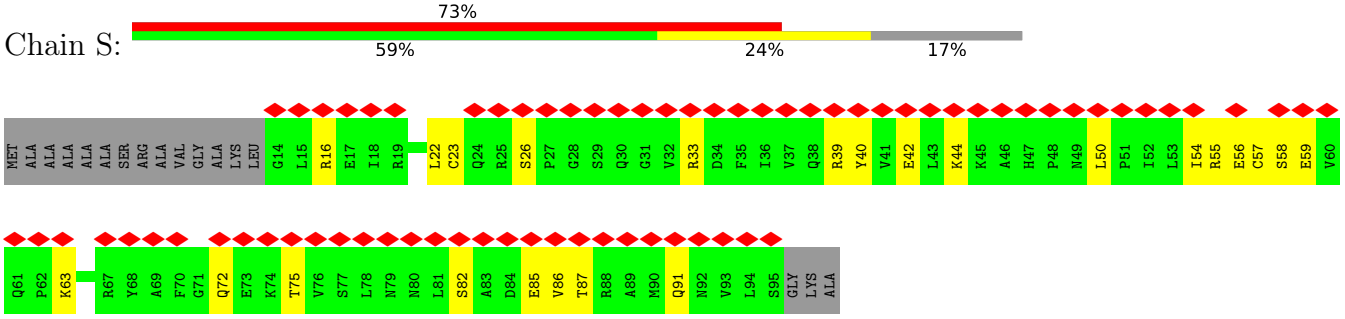
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain R:



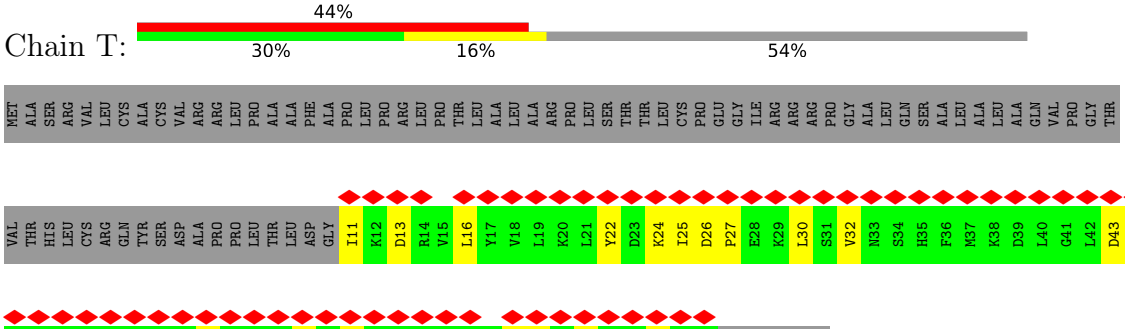
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain S:



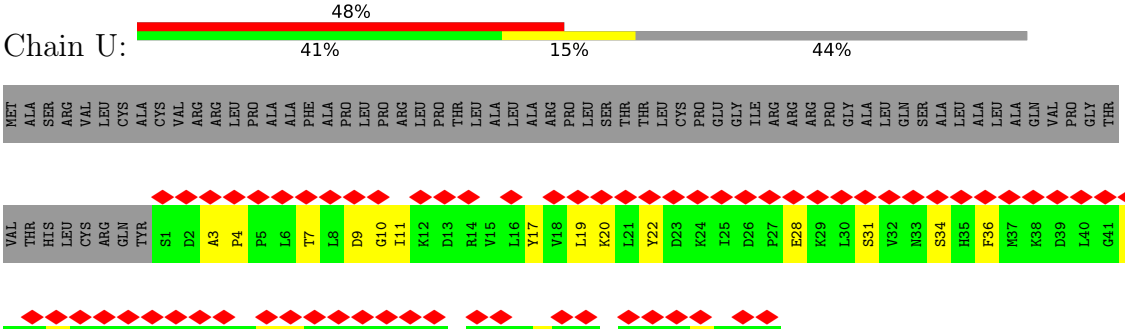
• Molecule 20: Acyl carrier protein, mitochondrial

Chain T:



• Molecule 20: Acyl carrier protein, mitochondrial

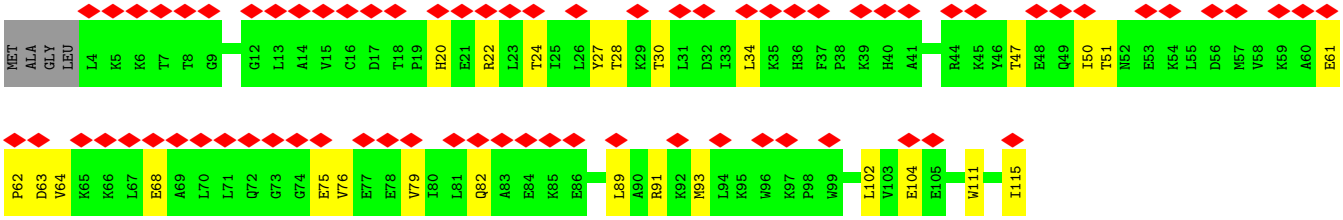
Chain U:



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

Chain V:

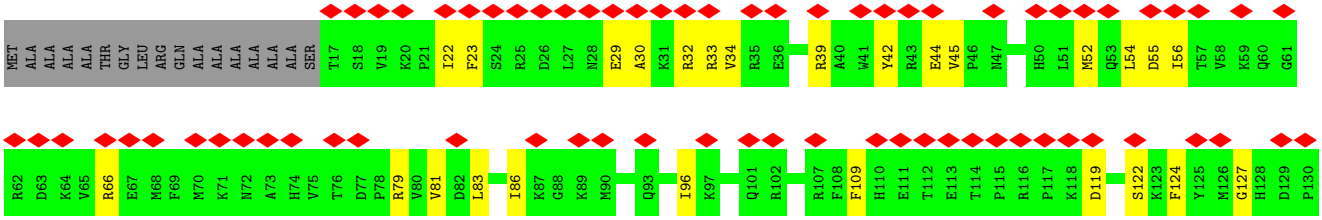




• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:

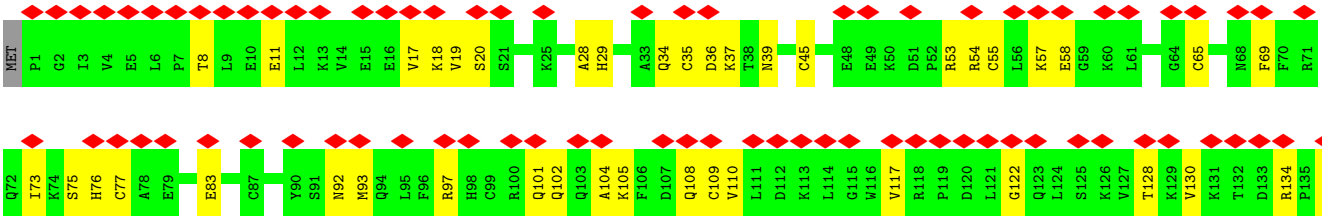


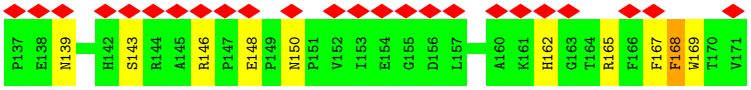


• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



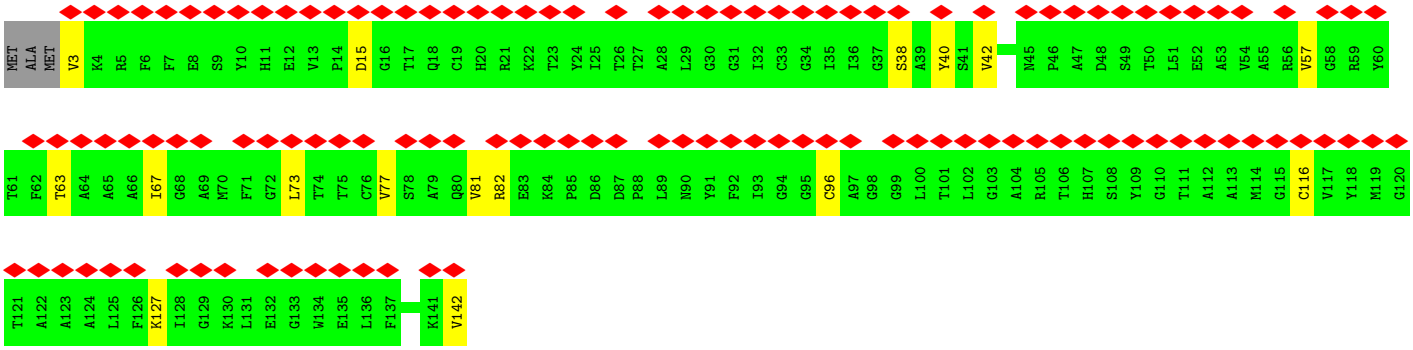




• Molecule 24: MCG5603

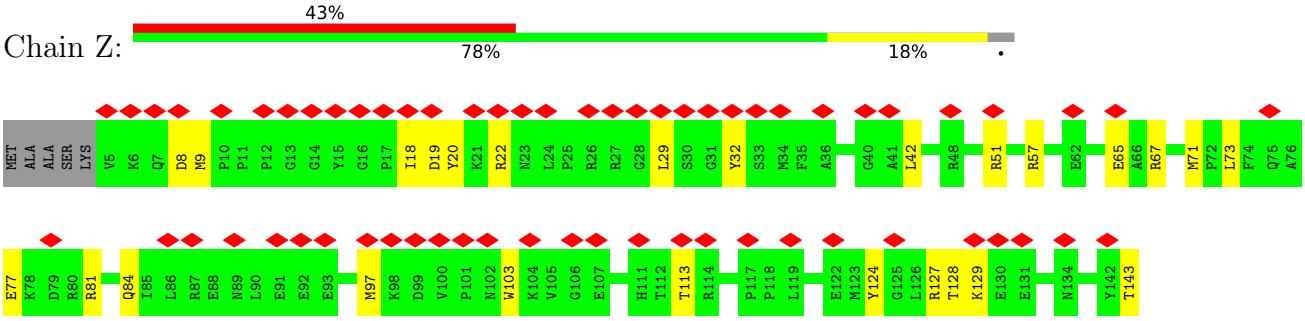
Chain Y:





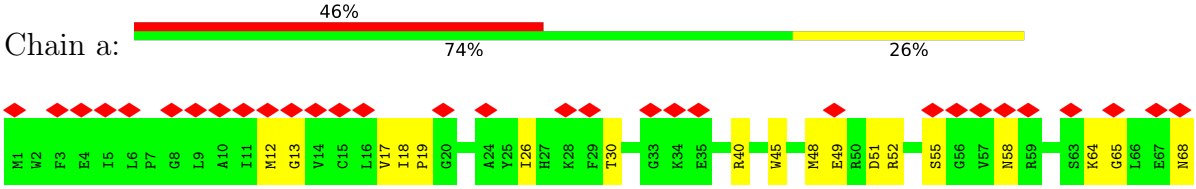
• Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:



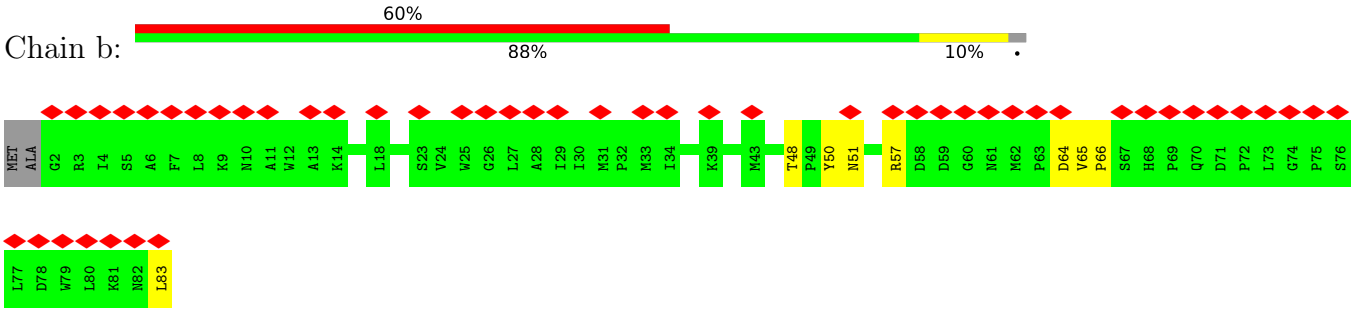
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain a:



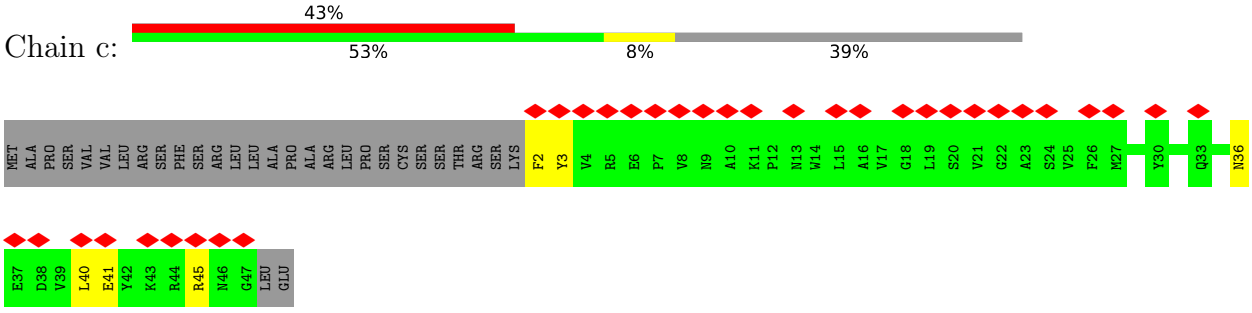
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:



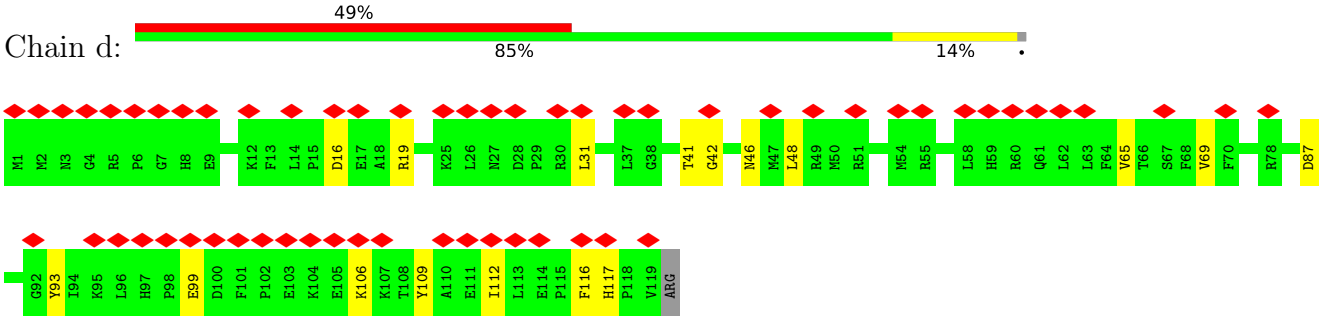
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain c:



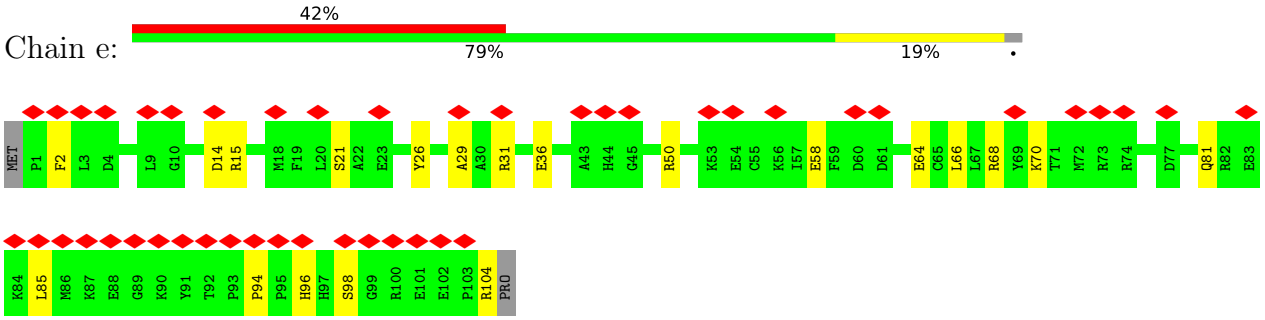
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain d:



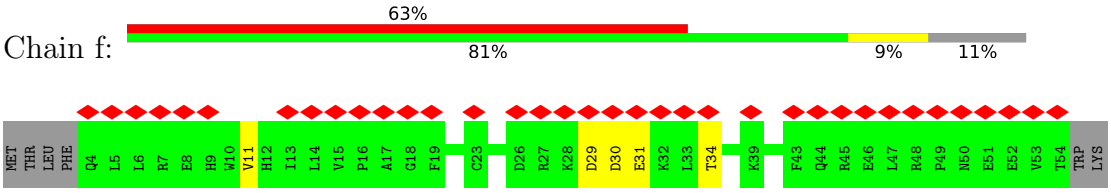
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:



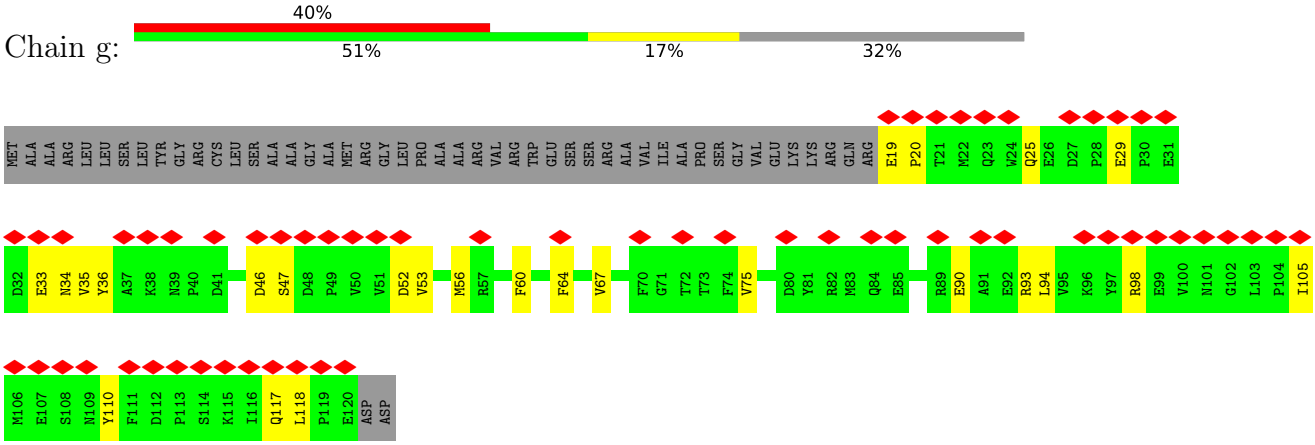
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:



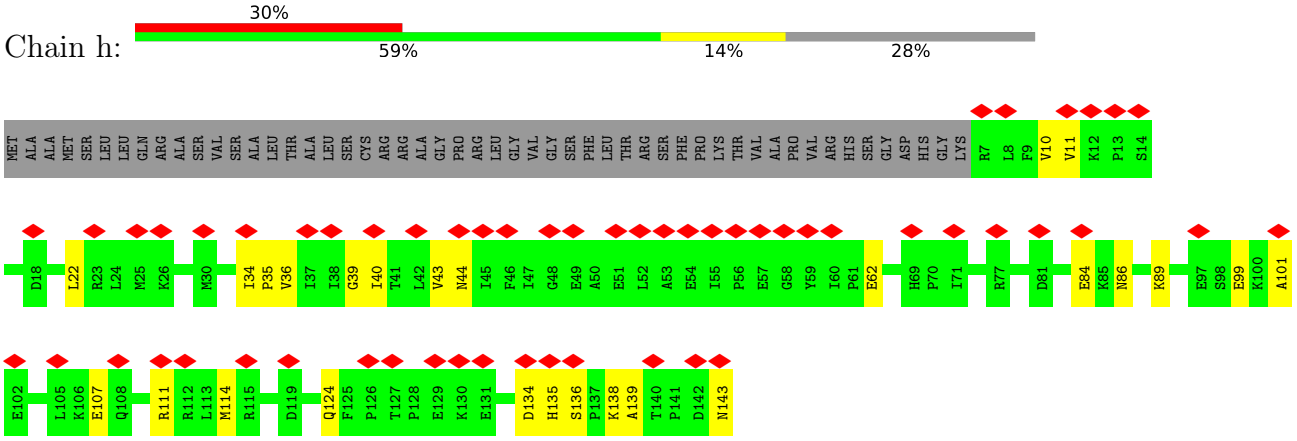
• Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain g:



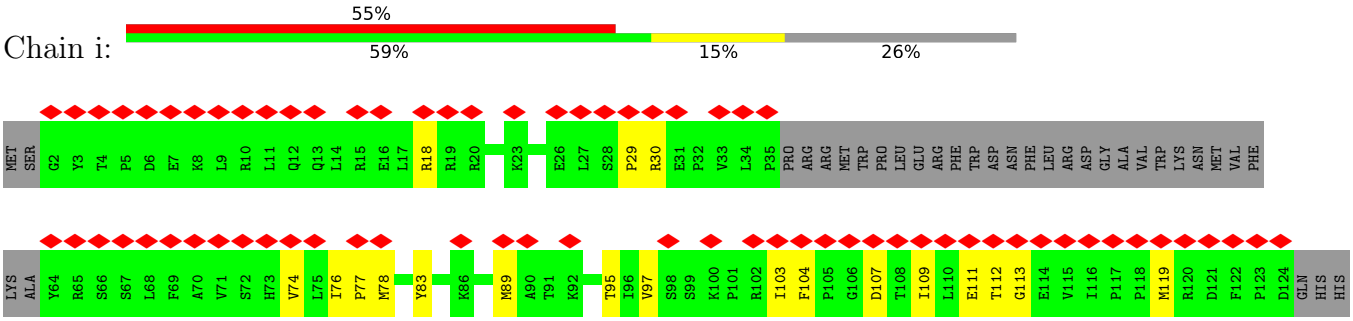
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h:



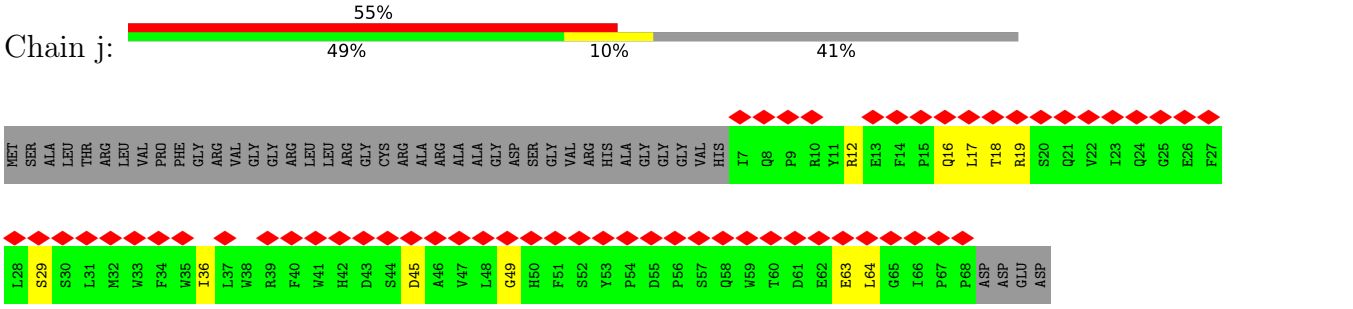
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i:



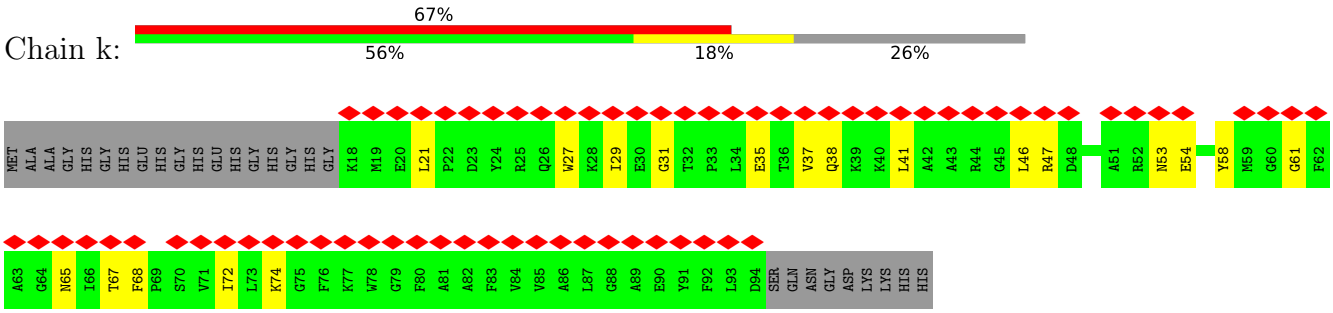
• Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain j:



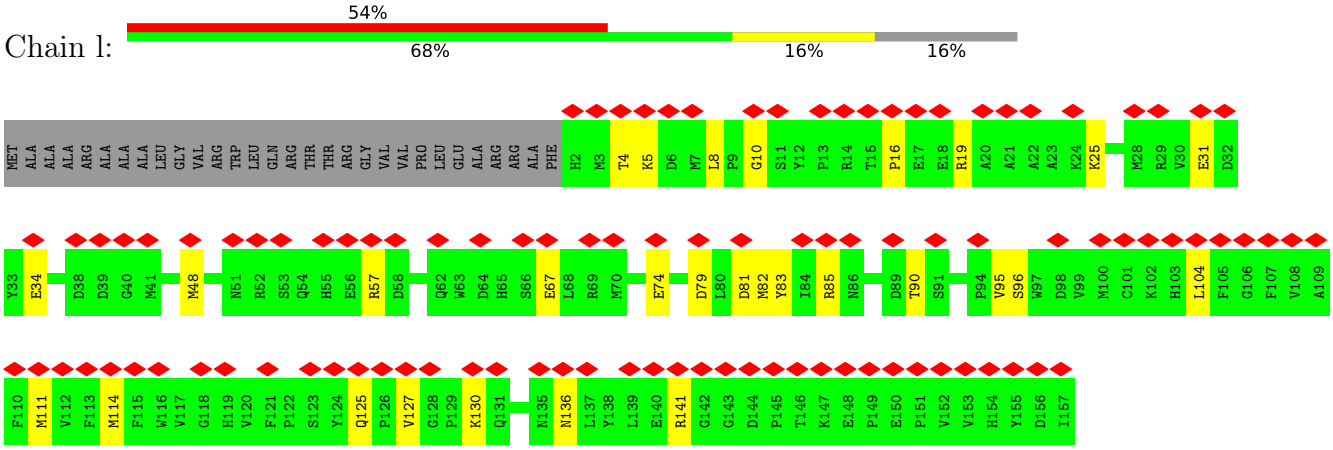
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain k:



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

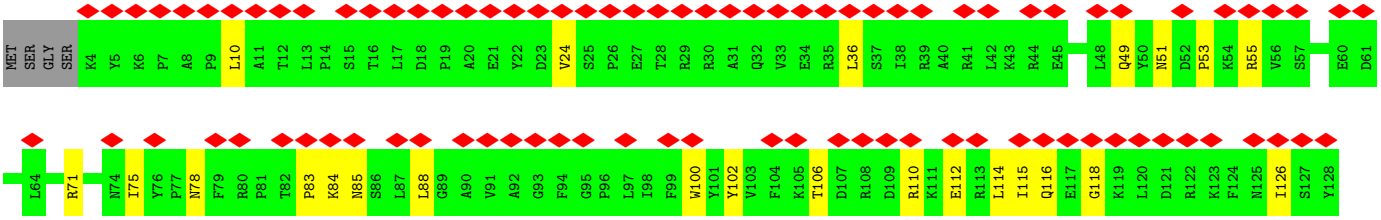
Chain l:



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

Chain m:

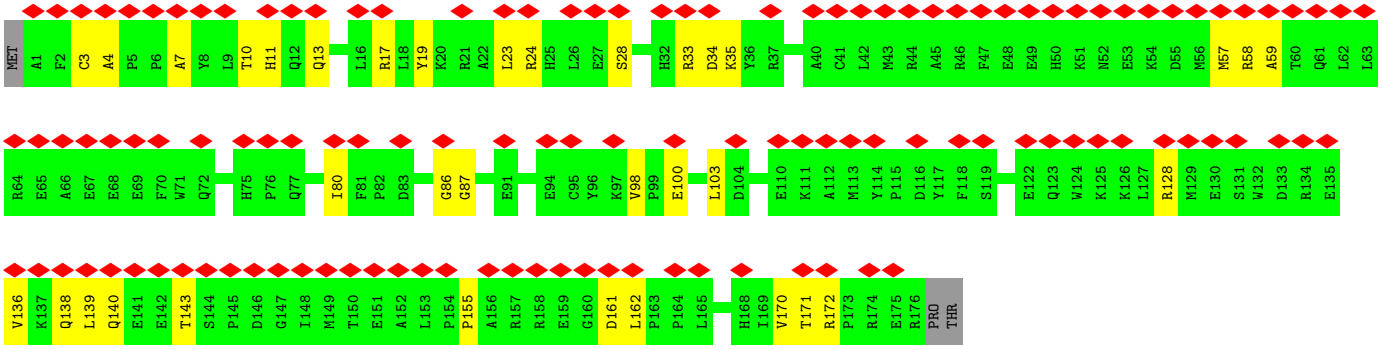




• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:

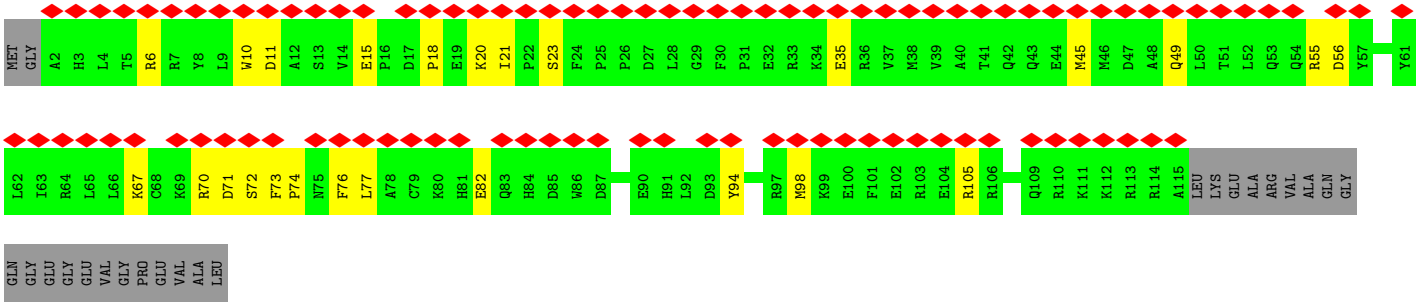




• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:

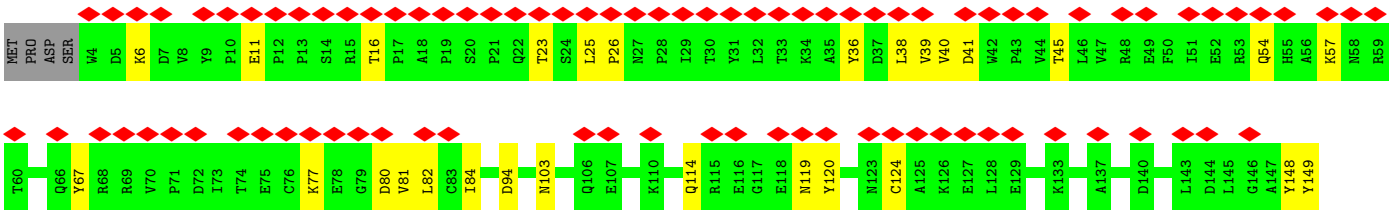


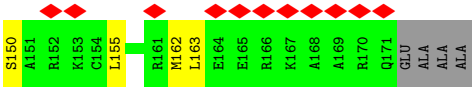


• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

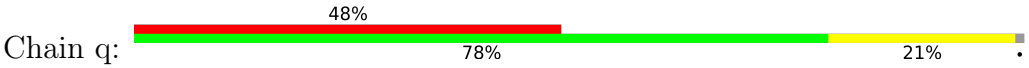
Chain p:

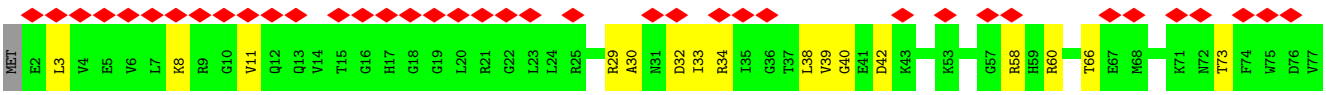


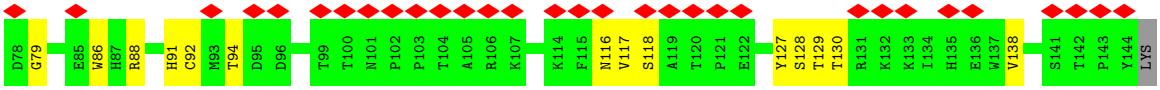




• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

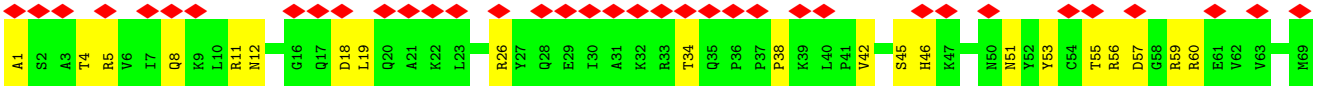


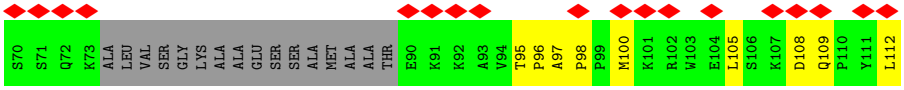




• Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7

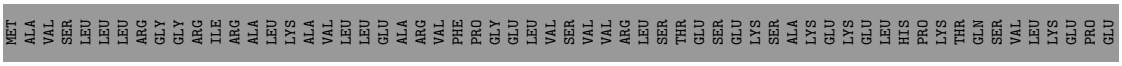


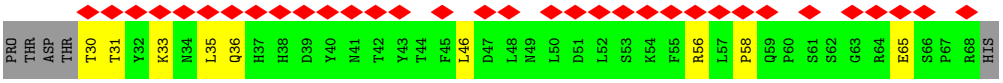




• Molecule 44: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	25629	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 ($e^-/Å^2$)	50.015	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.182	Depositor
Minimum map value	-0.046	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0268	Depositor
Map size (Å)	474.30002, 474.30002, 474.30002	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.054, 1.054, 1.054	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, FES, EHZ, AYA, FMN, ATP, CDL, PC1, 3PE, NDP, SF4, 2MR, FME

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	0.22	0/771	0.37	0/1054
2	B	0.32	0/1272	0.42	0/1722
3	C	0.28	0/1771	0.37	0/2412
4	D	0.28	0/3440	0.37	0/4656
5	E	0.20	0/1679	0.35	0/2288
6	F	0.22	0/3376	0.36	0/4561
7	G	0.25	0/5368	0.36	0/7273
8	H	0.25	0/2504	0.37	0/3420
9	I	0.33	0/1438	0.40	0/1946
10	J	0.21	0/1297	0.34	0/1764
11	K	0.23	0/738	0.32	0/1002
12	L	0.22	0/4913	0.36	0/6686
13	M	0.25	0/3709	0.37	0/5052
14	N	0.26	0/2748	0.36	0/3741
15	O	0.21	0/2666	0.34	0/3615
16	P	0.22	0/2329	0.38	0/3145
17	Q	0.24	0/1038	0.33	0/1401
18	R	0.24	0/751	0.34	0/1011
19	S	0.18	0/670	0.36	0/904
20	T	0.18	0/593	0.33	0/799
20	U	0.19	0/718	0.29	0/970
21	V	0.21	0/937	0.35	0/1270
22	W	0.22	0/993	0.38	0/1335
23	X	0.20	0/1434	0.36	0/1937
24	Y	0.19	0/1061	0.34	0/1439
25	Z	0.23	0/1183	0.36	0/1597
26	a	0.23	0/569	0.37	0/766
27	b	0.18	0/666	0.33	0/914
28	c	0.18	0/392	0.29	0/533
29	d	0.23	0/1017	0.33	0/1373
30	e	0.21	0/892	0.39	0/1187
31	f	0.18	0/443	0.34	0/596

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
32	g	0.21	0/887	0.34	0/1209
33	h	0.22	0/1188	0.35	0/1610
34	i	0.19	0/828	0.41	0/1125
35	j	0.17	0/561	0.34	0/768
36	k	0.16	0/646	0.37	0/873
37	l	0.19	0/1367	0.33	0/1866
38	m	0.21	0/1073	0.37	0/1455
39	n	0.20	0/1581	0.34	0/2140
40	o	0.17	0/1009	0.38	0/1355
41	p	0.22	0/1457	0.35	0/1969
42	q	0.23	0/1234	0.32	0/1681
43	r	0.21	0/786	0.37	0/1062
44	s	0.16	0/338	0.30	0/458
All	All	0.23	0/66331	0.36	0/89940

There are no bond length outliers.

There are no bond angle outliers.

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	761	0	813	30	0
2	B	1241	0	1250	30	0
3	C	1721	0	1680	61	0
4	D	3369	0	3316	90	0
5	E	1639	0	1631	37	0
6	F	3301	0	3252	68	0
7	G	5281	0	5311	127	0
8	H	2441	0	2518	84	0
9	I	1408	0	1344	58	0
10	J	1278	0	1292	45	0
11	K	737	0	768	26	0
12	L	4800	0	4985	149	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	M	3632	0	3853	128	0
14	N	2696	0	2895	86	0
15	O	2599	0	2552	64	0
16	P	2281	0	2305	63	0
17	Q	1015	0	1016	30	0
18	R	738	0	717	11	0
19	S	659	0	674	15	0
20	T	584	0	577	23	0
20	U	706	0	698	21	0
21	V	915	0	954	21	0
22	W	970	0	991	23	0
23	X	1396	0	1387	40	0
24	Y	1037	0	1022	11	0
25	Z	1152	0	1148	27	0
26	a	556	0	568	23	0
27	b	643	0	644	7	0
28	c	381	0	374	5	0
29	d	985	0	988	14	0
30	e	870	0	864	17	0
31	f	433	0	429	4	0
32	g	858	0	792	20	0
33	h	1153	0	1150	28	0
34	i	802	0	807	18	0
35	j	537	0	495	9	0
36	k	626	0	620	16	0
37	l	1312	0	1204	27	0
38	m	1044	0	1056	21	0
39	n	1527	0	1459	26	0
40	o	984	0	970	20	0
41	p	1424	0	1395	27	0
42	q	1192	0	1145	24	0
43	r	776	0	806	23	0
44	s	329	0	313	7	0
45	B	8	0	0	0	0
45	F	8	0	0	0	0
45	G	16	0	0	0	0
45	I	16	0	0	0	0
46	B	26	0	26	1	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	5	0
49	H	42	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	J	38	0	50	0	0
49	L	45	0	64	0	0
49	M	38	0	53	2	0
50	L	54	0	52	1	0
50	d	50	0	44	1	0
51	O	31	0	12	2	0
52	P	48	0	26	4	0
53	R	1	0	0	0	0
54	T	37	0	0	0	0
54	U	37	0	0	0	0
All	All	65323	0	65432	1451	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 11.

All (1451) 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)
26:a:64:LYS:CD	26:a:68:ASN:HD21	1.56	1.18
26:a:64:LYS:HD2	26:a:68:ASN:HD21	0.97	1.11
26:a:64:LYS:HD2	26:a:68:ASN:ND2	1.66	1.11
13:M:173:THR:HG23	33:h:101:ALA:HB2	1.46	0.95
2:B:187:TYR:O	16:P:102:ARG:NH1	2.01	0.94
14:N:20:THR:HG21	14:N:137:ALA:HB1	1.48	0.94
34:i:18:ARG:NH2	39:n:172:ARG:O	2.01	0.93
13:M:46:ASP:OD2	41:p:67:TYR:OH	1.89	0.90
9:I:17:LYS:NZ	9:I:21:ASP:OD2	2.05	0.90
8:H:24:GLU:OE1	8:H:228:TYR:OH	1.90	0.89
42:q:60:ARG:NH1	42:q:92:CYS:SG	2.47	0.88
17:Q:33:ARG:NH1	17:Q:60:ASP:O	2.07	0.88
7:G:548:HIS:O	7:G:549:HIS:ND1	2.08	0.87
29:d:106:LYS:O	41:p:77:LYS:NZ	2.07	0.86
5:E:104:THR:OG1	6:F:349:ARG:NH1	2.09	0.85
2:B:37:GLU:OE2	2:B:188:ARG:NH2	2.10	0.84
13:M:244:ILE:O	41:p:148:TYR:OH	1.94	0.84
25:Z:20:TYR:OH	43:r:108:ASP:OD2	1.94	0.84
13:M:452:LYS:NZ	49:M:501:3PE:O12	2.10	0.84
31:f:31:GLU:O	31:f:34:THR:OG1	1.95	0.83
20:U:7:THR:OG1	20:U:9:ASP:OD1	1.95	0.83
34:i:89:MET:O	34:i:95:THR:OG1	1.97	0.83
25:Z:84:GLN:OE1	30:e:104:ARG:NH1	2.12	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:233:ARG:NH2	9:I:25:ARG:O	2.12	0.82
10:J:2:ASN:OD1	10:J:3:ASN:ND2	2.13	0.82
12:L:282:ALA:O	12:L:285:THR:OG1	1.96	0.82
7:G:359:ARG:NH2	7:G:504:ASP:OD1	2.12	0.82
8:H:307:LEU:O	8:H:311:THR:OG1	1.97	0.82
37:l:81:ASP:OD2	38:m:71:ARG:NH1	2.13	0.81
8:H:31:MET:HE1	8:H:272:TRP:CD1	2.15	0.81
5:E:101:GLN:NE2	5:E:155:GLN:OE1	2.14	0.81
7:G:445:ASP:O	7:G:447:LYS:NZ	2.14	0.81
3:C:191:ALA:O	17:Q:74:SER:OG	1.98	0.81
12:L:594:ASN:ND2	24:Y:40:TYR:OH	2.13	0.81
7:G:140:LYS:NZ	7:G:182:GLN:OE1	2.15	0.80
7:G:229:ASP:OD1	7:G:230:VAL:N	2.16	0.80
15:O:52:PRO:O	15:O:107:GLN:NE2	2.14	0.80
14:N:258:THR:OG1	14:N:333:SER:O	1.98	0.79
3:C:194:PHE:O	17:Q:81:ASN:ND2	2.16	0.79
40:o:49:GLN:OE1	41:p:119:ASN:ND2	2.15	0.79
1:A:73:LEU:O	8:H:160:TYR:OH	2.01	0.79
12:L:396:ILE:O	12:L:400:ASN:ND2	2.16	0.78
15:O:309:ASN:ND2	28:c:3:TYR:OH	2.16	0.78
5:E:131:THR:OG1	5:E:137:PHE:O	2.01	0.78
16:P:128:ARG:NH1	16:P:218:THR:O	2.16	0.78
30:e:31:ARG:NH2	30:e:66:LEU:O	2.17	0.78
3:C:113:GLU:OE1	3:C:163:ARG:NH2	2.16	0.78
7:G:476:LYS:O	7:G:480:THR:HG23	1.84	0.78
2:B:172:GLN:NE2	42:q:118:SER:OG	2.16	0.78
6:F:358:SER:OG	6:F:365:CYS:SG	2.41	0.78
12:L:364:LYS:NZ	36:k:61:GLY:O	2.15	0.78
8:H:169:GLN:NE2	8:H:241:ILE:O	2.17	0.78
12:L:226:GLN:HA	12:L:284:THR:HG21	1.66	0.77
12:L:173:LEU:HD13	13:M:405:MET:HE3	1.66	0.77
15:O:65:ASP:OD1	28:c:2:PHE:N	2.17	0.77
19:S:26:SER:O	19:S:33:ARG:NH2	2.18	0.77
32:g:46:ASP:OD1	32:g:47:SER:N	2.18	0.77
7:G:620:ARG:NH1	7:G:633:TYR:OH	2.17	0.77
34:i:107:ASP:OD2	40:o:70:ARG:NH2	2.17	0.77
6:F:98:ASP:O	48:F:501:FMN:N3	2.18	0.77
15:O:25:ILE:HD11	15:O:48:MET:HE1	1.64	0.77
6:F:132:ARG:NH2	44:s:58:PRO:O	2.18	0.76
7:G:140:LYS:O	7:G:148:THR:OG1	2.04	0.76
13:M:329:LEU:HD23	13:M:437:MET:HE3	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:35:CYS:SG	23:X:65:CYS:HB3	2.26	0.76
26:a:64:LYS:HB3	26:a:68:ASN:ND2	1.99	0.76
41:p:120:TYR:O	41:p:124:CYS:HB3	1.86	0.75
3:C:205:ALA:O	43:r:60:ARG:NH1	2.19	0.75
12:L:237:MET:O	12:L:299:LYS:NZ	2.20	0.75
38:m:49:GLN:O	38:m:55:ARG:NH1	2.18	0.75
4:D:152:MET:SD	4:D:174:ARG:NH2	2.59	0.75
6:F:302:SER:OG	6:F:354:TYR:OH	2.00	0.75
8:H:283:ASP:OD1	8:H:284:GLN:N	2.19	0.75
5:E:115:SER:O	5:E:119:THR:HG23	1.87	0.75
15:O:83:TYR:HH	51:O:401:ATP:HO2'	0.77	0.75
6:F:84:LYS:O	6:F:91:LYS:NZ	2.18	0.75
13:M:168:GLN:NE2	13:M:172:GLY:O	2.19	0.75
16:P:212:LYS:O	16:P:216:ASN:ND2	2.20	0.75
7:G:372:GLU:O	7:G:402:ASN:ND2	2.19	0.75
13:M:300:SER:O	13:M:308:SER:OG	2.04	0.74
20:U:85:ASP:OD1	34:i:18:ARG:NH1	2.19	0.74
34:i:112:THR:HG23	34:i:113:GLY:H	1.53	0.74
7:G:325:ALA:HA	7:G:328:LEU:HD12	1.69	0.74
40:o:15:GLU:OE2	40:o:105:ARG:NH1	2.20	0.74
3:C:66:ASP:O	21:V:82:GLN:NE2	2.21	0.74
7:G:546:GLN:NE2	7:G:596:ASP:OD1	2.20	0.74
12:L:19:ILE:O	12:L:22:SER:OG	2.03	0.74
3:C:193:GLU:OE1	7:G:223:ARG:NH2	2.20	0.74
8:H:142:TYR:HE2	8:H:285:LEU:HD21	1.53	0.74
15:O:31:ILE:HD11	15:O:183:ILE:HD11	1.69	0.73
3:C:155:TYR:OH	4:D:79:HIS:ND1	2.20	0.73
7:G:31:GLU:OE2	7:G:39:ARG:NH2	2.21	0.73
7:G:213:TYR:O	7:G:216:THR:OG1	2.04	0.73
7:G:339:ASP:OD2	19:S:16:ARG:NH2	2.22	0.73
30:e:94:PRO:O	30:e:98:SER:OG	2.03	0.73
11:K:50:ASN:OD1	30:e:31:ARG:NH1	2.20	0.73
34:i:107:ASP:OD1	40:o:67:LYS:NZ	2.17	0.73
3:C:165:ASP:OD1	3:C:166:PHE:N	2.21	0.73
12:L:501:ALA:O	12:L:505:ASN:ND2	2.21	0.73
20:U:22:TYR:OH	20:U:46:ASP:OD2	2.06	0.72
2:B:80:ASP:OD2	8:H:34:ARG:NH2	2.21	0.72
12:L:361:ASN:O	12:L:365:ILE:HG22	1.88	0.72
39:n:139:LEU:O	39:n:143:THR:N	2.22	0.72
7:G:24:THR:HG22	7:G:25:THR:H	1.53	0.72
29:d:99:GLU:OE1	29:d:99:GLU:N	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:145:GLU:N	6:F:145:GLU:OE1	2.22	0.72
15:O:223:TYR:CE2	15:O:234:VAL:HG22	2.24	0.72
15:O:267:THR:O	15:O:271:ASN:ND2	2.22	0.72
12:L:386:LEU:O	12:L:387:THR:OG1	2.08	0.72
15:O:28:ASP:OD2	15:O:29:GLY:N	2.23	0.72
12:L:22:SER:HA	12:L:27:ILE:HD11	1.70	0.71
38:m:51:ASN:O	39:n:128:ARG:NH2	2.22	0.71
2:B:52:ARG:NH1	46:B:202:PC1:O12	2.22	0.71
12:L:295:GLN:NE2	12:L:524:THR:O	2.24	0.71
13:M:200:MET:HE1	13:M:246:ILE:HG23	1.72	0.71
32:g:110:TYR:OH	41:p:94:ASP:OD2	2.08	0.71
7:G:126:ASP:OD2	43:r:56:ARG:NH2	2.24	0.71
33:h:84:GLU:N	33:h:84:GLU:OE1	2.22	0.71
39:n:34:ASP:OD1	39:n:35:LYS:N	2.24	0.71
3:C:78:LEU:HD23	3:C:79:THR:N	2.05	0.71
16:P:236:TYR:OH	16:P:311:GLU:OE2	2.05	0.71
23:X:165:ARG:NH1	29:d:87:ASP:OD1	2.24	0.71
8:H:195:ARG:NH2	8:H:227:GLU:OE2	2.23	0.71
8:H:24:GLU:OE2	8:H:274:ARG:NH1	2.24	0.71
13:M:88:ASN:OD1	13:M:89:ASN:N	2.24	0.71
14:N:27:MET:HE1	14:N:71:LEU:HD11	1.72	0.71
6:F:199:LYS:NZ	17:Q:130:VAL:O	2.19	0.70
4:D:302:GLU:OE2	9:I:3:LYS:NZ	2.23	0.70
5:E:119:THR:HG21	5:E:166:PRO:HB3	1.72	0.70
6:F:189:GLU:OE1	6:F:206:LYS:NZ	2.24	0.70
7:G:98:LEU:HD21	7:G:116:LEU:HD11	1.73	0.70
8:H:4:ILE:O	8:H:8:THR:HG23	1.92	0.70
7:G:21:GLU:O	7:G:24:THR:OG1	2.05	0.70
9:I:97:GLU:OE1	9:I:109:THR:OG1	2.09	0.70
23:X:139:ASN:OD1	23:X:143:SER:N	2.24	0.70
25:Z:57:ARG:HH21	27:b:48:THR:HG21	1.55	0.70
33:h:136:SER:O	33:h:138:LYS:NZ	2.25	0.70
40:o:71:ASP:O	40:o:72:SER:OG	2.08	0.70
12:L:72:ASN:HB3	13:M:459:MET:HE1	1.73	0.70
14:N:1:FME:O	15:O:258:TYR:OH	2.09	0.70
9:I:116:THR:HG21	9:I:146:HIS:NE2	2.06	0.70
21:V:34:LEU:HD11	21:V:47:THR:HG23	1.74	0.70
44:s:65:GLU:OE1	44:s:65:GLU:N	2.24	0.70
20:T:47:GLN:NE2	20:T:67:ALA:O	2.26	0.69
9:I:64:ARG:NH1	9:I:121:CYS:O	2.25	0.69
13:M:310:MET:CE	13:M:459:MET:HE3	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:245:ALA:O	12:L:249:SER:OG	2.08	0.69
14:N:158:ALA:O	14:N:161:SER:OG	2.08	0.69
43:r:18:ASP:OD1	43:r:19:LEU:N	2.26	0.69
7:G:156:CYS:O	7:G:157:THR:OG1	2.09	0.69
9:I:81:ALA:O	9:I:106:ARG:NH2	2.25	0.69
15:O:281:GLU:N	15:O:281:GLU:OE1	2.26	0.69
20:T:24:LYS:NZ	20:T:46:ASP:OD1	2.24	0.69
22:W:83:LEU:HA	22:W:86:ILE:HD12	1.73	0.69
3:C:32:ILE:HG22	3:C:33:LEU:CD1	2.23	0.69
4:D:143:GLU:OE2	4:D:278:TYR:OH	2.06	0.69
7:G:229:ASP:OD1	7:G:231:MET:N	2.25	0.69
13:M:75:LEU:HD23	13:M:440:HIS:NE2	2.07	0.69
20:U:55:GLU:OE1	39:n:24:ARG:NH2	2.25	0.69
3:C:159:GLY:O	3:C:160:HIS:ND1	2.26	0.69
12:L:387:THR:OG1	12:L:461:SER:O	2.10	0.69
15:O:257:HIS:NE2	15:O:261:MET:SD	2.66	0.69
26:a:52:ARG:NH2	26:a:58:ASN:OD1	2.26	0.69
3:C:49:GLU:OE2	3:C:106:ARG:NH1	2.25	0.68
17:Q:54:LYS:NZ	21:V:115:ILE:O	2.26	0.68
13:M:310:MET:HE1	13:M:459:MET:HE3	1.74	0.68
9:I:58:PRO:O	9:I:59:LEU:HD23	1.94	0.68
13:M:269:MET:SD	13:M:399:ASN:ND2	2.67	0.68
15:O:58:TYR:O	15:O:62:THR:HG23	1.92	0.68
26:a:64:LYS:CG	26:a:68:ASN:HD21	2.06	0.68
7:G:389:PRO:O	7:G:392:ASN:N	2.26	0.68
10:J:21:LEU:HD11	10:J:91:PHE:HD2	1.58	0.68
10:J:22:LYS:NZ	11:K:21:MET:O	2.27	0.68
12:L:502:LEU:O	12:L:506:ASN:ND2	2.26	0.68
5:E:142:VAL:HG22	5:E:143:GLU:H	1.59	0.68
18:R:60:ASP:OD1	18:R:61:GLY:N	2.26	0.68
9:I:109:THR:O	42:q:129:THR:OG1	2.06	0.68
9:I:114:ASP:OD1	9:I:116:THR:OG1	2.05	0.68
2:B:94:ASP:OD1	8:H:58:LYS:NZ	2.23	0.67
7:G:46:LEU:HD11	7:G:202:ILE:HD11	1.74	0.67
7:G:379:LEU:HD23	7:G:452:VAL:CG1	2.24	0.67
12:L:221:THR:CG2	12:L:280:LEU:HD21	2.23	0.67
19:S:54:ILE:O	19:S:55:ARG:NH2	2.27	0.67
23:X:57:LYS:NZ	23:X:58:GLU:OE2	2.21	0.67
6:F:30:ASP:OD1	6:F:31:TRP:N	2.28	0.67
6:F:342:ASP:OD2	6:F:429:ARG:NH2	2.27	0.67
7:G:283:MET:HE3	7:G:293:TYR:HE1	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:64:LYS:CD	26:a:68:ASN:ND2	2.40	0.67
15:O:236:GLU:OE2	21:V:91:ARG:NH2	2.28	0.67
12:L:150:MET:HE3	50:L:702:CDL:H721	1.77	0.67
12:L:377:SER:O	12:L:381:THR:HG23	1.95	0.67
13:M:16:TRP:O	13:M:93:LYS:NZ	2.28	0.67
18:R:74:ASN:OD1	18:R:75:LEU:N	2.27	0.67
7:G:231:MET:HE3	7:G:677:ILE:HD12	1.75	0.67
23:X:104:ALA:O	23:X:108:GLN:NE2	2.28	0.67
1:A:49:LEU:HD12	1:A:50:PRO:HD2	1.77	0.66
10:J:25:LEU:HD13	10:J:71:THR:HG21	1.77	0.66
4:D:54:GLN:NE2	8:H:203:GLY:O	2.29	0.66
12:L:72:ASN:O	12:L:73:SER:OG	2.11	0.66
6:F:359:CYS:SG	6:F:360:GLY:N	2.67	0.66
14:N:58:LYS:NZ	14:N:117:GLU:OE1	2.20	0.66
7:G:276:ARG:NH1	7:G:680:ALA:O	2.29	0.66
17:Q:49:VAL:HG12	17:Q:49:VAL:O	1.95	0.66
29:d:93:TYR:CD2	33:h:114:MET:HE3	2.30	0.66
39:n:10:THR:N	39:n:13:GLN:OE1	2.28	0.66
2:B:172:GLN:NE2	42:q:116:ASN:OD1	2.28	0.66
14:N:317:GLN:HE22	15:O:106:LEU:HD21	1.59	0.66
15:O:80:GLU:N	15:O:80:GLU:OE1	2.28	0.66
4:D:151:ILE:HG13	4:D:304:MET:HE2	1.78	0.66
10:J:36:GLY:HA2	11:K:38:LEU:HD21	1.76	0.66
16:P:166:ILE:HG22	16:P:168:PRO:HD3	1.78	0.66
40:o:82:GLU:N	40:o:82:GLU:OE1	2.29	0.66
20:T:32:VAL:O	20:T:74:GLN:N	2.28	0.65
12:L:109:HIS:O	12:L:110:SER:OG	2.08	0.65
15:O:30:ASN:O	15:O:35:LYS:NZ	2.29	0.65
42:q:32:ASP:OD2	42:q:34:ARG:N	2.28	0.65
9:I:44:PHE:O	43:r:11:ARG:NH2	2.28	0.65
1:A:55:PHE:HB2	10:J:73:MET:HE1	1.78	0.65
2:B:139:SER:OG	4:D:85:2MR:O	2.13	0.65
5:E:24:THR:OG1	5:E:27:ASN:ND2	2.30	0.65
19:S:57:CYS:SG	19:S:58:SER:N	2.68	0.65
40:o:35:GLU:OE1	40:o:35:GLU:N	2.28	0.65
3:C:8:ARG:NH2	43:r:55:THR:O	2.27	0.65
6:F:96:ASN:ND2	48:F:501:FMN:O3'	2.28	0.65
7:G:522:LEU:HB2	7:G:543:ILE:HG22	1.77	0.65
12:L:433:THR:OG1	12:L:436:ARG:NH1	2.30	0.65
36:k:58:TYR:OH	39:n:34:ASP:OD2	2.15	0.65
12:L:62:MET:SD	12:L:199:GLN:NE2	2.69	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:MET:SD	1:A:88:MET:N	2.70	0.64
9:I:134:VAL:HG21	9:I:167:ILE:HG21	1.77	0.64
12:L:228:GLY:C	12:L:229:LEU:HD12	2.22	0.64
17:Q:33:ARG:NH2	17:Q:77:ASP:OD2	2.31	0.64
43:r:109:GLN:NE2	43:r:112:LEU:O	2.30	0.64
32:g:98:ARG:NH1	32:g:105:ILE:O	2.30	0.64
3:C:130:TYR:O	3:C:134:VAL:HG23	1.97	0.64
7:G:231:MET:CE	7:G:677:ILE:HD12	2.27	0.64
7:G:533:THR:HA	7:G:556:MET:HE3	1.78	0.64
14:N:106:LEU:HD21	14:N:138:PRO:HB2	1.79	0.64
27:b:64:ASP:OD1	27:b:65:VAL:N	2.30	0.64
5:E:110:LEU:HD11	6:F:260:GLY:HA2	1.79	0.64
15:O:240:TYR:OH	21:V:22:ARG:NH2	2.30	0.64
37:l:82:MET:HE3	37:l:83:TYR:CZ	2.33	0.64
35:j:16:GLN:NE2	35:j:17:LEU:O	2.30	0.64
19:S:23:CYS:SG	19:S:59:GLU:N	2.69	0.64
39:n:138:GLN:NE2	39:n:155:PRO:O	2.31	0.64
3:C:100:ARG:O	43:r:100:MET:N	2.31	0.64
9:I:121:CYS:SG	9:I:122:GLY:N	2.71	0.64
12:L:86:SER:O	12:L:90:THR:HG23	1.98	0.63
13:M:408:MET:HE2	13:M:408:MET:HA	1.80	0.63
17:Q:89:LYS:NZ	17:Q:107:GLU:OE2	2.31	0.63
42:q:42:ASP:OD1	42:q:86:TRP:NE1	2.32	0.63
16:P:313:LYS:O	16:P:317:VAL:HG23	1.98	0.63
6:F:378:ARG:NH1	7:G:132:GLU:OE2	2.31	0.63
14:N:57:THR:O	14:N:61:VAL:HG23	1.99	0.63
12:L:400:ASN:OD1	12:L:486:LEU:HD22	1.99	0.63
13:M:121:LEU:O	13:M:125:THR:HG23	1.99	0.63
32:g:90:GLU:OE2	32:g:93:ARG:NH1	2.32	0.63
15:O:178:GLU:OE2	15:O:182:ARG:NH2	2.31	0.63
26:a:64:LYS:CB	26:a:68:ASN:ND2	2.62	0.63
43:r:51:ASN:OD1	43:r:56:ARG:NH1	2.32	0.63
1:A:90:MET:HE3	10:J:149:THR:HB	1.81	0.63
5:E:190:ARG:NE	5:E:194:GLU:O	2.32	0.63
1:A:12:LEU:O	1:A:16:THR:HG23	1.98	0.62
12:L:359:MET:O	12:L:436:ARG:NH2	2.31	0.62
30:e:31:ARG:O	33:h:143:ASN:ND2	2.32	0.62
9:I:71:ARG:NH1	9:I:75:GLY:O	2.32	0.62
37:l:79:ASP:HB3	37:l:82:MET:HE2	1.81	0.62
13:M:346:ARG:NH1	37:l:67:GLU:OE1	2.32	0.62
15:O:70:ASP:OD1	15:O:71:ILE:N	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:8:SER:O	13:M:104:ILE:HD11	2.00	0.62
16:P:177:ARG:NH2	52:P:501:NDP:O2N	2.31	0.62
23:X:35:CYS:O	23:X:39:ASN:ND2	2.32	0.62
33:h:62:GLU:OE1	33:h:62:GLU:N	2.32	0.62
4:D:179:GLU:OE1	43:r:26:ARG:NH2	2.31	0.62
7:G:13:VAL:O	7:G:16:GLN:N	2.32	0.62
44:s:30:THR:OG1	44:s:31:THR:N	2.32	0.62
1:A:65:PHE:CE1	8:H:294:LEU:HD21	2.34	0.62
12:L:72:ASN:CB	13:M:459:MET:HE1	2.30	0.62
5:E:150:ASN:OD1	5:E:190:ARG:NH1	2.31	0.62
3:C:77:ASP:OD2	3:C:78:LEU:N	2.33	0.62
32:g:33:GLU:N	32:g:33:GLU:OE1	2.33	0.62
12:L:568:THR:O	12:L:572:ASN:ND2	2.32	0.61
13:M:173:THR:HG23	33:h:101:ALA:CB	2.26	0.61
14:N:240:MET:SD	29:d:48:LEU:HD22	2.41	0.61
23:X:162:HIS:NE2	33:h:99:GLU:OE1	2.31	0.61
10:J:115:ILE:HD12	10:J:117:LEU:HD21	1.81	0.61
12:L:71:MET:CE	13:M:314:MET:HE1	2.30	0.61
15:O:138:MET:HB3	15:O:144:ILE:HD12	1.83	0.61
15:O:210:PHE:HE1	15:O:214:MET:HE2	1.65	0.61
32:g:34:ASN:OD1	32:g:36:TYR:N	2.33	0.61
11:K:59:ILE:CG2	14:N:27:MET:HE2	2.30	0.61
12:L:399:ILE:CD1	12:L:412:THR:HG21	2.31	0.61
14:N:20:THR:CG2	14:N:137:ALA:HB1	2.27	0.61
15:O:231:PRO:O	15:O:234:VAL:N	2.32	0.61
42:q:88:ARG:HE	42:q:94:THR:HG21	1.66	0.61
25:Z:81:ARG:NH1	25:Z:124:TYR:OH	2.33	0.61
6:F:147:SER:O	6:F:151:VAL:HG23	2.01	0.61
6:F:380:VAL:O	6:F:429:ARG:NH1	2.33	0.61
8:H:177:PRO:HA	25:Z:42:LEU:HD12	1.82	0.61
12:L:237:MET:HE2	12:L:237:MET:N	2.15	0.61
14:N:214:PRO:HB2	14:N:247:MET:HE1	1.82	0.61
7:G:103:LEU:HD12	7:G:103:LEU:N	2.16	0.61
21:V:24:THR:O	21:V:28:THR:HG23	2.01	0.61
12:L:154:LEU:HD12	12:L:247:LEU:HD11	1.83	0.61
20:T:75:GLU:OE1	20:T:75:GLU:N	2.34	0.61
36:k:29:ILE:O	36:k:29:ILE:HG22	2.00	0.61
25:Z:57:ARG:NH2	27:b:48:THR:HG21	2.16	0.60
12:L:296:ASN:OD1	12:L:357:ARG:NE	2.32	0.60
41:p:41:ASP:OD1	41:p:45:THR:OG1	2.19	0.60
12:L:371:SER:OG	36:k:74:LYS:NZ	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:90:ASP:OD2	15:O:95:ARG:NH2	2.34	0.60
20:U:3:ALA:HB1	20:U:4:PRO:HD2	1.83	0.60
23:X:101:GLN:NE2	23:X:102:GLN:OE1	2.34	0.60
4:D:203:LEU:HD22	4:D:207:LEU:CD2	2.31	0.60
6:F:30:ASP:OD1	6:F:32:ARG:N	2.34	0.60
6:F:305:PRO:HG2	6:F:327:THR:HG22	1.83	0.60
3:C:112:ASP:OD1	3:C:113:GLU:N	2.35	0.60
12:L:193:MET:HE3	12:L:204:SER:OG	2.02	0.60
15:O:163:TYR:OH	15:O:269:VAL:HG13	2.02	0.60
4:D:238:ARG:NH2	4:D:412:ALA:O	2.34	0.60
7:G:52:CYS:SG	7:G:53:ARG:N	2.73	0.60
8:H:307:LEU:HD12	8:H:310:PHE:CZ	2.36	0.60
12:L:54:PHE:O	12:L:58:ASN:N	2.34	0.60
8:H:293:PHE:O	8:H:297:THR:OG1	2.16	0.60
13:M:296:LEU:CD2	13:M:396:MET:HE1	2.32	0.60
3:C:147:ASP:OD2	3:C:149:ARG:NH2	2.35	0.59
10:J:131:VAL:O	25:Z:67:ARG:NH1	2.34	0.59
7:G:197:GLY:O	7:G:268:ARG:NH2	2.34	0.59
8:H:185:TRP:CD1	8:H:238:THR:HG22	2.37	0.59
16:P:75:ALA:HB1	16:P:113:ILE:CD1	2.32	0.59
7:G:591:GLY:HA2	16:P:6:ILE:HG21	1.85	0.59
7:G:594:ARG:NH2	22:W:124:PHE:O	2.35	0.59
12:L:12:PHE:O	12:L:16:LEU:HD23	2.02	0.59
12:L:399:ILE:HD13	12:L:412:THR:HG21	1.84	0.59
13:M:176:LEU:O	13:M:177:MET:HG2	2.01	0.59
19:S:63:LYS:NZ	19:S:75:THR:OG1	2.34	0.59
20:T:22:TYR:OH	20:T:49:GLU:OE1	2.11	0.59
20:U:31:SER:N	20:U:34:SER:OG	2.34	0.59
13:M:419:LEU:HD12	13:M:420:THR:N	2.17	0.59
20:U:3:ALA:HB1	20:U:4:PRO:CD	2.33	0.59
21:V:27:TYR:O	21:V:30:THR:OG1	2.21	0.59
13:M:234:ILE:O	13:M:237:LYS:N	2.36	0.59
2:B:107:ALA:HB3	2:B:108:PRO:HD3	1.85	0.59
7:G:46:LEU:O	17:Q:116:LYS:NZ	2.35	0.59
8:H:195:ARG:HD2	8:H:231:ILE:HD11	1.85	0.59
8:H:276:SER:OG	9:I:39:THR:HG21	2.03	0.59
7:G:45:ARG:NH2	7:G:254:MET:HE3	2.18	0.58
10:J:3:ASN:O	10:J:7:VAL:HG23	2.02	0.58
1:A:94:LEU:HD11	10:J:152:MET:SD	2.43	0.58
3:C:192:GLN:OE1	9:I:117:LYS:NZ	2.36	0.58
13:M:210:TYR:O	13:M:213:HIS:ND1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:143:SER:O	16:P:147:ARG:NH2	2.35	0.58
16:P:311:GLU:OE1	16:P:311:GLU:N	2.35	0.58
8:H:89:LEU:HB3	8:H:91:MET:HE2	1.85	0.58
29:d:109:TYR:HA	29:d:112:ILE:HG22	1.84	0.58
12:L:131:LEU:HD23	12:L:131:LEU:O	2.02	0.58
23:X:36:ASP:OD1	23:X:37:LYS:N	2.36	0.58
42:q:38:LEU:HD23	42:q:39:VAL:N	2.18	0.58
4:D:293:CYS:SG	4:D:420:THR:HG21	2.44	0.58
7:G:385:ARG:NH1	7:G:414:ASP:OD2	2.37	0.58
12:L:261:VAL:HG23	12:L:322:PRO:HB2	1.85	0.58
16:P:41:MET:HE1	16:P:219:LYS:HD3	1.86	0.58
20:U:44:SER:O	20:U:48:VAL:HG23	2.03	0.58
40:o:20:LYS:O	40:o:23:SER:OG	2.12	0.58
41:p:81:VAL:O	41:p:84:ILE:N	2.36	0.58
7:G:53:ARG:O	7:G:93:VAL:HG21	2.03	0.58
8:H:277:TYR:CZ	9:I:36:LEU:HD21	2.38	0.58
4:D:381:ASP:OD1	4:D:382:GLY:N	2.35	0.58
48:F:501:FMN:O4'	48:F:501:FMN:O2'	2.16	0.58
35:j:45:ASP:O	35:j:49:GLY:N	2.37	0.58
38:m:110:ARG:O	38:m:114:LEU:HD23	2.04	0.58
6:F:297:VAL:HG12	6:F:298:ILE:N	2.19	0.58
13:M:286:ILE:O	13:M:289:SER:OG	2.20	0.58
15:O:45:GLN:OE1	15:O:235:VAL:HG21	2.04	0.58
16:P:238:LEU:O	16:P:242:VAL:HG23	2.04	0.58
18:R:50:ASN:OD1	18:R:51:GLU:N	2.36	0.58
24:Y:38:SER:HB2	24:Y:57:VAL:HG22	1.86	0.58
29:d:42:GLY:O	29:d:46:ASN:ND2	2.37	0.58
4:D:203:LEU:HD22	4:D:207:LEU:HD23	1.86	0.57
4:D:414:VAL:HA	4:D:417:ILE:HD12	1.85	0.57
7:G:43:HIS:HB3	7:G:46:LEU:HD12	1.86	0.57
8:H:183:MET:O	8:H:187:ILE:HD12	2.04	0.57
14:N:137:ALA:HB3	14:N:138:PRO:HD3	1.84	0.57
6:F:215:VAL:HG22	6:F:216:PHE:CD2	2.39	0.57
7:G:588:THR:HG21	17:Q:63:GLU:HA	1.86	0.57
9:I:66:GLU:OE2	9:I:159:ASN:ND2	2.36	0.57
14:N:215:MET:SD	14:N:247:MET:HE3	2.44	0.57
4:D:109:VAL:HG11	4:D:149:ASN:HA	1.86	0.57
23:X:92:ASN:OD1	23:X:93:MET:N	2.37	0.57
4:D:150:HIS:HB3	4:D:304:MET:HE3	1.85	0.57
6:F:212:ASP:OD1	6:F:213:VAL:N	2.37	0.57
12:L:572:ASN:O	12:L:575:THR:OG1	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:365:ALA:O	13:M:374:ASN:ND2	2.36	0.57
20:T:44:SER:O	20:T:48:VAL:HG23	2.04	0.57
7:G:285:ARG:NH2	7:G:289:GLY:O	2.37	0.57
10:J:32:LEU:O	10:J:35:SER:OG	2.16	0.57
19:S:82:SER:N	19:S:85:GLU:OE1	2.35	0.57
22:W:119:ASP:O	22:W:122:SER:OG	2.12	0.57
6:F:423:ARG:NH2	6:F:427:GLU:OE2	2.37	0.57
7:G:24:THR:HG22	7:G:25:THR:N	2.20	0.57
13:M:41:LEU:O	13:M:50:LYS:NZ	2.37	0.57
13:M:173:THR:CG2	33:h:101:ALA:HB2	2.29	0.57
11:K:40:LEU:HD12	14:N:71:LEU:HD23	1.85	0.57
42:q:128:SER:OG	42:q:130:THR:HG22	2.05	0.56
2:B:74:ALA:HB1	2:B:75:PRO:CD	2.36	0.56
16:P:172:PHE:CD1	16:P:310:LEU:HD13	2.40	0.56
3:C:41:GLN:NE2	3:C:49:GLU:OE1	2.38	0.56
3:C:123:VAL:O	4:D:252:ASN:ND2	2.37	0.56
4:D:342:MET:HE1	7:G:105:CYS:SG	2.46	0.56
14:N:233:LEU:HD23	14:N:241:LEU:HD23	1.87	0.56
19:S:82:SER:O	19:S:86:VAL:HG23	2.05	0.56
24:Y:3:VAL:HG12	24:Y:3:VAL:O	2.05	0.56
36:k:37:VAL:O	36:k:41:LEU:HD23	2.04	0.56
12:L:320:ASN:O	12:L:321:GLN:NE2	2.39	0.56
26:a:51:ASP:O	26:a:55:SER:OG	2.22	0.56
24:Y:81:VAL:HG23	24:Y:82:ARG:N	2.21	0.56
4:D:327:ASP:OD1	43:r:53:TYR:OH	2.12	0.56
6:F:47:GLU:N	6:F:47:GLU:OE1	2.39	0.56
14:N:53:THR:O	14:N:57:THR:HG23	2.06	0.56
32:g:117:GLN:C	32:g:118:LEU:HD12	2.30	0.56
4:D:64:LEU:HD23	4:D:78:PRO:HA	1.88	0.56
4:D:241:ASP:OD1	4:D:290:ARG:NH1	2.39	0.56
15:O:63:THR:OG1	15:O:302:ARG:NH2	2.38	0.56
13:M:156:GLY:O	13:M:202:ALA:HB2	2.05	0.56
14:N:27:MET:HE1	14:N:71:LEU:CD1	2.35	0.56
34:i:109:ILE:HG22	34:i:111:GLU:H	1.70	0.56
8:H:55:LEU:HD13	8:H:221:ALA:HB2	1.88	0.56
13:M:126:LEU:HD21	13:M:153:THR:HG21	1.88	0.56
4:D:107:ASP:OD2	4:D:110:SER:OG	2.23	0.55
8:H:285:LEU:HD23	8:H:285:LEU:C	2.32	0.55
12:L:67:HIS:NE2	12:L:69:VAL:O	2.39	0.55
12:L:76:LEU:HD21	12:L:196:TRP:CE3	2.41	0.55
14:N:233:LEU:HD23	14:N:241:LEU:CD2	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:163:GLN:OE1	26:a:40:ARG:NH1	2.39	0.55
10:J:132:GLY:O	10:J:135:LEU:HD22	2.06	0.55
13:M:127:ILE:HD11	14:N:254:LEU:HD23	1.88	0.55
20:U:65:ILE:HD11	39:n:4:ALA:C	2.30	0.55
1:A:51:PHE:CZ	10:J:73:MET:HE2	2.41	0.55
3:C:114:LEU:CD1	17:Q:17:LEU:HD11	2.37	0.55
14:N:300:THR:HG23	14:N:301:SER:N	2.22	0.55
15:O:317:ILE:HG22	15:O:317:ILE:O	2.06	0.55
21:V:64:VAL:HG13	21:V:76:VAL:HG11	1.89	0.55
37:l:31:GLU:OE1	37:l:31:GLU:N	2.35	0.55
7:G:456:SER:OG	7:G:495:ARG:NH1	2.40	0.55
12:L:295:GLN:O	12:L:301:ILE:HD11	2.07	0.55
13:M:271:MET:O	13:M:274:SER:OG	2.24	0.55
22:W:30:ALA:O	22:W:34:VAL:HG23	2.07	0.55
8:H:192:GLU:CG	8:H:234:MET:HE1	2.36	0.55
9:I:56:LYS:NZ	42:q:79:GLY:O	2.37	0.55
10:J:44:LEU:HD23	10:J:49:SER:HA	1.89	0.55
15:O:176:VAL:HG21	15:O:196:SER:HB3	1.88	0.55
2:B:76:ARG:NH1	4:D:179:GLU:OE2	2.40	0.55
4:D:366:ALA:O	4:D:367:ILE:HD13	2.06	0.55
5:E:55:GLN:NE2	5:E:89:MET:O	2.40	0.55
20:T:49:GLU:OE2	22:W:66:ARG:NH2	2.38	0.55
15:O:115:LEU:C	15:O:115:LEU:HD23	2.31	0.55
4:D:230:THR:O	4:D:294:TYR:OH	2.24	0.55
10:J:115:ILE:HG22	11:K:3:SER:HB3	1.89	0.55
13:M:396:MET:HA	13:M:396:MET:HE2	1.89	0.55
32:g:34:ASN:OD1	32:g:35:VAL:N	2.40	0.55
37:l:130:LYS:NZ	40:o:56:ASP:OD2	2.33	0.55
42:q:138:VAL:HG23	42:q:138:VAL:O	2.06	0.55
4:D:154:VAL:HG13	4:D:297:TYR:HE1	1.72	0.54
25:Z:127:ARG:NH1	30:e:96:HIS:O	2.40	0.54
37:l:136:ASN:OD1	37:l:141:ARG:NE	2.39	0.54
2:B:46:LEU:O	2:B:49:TRP:HB3	2.08	0.54
7:G:131:LEU:N	7:G:132:GLU:OE1	2.40	0.54
7:G:379:LEU:HD23	7:G:452:VAL:HG13	1.89	0.54
16:P:53:VAL:HG12	16:P:57:MET:SD	2.47	0.54
20:T:65:ILE:HD12	20:T:65:ILE:H	1.73	0.54
6:F:318:ASP:OD2	6:F:318:ASP:N	2.39	0.54
6:F:326:GLN:OE1	6:F:420:ARG:NE	2.40	0.54
10:J:114:VAL:HG12	10:J:115:ILE:HG23	1.88	0.54
16:P:157:ARG:NH2	16:P:226:LYS:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:i:119:MET:SD	34:i:119:MET:N	2.81	0.54
7:G:440:CYS:SG	7:G:441:GLU:N	2.80	0.54
12:L:532:ILE:HD11	37:l:104:LEU:HD23	1.89	0.54
14:N:118:VAL:CG1	14:N:122:ILE:HD11	2.38	0.54
21:V:47:THR:HA	21:V:50:ILE:HD12	1.89	0.54
8:H:96:ILE:CG2	8:H:98:LEU:HD21	2.37	0.54
11:K:19:THR:HG21	11:K:33:LEU:HD12	1.88	0.54
11:K:43:MET:O	11:K:47:THR:HG23	2.08	0.54
12:L:173:LEU:HD13	13:M:405:MET:CE	2.35	0.54
13:M:172:GLY:HA3	33:h:101:ALA:HB1	1.89	0.54
28:c:41:GLU:OE1	29:d:19:ARG:NH1	2.37	0.54
1:A:79:ILE:HG13	1:A:87:MET:HE3	1.90	0.54
4:D:141:PHE:O	4:D:145:THR:HG23	2.08	0.54
6:F:94:VAL:HG11	6:F:192:LEU:HD21	1.89	0.54
9:I:125:GLN:OE1	9:I:135:GLU:N	2.40	0.54
13:M:259:TYR:O	13:M:263:LEU:HD23	2.07	0.54
37:l:10:GLY:O	38:m:78:ASN:ND2	2.40	0.54
44:s:36:GLN:OE1	44:s:36:GLN:N	2.40	0.54
1:A:104:TYR:OH	14:N:2:ASN:ND2	2.41	0.54
3:C:116:PRO:O	3:C:117:ILE:HD13	2.08	0.54
7:G:261:GLU:OE1	17:Q:42:ARG:NH2	2.40	0.54
14:N:98:THR:O	14:N:102:LEU:HD23	2.08	0.54
20:T:26:ASP:OD2	20:T:30:LEU:HD13	2.08	0.54
2:B:106:MET:SD	4:D:82:LEU:HD23	2.48	0.54
4:D:207:LEU:H	25:Z:9:MET:HE2	1.73	0.54
6:F:255:LEU:HD23	6:F:268:VAL:O	2.07	0.54
11:K:1:FME:HE1	11:K:5:PHE:CD1	2.43	0.54
6:F:224:ASN:OD1	6:F:225:VAL:N	2.41	0.53
7:G:644:GLN:N	7:G:644:GLN:OE1	2.39	0.53
8:H:96:ILE:HG22	8:H:98:LEU:HD21	1.88	0.53
10:J:145:TYR:CZ	10:J:152:MET:HE3	2.43	0.53
20:T:43:ASP:OD1	20:T:44:SER:N	2.41	0.53
13:M:63:THR:HA	13:M:66:ILE:HD12	1.90	0.53
15:O:31:ILE:CD1	15:O:183:ILE:HD11	2.36	0.53
23:X:150:ASN:OD1	30:e:50:ARG:NH2	2.40	0.53
7:G:285:ARG:NE	7:G:557:ALA:O	2.41	0.53
34:i:29:PRO:O	34:i:30:ARG:HG3	2.09	0.53
7:G:360:SER:HG	7:G:639:THR:CB	2.20	0.53
9:I:84:LEU:O	9:I:88:ILE:HG22	2.08	0.53
12:L:400:ASN:CG	12:L:486:LEU:HD22	2.33	0.53
12:L:416:THR:O	12:L:419:THR:OG1	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:64:LYS:CB	26:a:68:ASN:HD21	2.21	0.53
39:n:136:VAL:HG12	39:n:140:GLN:HG3	1.90	0.53
2:B:71:HIS:O	2:B:74:ALA:HB3	2.08	0.53
6:F:94:VAL:HG11	6:F:192:LEU:CD2	2.38	0.53
15:O:90:ASP:O	32:g:25:GLN:NE2	2.42	0.53
4:D:112:MET:HB2	4:D:145:THR:HG21	1.89	0.53
14:N:42:PRO:HA	14:N:45:ILE:HG22	1.90	0.53
22:W:22:ILE:O	22:W:22:ILE:HG23	2.09	0.53
26:a:13:GLY:O	26:a:17:VAL:HG23	2.08	0.53
34:i:109:ILE:HG22	34:i:111:GLU:N	2.22	0.53
5:E:16:ASN:H	5:E:19:THR:HG1	1.57	0.53
7:G:13:VAL:N	7:G:16:GLN:O	2.41	0.53
8:H:235:ASN:O	8:H:239:THR:HG23	2.09	0.53
12:L:378:LEU:HD23	12:L:383:MET:CE	2.39	0.53
13:M:17:LEU:HD12	13:M:17:LEU:C	2.34	0.53
25:Z:143:THR:HG23	26:a:48:MET:CE	2.39	0.53
7:G:359:ARG:O	7:G:363:LEU:HD12	2.08	0.53
29:d:65:VAL:O	29:d:69:VAL:HG23	2.08	0.53
13:M:422:HIS:CE1	13:M:423:MET:HE2	2.44	0.53
16:P:75:ALA:HB1	16:P:113:ILE:HD11	1.90	0.53
36:k:38:GLN:OE1	36:k:47:ARG:NH1	2.42	0.53
2:B:74:ALA:HB1	2:B:75:PRO:HD2	1.92	0.52
5:E:124:LEU:HD21	5:E:137:PHE:HD2	1.74	0.52
3:C:17:VAL:HG23	3:C:18:THR:N	2.24	0.52
12:L:366:MET:SD	12:L:369:THR:OG1	2.59	0.52
12:L:378:LEU:O	12:L:381:THR:OG1	2.22	0.52
33:h:40:ILE:HG22	33:h:44:ASN:HD21	1.73	0.52
7:G:306:MET:HE1	7:G:542:PHE:CG	2.44	0.52
8:H:281:ARG:NH2	8:H:284:GLN:OE1	2.42	0.52
7:G:145:LEU:HD13	7:G:269:PHE:CE2	2.44	0.52
7:G:266:LYS:NZ	7:G:671:PHE:O	2.39	0.52
3:C:64:LEU:HD22	3:C:72:PHE:HD1	1.74	0.52
3:C:168:LEU:HD11	4:D:90:LEU:HD23	1.92	0.52
4:D:208:LEU:H	25:Z:9:MET:HE3	1.75	0.52
11:K:78:LEU:C	11:K:78:LEU:HD23	2.34	0.52
12:L:150:MET:HE2	12:L:150:MET:HA	1.91	0.52
20:U:36:PHE:HB3	20:U:42:LEU:HD12	1.91	0.52
5:E:53:LEU:HD12	44:s:46:LEU:HD13	1.92	0.52
5:E:214:GLN:NE2	6:F:59:GLU:OE2	2.43	0.52
7:G:199:VAL:HA	7:G:202:ILE:HG22	1.92	0.52
12:L:76:LEU:HD21	12:L:196:TRP:CZ3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:230:HIS:N	12:L:231:PRO:CD	2.73	0.52
16:P:88:SER:OG	16:P:89:ASN:N	2.42	0.52
4:D:88:GLU:OE2	4:D:430:ARG:NH1	2.38	0.52
12:L:154:LEU:CD1	12:L:247:LEU:HD11	2.39	0.52
14:N:321:LYS:N	14:N:322:PRO:CD	2.73	0.52
16:P:319:ARG:NH2	22:W:54:LEU:O	2.42	0.52
20:U:20:LYS:NZ	20:U:28:GLU:O	2.41	0.52
4:D:47:MET:HE1	8:H:126:LYS:HB2	1.92	0.52
9:I:65:GLY:N	9:I:136:GLY:O	2.43	0.52
19:S:87:THR:O	19:S:91:GLN:NE2	2.42	0.52
23:X:75:SER:OG	23:X:76:HIS:ND1	2.42	0.52
8:H:192:GLU:HG2	8:H:234:MET:HE1	1.92	0.52
3:C:64:LEU:HD22	3:C:72:PHE:CD1	2.45	0.52
9:I:51:ASN:O	9:I:55:GLU:N	2.43	0.52
13:M:243:MET:HE2	13:M:301:ILE:HG21	1.92	0.52
3:C:151:ILE:HG23	3:C:152:LEU:N	2.25	0.51
5:E:50:VAL:HG11	5:E:69:VAL:HG13	1.90	0.51
8:H:96:ILE:HG22	8:H:98:LEU:CD2	2.40	0.51
10:J:168:GLU:OE2	14:N:1:FME:N	2.43	0.51
11:K:40:LEU:CD1	14:N:71:LEU:HD23	2.39	0.51
16:P:138:SER:OG	16:P:139:MET:N	2.43	0.51
28:c:36:ASN:O	28:c:40:LEU:HD23	2.10	0.51
30:e:21:SER:N	30:e:36:GLU:OE1	2.43	0.51
7:G:281:GLU:HG2	7:G:592:LEU:HD12	1.91	0.51
13:M:266:LEU:HD13	13:M:395:LEU:HD12	1.90	0.51
13:M:429:SER:HB3	13:M:434:LEU:HD21	1.92	0.51
16:P:57:MET:HE1	16:P:60:ARG:HE	1.75	0.51
3:C:16:ASP:OD1	3:C:17:VAL:N	2.43	0.51
4:D:184:VAL:HG13	4:D:185:SER:N	2.25	0.51
44:s:33:LYS:C	44:s:35:LEU:HD12	2.35	0.51
9:I:134:VAL:O	9:I:134:VAL:HG23	2.09	0.51
10:J:151:MET:HE1	14:N:28:LEU:HD21	1.93	0.51
12:L:224:SER:OG	12:L:253:VAL:O	2.27	0.51
16:P:51:CYS:SG	16:P:52:ASP:N	2.79	0.51
23:X:150:ASN:ND2	33:h:124:GLN:OE1	2.44	0.51
4:D:133:ARG:NH1	25:Z:8:ASP:O	2.43	0.51
8:H:140:ILE:HD11	10:J:65:VAL:HG11	1.92	0.51
8:H:157:ASN:ND2	8:H:165:LEU:HD12	2.26	0.51
13:M:156:GLY:C	13:M:202:ALA:HB2	2.35	0.51
18:R:38:ASN:HB3	18:R:43:LEU:HD11	1.93	0.51
20:U:17:TYR:OH	36:k:27:TRP:NE1	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:14:ASP:OD1	30:e:15:ARG:N	2.44	0.51
6:F:360:GLY:O	6:F:366:ARG:NH1	2.37	0.51
11:K:19:THR:CG2	11:K:33:LEU:HD12	2.41	0.51
14:N:250:SER:O	14:N:253:GLY:N	2.44	0.51
8:H:314:VAL:O	8:H:314:VAL:HG13	2.10	0.51
12:L:51:LEU:HD21	12:L:87:ILE:O	2.10	0.51
12:L:562:ILE:HB	12:L:563:PRO:HD3	1.92	0.51
35:j:12:ARG:NH1	36:k:53:ASN:OD1	2.40	0.51
11:K:42:ILE:O	11:K:46:VAL:HG23	2.11	0.51
25:Z:113:THR:HG22	25:Z:113:THR:O	2.10	0.51
4:D:349:PHE:CE2	9:I:84:LEU:HD11	2.46	0.50
9:I:59:LEU:HD11	42:q:91:HIS:HD2	1.76	0.50
13:M:73:LEU:HD22	13:M:103:GLN:CD	2.37	0.50
13:M:230:ILE:CD1	13:M:234:ILE:HD12	2.40	0.50
16:P:315:ILE:HD12	16:P:315:ILE:H	1.76	0.50
20:T:13:ASP:N	20:T:13:ASP:OD1	2.44	0.50
23:X:83:GLU:OE2	23:X:105:LYS:NZ	2.35	0.50
23:X:130:VAL:HG13	23:X:130:VAL:O	2.12	0.50
12:L:350:LEU:HD13	12:L:353:GLU:OE2	2.11	0.50
14:N:29:MET:HE1	14:N:144:GLN:OE1	2.11	0.50
7:G:503:LEU:HD21	7:G:509:PRO:HB3	1.92	0.50
12:L:7:SER:O	12:L:11:ILE:HG23	2.10	0.50
12:L:561:THR:O	12:L:565:SER:OG	2.26	0.50
1:A:2:ASN:O	1:A:5:THR:OG1	2.26	0.50
2:B:159:CYS:SG	4:D:105:ARG:NH1	2.74	0.50
7:G:337:LYS:NZ	7:G:609:ILE:O	2.43	0.50
15:O:223:TYR:HE2	15:O:234:VAL:HG22	1.74	0.50
16:P:295:THR:HG23	16:P:295:THR:O	2.12	0.50
37:l:34:GLU:HG3	37:l:48:MET:HE3	1.93	0.50
26:a:49:GLU:OE1	26:a:52:ARG:NE	2.42	0.50
1:A:49:LEU:HD13	4:D:47:MET:HE3	1.93	0.50
2:B:64:CYS:HB3	4:D:108:TYR:CB	2.42	0.50
12:L:304:PHE:CZ	12:L:526:LEU:HD11	2.46	0.50
12:L:327:LEU:O	12:L:331:THR:HG23	2.12	0.50
13:M:419:LEU:HD12	13:M:420:THR:H	1.76	0.50
14:N:308:ASN:OD1	15:O:282:ILE:HD12	2.11	0.50
23:X:34:GLN:O	23:X:35:CYS:HB2	2.11	0.50
24:Y:81:VAL:HG23	24:Y:82:ARG:H	1.77	0.50
32:g:46:ASP:N	32:g:52:ASP:OD1	2.41	0.50
41:p:6:LYS:NZ	41:p:11:GLU:OE1	2.32	0.50
7:G:254:MET:HE1	17:Q:111:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:272:TRP:CH2	9:I:40:LEU:HD13	2.47	0.50
9:I:101:ARG:O	9:I:104:GLY:N	2.40	0.50
14:N:1:FME:HE1	14:N:43:MET:SD	2.52	0.50
15:O:110:ASP:OD1	15:O:266:LYS:NZ	2.39	0.50
37:l:57:ARG:NH2	37:l:74:GLU:OE2	2.40	0.50
7:G:28:GLN:NE2	17:Q:114:LYS:O	2.44	0.50
8:H:17:MET:HE1	8:H:225:MET:HG2	1.93	0.50
12:L:536:ILE:HG22	38:m:10:LEU:HD11	1.93	0.50
13:M:158:ILE:HB	13:M:159:PRO:HD3	1.94	0.50
18:R:34:GLU:O	42:q:127:TYR:OH	2.26	0.50
26:a:64:LYS:CG	26:a:68:ASN:ND2	2.73	0.50
33:h:40:ILE:O	33:h:44:ASN:ND2	2.45	0.50
3:C:178:ASP:OD2	16:P:62:MET:HE1	2.12	0.49
12:L:273:ILE:HA	12:L:276:THR:HG22	1.94	0.49
12:L:313:MET:O	12:L:316:THR:HG22	2.12	0.49
43:r:34:THR:HG22	43:r:34:THR:O	2.12	0.49
4:D:199:VAL:HG12	4:D:200:HIS:N	2.26	0.49
48:F:501:FMN:O2'	48:F:501:FMN:H9	2.12	0.49
10:J:33:ILE:CG1	10:J:64:LEU:HD23	2.42	0.49
16:P:76:ARG:NH1	16:P:103:ASN:O	2.44	0.49
6:F:21:ILE:O	6:F:23:THR:N	2.43	0.49
11:K:57:MET:N	11:K:58:PRO:CD	2.76	0.49
12:L:230:HIS:O	12:L:232:TRP:N	2.45	0.49
15:O:305:ALA:HB1	15:O:306:PRO:CD	2.41	0.49
23:X:165:ARG:NH2	33:h:107:GLU:OE1	2.41	0.49
6:F:111:MET:SD	6:F:138:ILE:HD12	2.53	0.49
7:G:587:VAL:HG12	7:G:588:THR:N	2.28	0.49
16:P:61:LEU:C	16:P:61:LEU:HD12	2.37	0.49
3:C:45:LEU:HD12	3:C:45:LEU:O	2.12	0.49
4:D:287:ILE:O	9:I:5:VAL:HG22	2.13	0.49
5:E:166:PRO:HA	5:E:169:ILE:HG22	1.95	0.49
6:F:24:ASN:ND2	6:F:30:ASP:O	2.45	0.49
12:L:204:SER:O	12:L:209:ASN:ND2	2.45	0.49
13:M:119:TYR:HD1	13:M:160:LEU:HD23	1.76	0.49
13:M:153:THR:HG23	13:M:206:LYS:CE	2.42	0.49
4:D:205:LEU:HD11	43:r:38:PRO:HB3	1.93	0.49
7:G:306:MET:HE1	7:G:542:PHE:CD1	2.48	0.49
14:N:285:MET:CE	14:N:288:LEU:HD11	2.43	0.49
20:T:16:LEU:HB2	20:T:30:LEU:HD11	1.95	0.49
1:A:57:LEU:O	1:A:61:THR:HG23	2.11	0.49
3:C:175:ARG:NH2	3:C:186:GLU:OE2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:281:VAL:HG22	4:D:282:GLU:N	2.26	0.49
7:G:145:LEU:HD13	7:G:269:PHE:HE2	1.78	0.49
49:M:501:3PE:H342	32:g:75:VAL:HG11	1.95	0.49
15:O:147:GLN:OE1	15:O:147:GLN:N	2.37	0.49
20:U:11:ILE:HG22	20:U:77:VAL:HG22	1.94	0.49
3:C:114:LEU:HD11	17:Q:17:LEU:HD11	1.94	0.49
12:L:536:ILE:HG13	12:L:537:THR:N	2.28	0.49
12:L:549:SER:OG	13:M:275:ILE:HD11	2.11	0.49
24:Y:96:CYS:HA	24:Y:116:CYS:HA	1.94	0.49
1:A:65:PHE:CZ	8:H:294:LEU:HD21	2.48	0.49
4:D:357:GLN:O	43:r:59:ARG:NH1	2.46	0.49
36:k:31:GLY:N	36:k:35:GLU:OE1	2.43	0.49
3:C:138:PHE:O	3:C:163:ARG:NE	2.39	0.49
7:G:424:ASP:N	7:G:424:ASP:OD1	2.45	0.49
12:L:467:VAL:O	12:L:471:ASN:ND2	2.46	0.49
16:P:159:VAL:HG23	16:P:160:PHE:H	1.78	0.49
4:D:150:HIS:CB	4:D:304:MET:HE3	2.42	0.48
5:E:65:ALA:O	5:E:69:VAL:HG23	2.12	0.48
8:H:100:LEU:HB3	10:J:53:LEU:HD13	1.95	0.48
20:T:25:ILE:HG22	20:T:26:ASP:N	2.28	0.48
34:i:97:VAL:HG11	41:p:114:GLN:HB3	1.95	0.48
41:p:149:TYR:O	41:p:150:SER:OG	2.25	0.48
3:C:85:THR:HG21	21:V:115:ILE:CG1	2.43	0.48
7:G:627:SER:HB2	7:G:630:LEU:HD12	1.95	0.48
10:J:2:ASN:OD1	10:J:3:ASN:N	2.46	0.48
23:X:53:ARG:O	23:X:54:ARG:NH2	2.45	0.48
7:G:145:LEU:HD21	7:G:687:CYS:SG	2.53	0.48
7:G:324:ASP:HB2	7:G:571:ALA:HB1	1.94	0.48
10:J:82:TRP:CG	10:J:82:TRP:O	2.65	0.48
12:L:442:SER:CB	20:U:3:ALA:HB2	2.43	0.48
13:M:176:LEU:O	13:M:177:MET:CG	2.62	0.48
14:N:332:MET:O	14:N:336:THR:HG21	2.12	0.48
16:P:177:ARG:NH1	52:P:501:NDP:O2N	2.46	0.48
30:e:64:GLU:OE2	30:e:70:LYS:N	2.40	0.48
39:n:143:THR:HG23	39:n:143:THR:O	2.13	0.48
4:D:182:GLU:OE2	9:I:59:LEU:HD22	2.13	0.48
7:G:384:PRO:HA	7:G:387:GLU:O	2.12	0.48
7:G:556:MET:SD	7:G:556:MET:O	2.72	0.48
20:U:64:ASP:OD2	39:n:17:ARG:NH1	2.46	0.48
21:V:20:HIS:HE1	21:V:64:VAL:HG23	1.77	0.48
9:I:78:ARG:NH1	18:R:66:LEU:O	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:257:ILE:HG23	12:L:317:LEU:HD11	1.95	0.48
12:L:378:LEU:HD23	12:L:383:MET:HE3	1.95	0.48
26:a:64:LYS:HB3	26:a:68:ASN:HD21	1.70	0.48
2:B:36:ALA:O	2:B:40:VAL:HG23	2.13	0.48
6:F:175:VAL:O	44:s:56:ARG:NH1	2.46	0.48
7:G:461:ASP:OD1	7:G:462:ASP:N	2.43	0.48
8:H:81:LEU:HD13	8:H:111:LEU:HB2	1.94	0.48
8:H:157:ASN:HD21	8:H:165:LEU:HD12	1.78	0.48
15:O:56:ILE:O	15:O:57:GLN:NE2	2.46	0.48
25:Z:73:LEU:HD11	25:Z:77:GLU:OE2	2.14	0.48
3:C:117:ILE:HG22	3:C:118:ASP:N	2.28	0.48
7:G:132:GLU:OE1	7:G:132:GLU:N	2.47	0.48
40:o:70:ARG:NE	40:o:71:ASP:OD1	2.45	0.48
41:p:81:VAL:O	41:p:82:LEU:C	2.56	0.48
42:q:3:LEU:N	42:q:3:LEU:HD12	2.28	0.48
5:E:67:ASN:OD1	5:E:81:TYR:OH	2.19	0.48
13:M:71:TRP:HZ3	32:g:67:VAL:HG11	1.79	0.48
41:p:80:ASP:OD1	41:p:81:VAL:N	2.46	0.48
3:C:186:GLU:HB3	3:C:187:PRO:HD2	1.96	0.48
10:J:92:LEU:C	10:J:92:LEU:HD23	2.39	0.48
10:J:147:CYS:O	10:J:148:ALA:HB3	2.14	0.48
13:M:424:ILE:HG22	13:M:424:ILE:O	2.13	0.48
14:N:27:MET:O	14:N:31:VAL:HG23	2.13	0.48
16:P:95:ILE:O	52:P:501:NDP:O3D	2.32	0.48
23:X:45:CYS:HB3	23:X:55:CYS:SG	2.54	0.48
26:a:26:ILE:O	26:a:30:THR:HG23	2.13	0.48
3:C:32:ILE:HG22	3:C:33:LEU:HD12	1.94	0.48
6:F:313:GLU:O	6:F:314:THR:OG1	2.23	0.48
9:I:150:LEU:HB3	17:Q:70:MET:HE1	1.96	0.48
10:J:67:PHE:O	10:J:71:THR:OG1	2.24	0.48
22:W:52:MET:O	22:W:54:LEU:N	2.47	0.48
24:Y:73:LEU:O	24:Y:77:VAL:HG23	2.14	0.48
43:r:4:THR:HG22	43:r:5:ARG:N	2.29	0.48
3:C:189:GLU:OE1	16:P:15:SER:OG	2.29	0.47
8:H:24:GLU:HA	8:H:271:LEU:HD13	1.96	0.47
8:H:24:GLU:HG3	8:H:271:LEU:HD22	1.96	0.47
9:I:116:THR:HG21	9:I:146:HIS:CD2	2.48	0.47
16:P:113:ILE:HB	16:P:114:PRO:CD	2.44	0.47
38:m:24:VAL:HG12	38:m:24:VAL:O	2.14	0.47
6:F:372:MET:HE3	6:F:399:ILE:HD12	1.96	0.47
7:G:675:ASP:C	7:G:679:ARG:HE	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:157:ASN:O	8:H:159:SER:N	2.41	0.47
12:L:226:GLN:NE2	12:L:314:MET:SD	2.87	0.47
12:L:424:MET:HE1	36:k:68:PHE:CD1	2.49	0.47
15:O:210:PHE:CE1	15:O:214:MET:HE2	2.47	0.47
4:D:226:GLU:OE2	25:Z:22:ARG:NH1	2.47	0.47
7:G:338:VAL:O	7:G:338:VAL:CG1	2.62	0.47
7:G:396:ARG:HH12	7:G:400:LEU:HD13	1.79	0.47
14:N:43:MET:CB	14:N:126:MET:HE2	2.44	0.47
14:N:330:ALA:O	14:N:334:THR:HG23	2.14	0.47
15:O:247:PRO:O	15:O:250:LYS:N	2.47	0.47
16:P:53:VAL:HA	16:P:56:ILE:HG22	1.96	0.47
25:Z:51:ARG:NH1	27:b:83:LEU:O	2.45	0.47
30:e:64:GLU:O	30:e:68:ARG:N	2.47	0.47
37:l:114:MET:N	37:l:114:MET:HE2	2.29	0.47
1:A:87:MET:SD	8:H:309:ILE:HD11	2.54	0.47
7:G:437:HIS:O	7:G:440:CYS:N	2.40	0.47
16:P:6:ILE:HG22	16:P:7:PRO:HD2	1.95	0.47
23:X:167:PHE:O	23:X:169:TRP:N	2.47	0.47
7:G:592:LEU:O	7:G:594:ARG:NH1	2.44	0.47
13:M:73:LEU:HD22	13:M:103:GLN:OE1	2.15	0.47
14:N:300:THR:CG2	14:N:301:SER:N	2.78	0.47
39:n:11:HIS:CE1	39:n:59:ALA:HB1	2.50	0.47
4:D:142:GLY:O	4:D:146:ARG:HG2	2.15	0.47
4:D:417:ILE:O	4:D:420:THR:OG1	2.25	0.47
5:E:8:VAL:HG12	5:E:9:HIS:N	2.30	0.47
7:G:594:ARG:NE	22:W:127:GLY:O	2.43	0.47
9:I:145:THR:HG22	9:I:146:HIS:N	2.30	0.47
13:M:409:TYR:CE1	13:M:413:THR:HG21	2.49	0.47
16:P:61:LEU:HD12	16:P:62:MET:N	2.30	0.47
1:A:8:PHE:O	1:A:12:LEU:HD23	2.14	0.47
3:C:180:VAL:HG23	3:C:182:ARG:H	1.79	0.47
5:E:105:THR:HG22	5:E:106:THR:H	1.79	0.47
5:E:149:VAL:HG13	5:E:150:ASN:N	2.30	0.47
6:F:45:THR:O	6:F:49:LEU:HG	2.15	0.47
6:F:98:ASP:OD1	6:F:99:GLU:N	2.48	0.47
6:F:400:GLU:OE2	6:F:416:GLN:NE2	2.47	0.47
9:I:96:ILE:HD11	9:I:111:TYR:CE1	2.50	0.47
13:M:217:PRO:O	13:M:221:VAL:HG23	2.15	0.47
16:P:45:VAL:HG12	16:P:47:ILE:HG13	1.97	0.47
16:P:244:TYR:CZ	16:P:248:MET:HE3	2.50	0.47
20:U:11:ILE:CG2	20:U:77:VAL:HG22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:V:102:LEU:HD23	21:V:104:GLU:N	2.29	0.47
23:X:19:VAL:HG12	23:X:20:SER:N	2.28	0.47
23:X:77:CYS:SG	23:X:110:VAL:HG22	2.55	0.47
7:G:358:LEU:HD12	7:G:645:ALA:HB2	1.97	0.47
7:G:585:VAL:HG13	7:G:585:VAL:O	2.15	0.47
12:L:537:THR:HB	12:L:538:PRO:HD3	1.97	0.47
15:O:55:GLY:O	15:O:100:LEU:HD23	2.14	0.47
16:P:159:VAL:HG23	16:P:160:PHE:N	2.30	0.47
30:e:29:ALA:HB2	33:h:138:LYS:HB3	1.95	0.47
13:M:63:THR:HB	13:M:64:PRO:HD3	1.97	0.47
13:M:317:ILE:HG13	13:M:454:ILE:HD11	1.97	0.47
15:O:31:ILE:HG13	15:O:32:CYS:N	2.30	0.47
23:X:77:CYS:HB3	23:X:109:CYS:SG	2.55	0.47
31:f:30:ASP:OD1	33:h:89:LYS:NZ	2.43	0.47
3:C:178:ASP:OD1	16:P:36:ASN:ND2	2.48	0.47
6:F:261:HIS:ND1	6:F:338:ASP:OD1	2.48	0.47
7:G:127:ARG:NH1	43:r:45:SER:O	2.48	0.47
7:G:574:VAL:HG12	7:G:575:ASN:O	2.15	0.47
33:h:10:VAL:HG23	33:h:10:VAL:O	2.15	0.47
4:D:295:ASP:OD1	9:I:6:ASN:ND2	2.48	0.46
8:H:125:SER:O	8:H:128:SER:OG	2.22	0.46
9:I:66:GLU:OE1	9:I:138:ASN:ND2	2.45	0.46
12:L:72:ASN:C	12:L:73:SER:HG	2.16	0.46
13:M:313:THR:OG1	13:M:455:THR:O	2.30	0.46
13:M:368:ALA:HB1	13:M:375:LEU:HD13	1.97	0.46
17:Q:13:VAL:O	17:Q:13:VAL:HG13	2.14	0.46
24:Y:15:ASP:OD2	24:Y:127:LYS:NZ	2.45	0.46
7:G:273:GLY:O	7:G:549:HIS:NE2	2.48	0.46
9:I:146:HIS:O	9:I:146:HIS:CG	2.68	0.46
12:L:3:ILE:HD13	41:p:36:TYR:CG	2.50	0.46
13:M:49:TYR:O	33:h:86:ASN:ND2	2.39	0.46
35:j:63:GLU:C	35:j:64:LEU:HD23	2.39	0.46
1:A:84:THR:HA	1:A:87:MET:HG3	1.97	0.46
2:B:96:MET:HB2	2:B:117:MET:HE1	1.96	0.46
6:F:95:VAL:HG21	6:F:122:CYS:SG	2.55	0.46
7:G:8:LEU:HD13	7:G:20:VAL:O	2.16	0.46
9:I:54:PHE:CE2	42:q:30:ALA:HB2	2.51	0.46
16:P:206:TYR:CE2	16:P:208:ALA:HB3	2.50	0.46
21:V:68:GLU:CG	21:V:76:VAL:HG13	2.46	0.46
23:X:134:ARG:O	27:b:57:ARG:NH2	2.48	0.46
4:D:90:LEU:HD13	4:D:102:TYR:OH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:253:THR:OG1	6:F:270:GLU:O	2.21	0.46
12:L:437:PHE:HB2	12:L:438:PRO:CD	2.45	0.46
13:M:176:LEU:C	13:M:178:ILE:H	2.24	0.46
17:Q:11:ILE:HG22	17:Q:12:THR:N	2.31	0.46
21:V:20:HIS:NE2	21:V:62:PRO:O	2.48	0.46
41:p:25:LEU:HD12	41:p:26:PRO:HD2	1.97	0.46
3:C:9:PRO:HG2	3:C:10:THR:HG23	1.96	0.46
6:F:139:ARG:NH1	6:F:141:GLU:OE2	2.41	0.46
7:G:294:THR:HG21	7:G:298:ASP:OD2	2.15	0.46
14:N:2:ASN:HB2	14:N:3:PRO:CD	2.45	0.46
14:N:166:ALA:HB1	14:N:288:LEU:HB2	1.97	0.46
7:G:639:THR:HG22	19:S:56:GLU:CD	2.41	0.46
16:P:155:GLU:O	16:P:159:VAL:HG22	2.15	0.46
16:P:167:ARG:O	16:P:167:ARG:HG3	2.16	0.46
23:X:122:GLY:N	25:Z:65:GLU:OE2	2.46	0.46
33:h:34:ILE:HB	33:h:35:PRO:HD3	1.98	0.46
10:J:33:ILE:HG13	10:J:64:LEU:HD23	1.98	0.46
12:L:75:GLU:OE2	41:p:103:ASN:ND2	2.49	0.46
12:L:131:LEU:HD23	12:L:131:LEU:C	2.41	0.46
22:W:29:GLU:O	22:W:32:ARG:HG2	2.15	0.46
7:G:148:THR:HG22	7:G:208:LEU:HD22	1.98	0.46
8:H:37:PRO:O	8:H:38:ASN:ND2	2.49	0.46
10:J:9:SER:OG	11:K:7:ASN:HB2	2.15	0.46
12:L:247:LEU:O	12:L:248:HIS:ND1	2.49	0.46
13:M:119:TYR:CD1	13:M:160:LEU:HD23	2.51	0.46
13:M:126:LEU:HD13	13:M:150:LEU:CD1	2.45	0.46
20:U:65:ILE:HD13	39:n:3:CYS:O	2.16	0.46
36:k:54:GLU:OE1	39:n:33:ARG:NE	2.46	0.46
41:p:80:ASP:O	41:p:84:ILE:HD12	2.16	0.46
1:A:1:FME:O	1:A:5:THR:HG23	2.16	0.46
4:D:23:LYS:HZ3	12:L:575:THR:HB	1.81	0.46
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.98	0.46
8:H:97:ASN:O	8:H:98:LEU:HD23	2.16	0.46
16:P:20:VAL:HG11	16:P:88:SER:HA	1.98	0.46
20:T:52:MET:HE1	22:W:42:TYR:HB3	1.98	0.46
34:i:76:ILE:HB	34:i:77:PRO:HD3	1.98	0.46
37:l:111:MET:HE2	37:l:111:MET:N	2.30	0.46
3:C:11:VAL:HG12	3:C:12:ARG:O	2.16	0.46
9:I:49:THR:HG22	9:I:50:ILE:N	2.30	0.46
11:K:70:GLU:O	11:K:73:VAL:HG22	2.16	0.46
16:P:113:ILE:HB	16:P:114:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:61:GLU:N	20:T:61:GLU:OE2	2.49	0.46
25:Z:128:THR:HG22	25:Z:129:LYS:N	2.30	0.46
38:m:115:ILE:O	38:m:118:GLY:N	2.49	0.46
1:A:49:LEU:HD12	1:A:50:PRO:CD	2.45	0.45
2:B:38:TYR:O	2:B:41:THR:OG1	2.29	0.45
2:B:64:CYS:HB3	4:D:108:TYR:HB2	1.98	0.45
7:G:554:ALA:HB3	7:G:555:PRO:HD3	1.98	0.45
8:H:277:TYR:OH	9:I:36:LEU:HD21	2.15	0.45
13:M:296:LEU:HD21	13:M:396:MET:HE1	1.97	0.45
14:N:42:PRO:O	14:N:45:ILE:N	2.48	0.45
14:N:340:ALA:N	14:N:341:PRO:CD	2.79	0.45
17:Q:132:THR:HG22	17:Q:133:LYS:N	2.31	0.45
20:U:19:LEU:HD22	20:U:50:ILE:HD12	1.97	0.45
40:o:45:MET:HE3	40:o:55:ARG:HG3	1.98	0.45
4:D:347:HIS:O	4:D:351:LEU:HG	2.15	0.45
5:E:108:CYS:SG	5:E:151:ALA:O	2.74	0.45
7:G:522:LEU:HD11	7:G:537:LEU:HD11	1.98	0.45
13:M:23:THR:HG23	13:M:24:TRP:N	2.31	0.45
13:M:344:MET:HE2	13:M:423:MET:HE1	1.97	0.45
41:p:155:LEU:C	41:p:155:LEU:HD23	2.41	0.45
42:q:38:LEU:HD21	42:q:40:GLY:O	2.15	0.45
1:A:62:PHE:CZ	1:A:66:ASP:OD2	2.69	0.45
3:C:104:ARG:NH2	4:D:373:GLU:OE2	2.46	0.45
4:D:261:ARG:NH2	4:D:267:TRP:O	2.49	0.45
6:F:109:GLU:OE2	6:F:112:ARG:NE	2.48	0.45
7:G:318:ILE:HG21	7:G:346:GLU:OE1	2.15	0.45
8:H:95:LEU:O	8:H:96:ILE:HD13	2.16	0.45
13:M:116:ILE:O	13:M:120:ILE:HG23	2.17	0.45
13:M:127:ILE:HB	13:M:128:PRO:HD3	1.97	0.45
17:Q:104:ASP:OD1	17:Q:105:VAL:N	2.49	0.45
18:R:41:ILE:HG23	18:R:42:ASP:N	2.32	0.45
20:U:64:ASP:N	20:U:64:ASP:OD1	2.47	0.45
21:V:64:VAL:CG1	21:V:76:VAL:HG11	2.46	0.45
33:h:39:GLY:O	33:h:43:VAL:HG23	2.16	0.45
34:i:103:ILE:HG22	34:i:104:PHE:N	2.31	0.45
4:D:184:VAL:O	9:I:62:ARG:NH2	2.45	0.45
9:I:96:ILE:HD11	9:I:111:TYR:HE1	1.81	0.45
13:M:354:LEU:HD11	33:h:22:LEU:HD21	1.99	0.45
14:N:221:LEU:HD23	14:N:222:ASN:OD1	2.16	0.45
15:O:25:ILE:CD1	15:O:48:MET:HE1	2.39	0.45
15:O:125:GLU:O	15:O:126:ARG:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:22:LEU:HD21	19:S:56:GLU:HB3	1.98	0.45
19:S:44:LYS:NZ	19:S:50:LEU:O	2.49	0.45
33:h:134:ASP:OD1	33:h:135:HIS:N	2.49	0.45
35:j:63:GLU:O	35:j:64:LEU:C	2.60	0.45
39:n:170:VAL:HG12	39:n:171:THR:HG23	1.97	0.45
1:A:57:LEU:HD21	10:J:170:THR:HG21	1.97	0.45
2:B:189:ARG:NH2	52:P:501:NDP:O3X	2.45	0.45
8:H:179:TRP:N	8:H:180:PRO:CD	2.79	0.45
36:k:21:LEU:N	36:k:21:LEU:HD12	2.31	0.45
8:H:70:LEU:HA	8:H:73:ILE:HG12	1.99	0.45
8:H:296:LEU:O	8:H:300:LEU:HD23	2.17	0.45
25:Z:67:ARG:O	25:Z:71:MET:HG3	2.17	0.45
38:m:36:LEU:HB2	39:n:7:ALA:HB2	1.99	0.45
39:n:80:ILE:HG21	39:n:86:GLY:C	2.42	0.45
42:q:32:ASP:OD2	42:q:33:ILE:N	2.49	0.45
12:L:229:LEU:HD12	12:L:229:LEU:N	2.32	0.45
13:M:230:ILE:HD11	13:M:234:ILE:HD12	1.98	0.45
13:M:268:GLY:O	13:M:272:THR:HG23	2.16	0.45
13:M:454:ILE:O	13:M:454:ILE:HG23	2.16	0.45
33:h:11:VAL:HB	39:n:98:VAL:HG23	1.97	0.45
4:D:2:ARG:NE	32:g:29:GLU:OE2	2.50	0.45
4:D:117:ALA:HB2	4:D:367:ILE:HG13	1.98	0.45
12:L:194:ASN:CG	38:m:126:ILE:HD11	2.42	0.45
12:L:230:HIS:N	12:L:231:PRO:HD3	2.31	0.45
13:M:370:PRO:HB3	13:M:375:LEU:HD23	1.98	0.45
14:N:175:MET:HE2	14:N:219:LEU:HD11	1.99	0.45
22:W:44:GLU:CD	22:W:96:ILE:HG22	2.41	0.45
22:W:56:ILE:HG21	22:W:109:PHE:HE1	1.82	0.45
38:m:102:TYR:O	38:m:106:THR:HG23	2.17	0.45
7:G:11:VAL:HG12	7:G:12:PHE:N	2.32	0.45
13:M:134:THR:O	13:M:142:ARG:NE	2.45	0.45
14:N:221:LEU:CD2	14:N:240:MET:HE3	2.47	0.45
23:X:136:LEU:HD23	23:X:136:LEU:H	1.81	0.45
4:D:335:ARG:NH2	9:I:128:CYS:O	2.48	0.45
7:G:171:ASP:OD1	7:G:172:LEU:N	2.49	0.45
12:L:114:ILE:O	12:L:118:ILE:HG12	2.17	0.45
12:L:294:THR:CB	12:L:524:THR:HG1	2.22	0.45
13:M:130:LEU:O	13:M:134:THR:HG23	2.17	0.45
15:O:3:TYR:O	15:O:3:TYR:CD2	2.69	0.45
22:W:23:PHE:O	22:W:33:ARG:NH1	2.50	0.45
40:o:10:TRP:O	40:o:11:ASP:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:284:ASP:OD1	9:I:1:THR:OG1	2.33	0.44
6:F:60:MET:O	6:F:63:SER:OG	2.25	0.44
6:F:351:ILE:HD11	6:F:415:VAL:HG23	1.98	0.44
7:G:322:LEU:N	7:G:322:LEU:HD12	2.31	0.44
7:G:362:TYR:O	7:G:363:LEU:HD23	2.17	0.44
8:H:45:ILE:C	8:H:46:LEU:HD22	2.42	0.44
8:H:89:LEU:CB	8:H:91:MET:HE2	2.47	0.44
10:J:13:LEU:HD11	11:K:10:MET:HE2	2.00	0.44
12:L:241:THR:N	12:L:242:PRO:CD	2.80	0.44
13:M:17:LEU:HD12	13:M:18:SER:N	2.32	0.44
13:M:115:LEU:HD21	13:M:176:LEU:HD21	1.99	0.44
13:M:165:ILE:HG21	14:N:271:MET:HG3	1.99	0.44
13:M:168:GLN:HG2	23:X:167:PHE:CZ	2.51	0.44
13:M:344:MET:CE	13:M:423:MET:HE1	2.46	0.44
14:N:24:THR:O	14:N:24:THR:HG22	2.16	0.44
15:O:305:ALA:HB1	15:O:306:PRO:HD2	1.99	0.44
21:V:64:VAL:HG13	21:V:76:VAL:CG1	2.47	0.44
37:l:127:VAL:HG11	40:o:94:TYR:CZ	2.52	0.44
40:o:6:ARG:HA	40:o:10:TRP:HB2	1.99	0.44
3:C:78:LEU:HD23	3:C:78:LEU:C	2.42	0.44
4:D:80:ILE:CG2	4:D:81:GLY:N	2.80	0.44
11:K:1:FME:HE1	11:K:5:PHE:HD1	1.80	0.44
12:L:245:ALA:HB2	12:L:340:PHE:CB	2.47	0.44
14:N:146:TYR:N	14:N:147:PRO:CD	2.80	0.44
16:P:205:VAL:HG22	16:P:206:TYR:N	2.32	0.44
22:W:22:ILE:HG22	22:W:79:ARG:HG2	1.99	0.44
38:m:112:GLU:OE2	38:m:116:GLN:NE2	2.50	0.44
6:F:399:ILE:O	6:F:400:GLU:C	2.60	0.44
13:M:175:ASN:OD1	13:M:176:LEU:N	2.50	0.44
16:P:143:SER:OG	16:P:144:LYS:N	2.49	0.44
41:p:54:GLN:O	41:p:57:LYS:HG2	2.16	0.44
7:G:114:CYS:SG	7:G:117:GLN:N	2.78	0.44
8:H:145:THR:O	8:H:149:ILE:HG12	2.17	0.44
8:H:166:ILE:CG2	8:H:247:TYR:HB2	2.48	0.44
12:L:221:THR:HG22	12:L:280:LEU:HD21	1.99	0.44
13:M:171:VAL:CG1	13:M:172:GLY:N	2.81	0.44
14:N:45:ILE:HD11	14:N:53:THR:HG22	1.98	0.44
18:R:22:ASP:OD2	18:R:24:ARG:NH2	2.46	0.44
34:i:74:VAL:O	34:i:78:MET:HB2	2.18	0.44
34:i:109:ILE:HG23	41:p:16:THR:O	2.17	0.44
5:E:95:VAL:HG12	5:E:96:GLY:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:591:GLY:CA	16:P:6:ILE:HG21	2.48	0.44
20:T:77:VAL:HA	20:T:80:ILE:HG22	2.00	0.44
29:d:116:PHE:O	29:d:117:HIS:ND1	2.51	0.44
38:m:83:PRO:C	38:m:85:ASN:H	2.25	0.44
5:E:63:ILE:HD12	5:E:81:TYR:CE1	2.53	0.44
13:M:237:LYS:HG3	13:M:316:MET:CG	2.48	0.44
15:O:191:GLU:OE2	51:O:401:ATP:O3'	2.35	0.44
17:Q:105:VAL:HG12	17:Q:106:GLU:N	2.32	0.44
20:U:46:ASP:O	20:U:50:ILE:HG12	2.17	0.44
21:V:47:THR:O	21:V:51:THR:HG23	2.17	0.44
22:W:30:ALA:HB1	22:W:81:VAL:HG11	1.99	0.44
33:h:107:GLU:OE2	33:h:111:ARG:NH2	2.50	0.44
4:D:80:ILE:HD11	4:D:399:LEU:HD11	1.99	0.44
6:F:109:GLU:OE2	6:F:112:ARG:NH2	2.47	0.44
8:H:96:ILE:HG22	8:H:98:LEU:HG	2.00	0.44
9:I:1:THR:OG1	9:I:1:THR:O	2.35	0.44
9:I:16:MET:O	9:I:20:THR:OG1	2.29	0.44
14:N:211:LEU:HD21	14:N:333:SER:HB2	2.00	0.44
15:O:5:LEU:HD12	15:O:257:HIS:NE2	2.33	0.44
16:P:48:PRO:HB2	16:P:73:TRP:CD1	2.53	0.44
24:Y:38:SER:O	24:Y:42:VAL:HG23	2.17	0.44
3:C:32:ILE:HG22	3:C:33:LEU:HD13	1.98	0.44
5:E:149:VAL:HG13	5:E:150:ASN:H	1.82	0.44
12:L:194:ASN:ND2	38:m:126:ILE:HD11	2.33	0.44
12:L:574:THR:HG23	14:N:167:TRP:O	2.18	0.44
13:M:282:LEU:HD12	13:M:342:MET:HE3	1.98	0.44
14:N:277:ILE:HG23	14:N:278:MET:N	2.32	0.44
22:W:56:ILE:HD13	22:W:109:PHE:HE1	1.83	0.44
30:e:21:SER:O	30:e:21:SER:OG	2.32	0.44
4:D:402:LEU:HD12	4:D:417:ILE:HG21	1.99	0.44
4:D:415:VAL:HG13	4:D:416:ALA:N	2.33	0.44
14:N:273:ASN:OD1	24:Y:142:VAL:N	2.50	0.44
14:N:304:MET:HB2	15:O:286:ALA:HB1	2.00	0.44
32:g:19:GLU:N	32:g:20:PRO:CD	2.81	0.44
3:C:57:VAL:O	3:C:61:LEU:HD23	2.18	0.43
4:D:83:LEU:N	4:D:429:ASP:OD2	2.50	0.43
4:D:174:ARG:HA	4:D:177:MET:HE2	2.00	0.43
10:J:115:ILE:HG22	11:K:3:SER:CB	2.48	0.43
12:L:313:MET:HA	12:L:316:THR:HG22	2.00	0.43
13:M:306:PRO:HA	13:M:458:THR:HG21	2.00	0.43
17:Q:17:LEU:HD12	17:Q:18:ASP:H	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:50:TYR:O	27:b:51:ASN:ND2	2.51	0.43
28:c:45:ARG:NH2	29:d:16:ASP:OD1	2.46	0.43
4:D:236:ARG:O	4:D:240:VAL:HG23	2.17	0.43
4:D:342:MET:HE3	4:D:346:ILE:HD11	2.00	0.43
7:G:283:MET:HE3	7:G:293:TYR:CE1	2.46	0.43
10:J:13:LEU:C	10:J:13:LEU:HD23	2.43	0.43
13:M:83:HIS:O	13:M:84:LEU:HG	2.18	0.43
13:M:126:LEU:O	13:M:127:ILE:C	2.61	0.43
14:N:317:GLN:NE2	15:O:106:LEU:HD21	2.30	0.43
23:X:17:VAL:HG23	23:X:18:LYS:N	2.32	0.43
23:X:128:THR:OG1	27:b:66:PRO:O	2.23	0.43
25:Z:29:LEU:HD23	25:Z:29:LEU:N	2.33	0.43
25:Z:143:THR:HG23	26:a:48:MET:HE1	2.00	0.43
34:i:112:THR:HG23	34:i:113:GLY:N	2.28	0.43
36:k:68:PHE:CE1	36:k:72:ILE:HG13	2.53	0.43
4:D:208:LEU:HG	25:Z:9:MET:HE3	1.99	0.43
6:F:297:VAL:CG1	6:F:298:ILE:N	2.81	0.43
10:J:101:PHE:O	10:J:105:VAL:HG23	2.19	0.43
11:K:57:MET:O	11:K:60:PRO:HG2	2.19	0.43
12:L:174:TYR:HD1	12:L:229:LEU:HD23	1.83	0.43
15:O:56:ILE:O	15:O:56:ILE:HG22	2.18	0.43
23:X:148:GLU:OE1	23:X:148:GLU:N	2.50	0.43
6:F:388:GLU:O	6:F:391:SER:OG	2.26	0.43
7:G:411:SER:O	7:G:413:VAL:HG23	2.17	0.43
12:L:86:SER:OG	12:L:132:THR:O	2.34	0.43
12:L:130:ILE:O	12:L:134:ALA:HB2	2.18	0.43
12:L:180:ILE:HD12	13:M:397:GLY:CA	2.48	0.43
13:M:368:ALA:HB1	13:M:375:LEU:CD1	2.49	0.43
14:N:43:MET:HB3	14:N:126:MET:HE2	1.99	0.43
14:N:97:MET:HA	14:N:100:MET:HE2	2.01	0.43
40:o:45:MET:HE3	40:o:55:ARG:CG	2.48	0.43
41:p:38:LEU:C	41:p:38:LEU:HD23	2.44	0.43
1:A:24:LEU:HD12	8:H:56:PHE:HB3	2.01	0.43
3:C:79:THR:HG22	3:C:80:ALA:N	2.33	0.43
7:G:105:CYS:HB2	7:G:106:PRO:HD3	2.01	0.43
13:M:225:ILE:HG23	13:M:226:ALA:N	2.34	0.43
14:N:190:MET:O	14:N:193:ILE:HG22	2.18	0.43
14:N:276:LEU:HD23	14:N:276:LEU:H	1.84	0.43
15:O:144:ILE:CG2	15:O:145:ARG:N	2.82	0.43
17:Q:82:MET:HE2	17:Q:82:MET:HA	2.00	0.43
23:X:167:PHE:O	23:X:168:PHE:CD1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:10:THR:HG22	4:D:325:VAL:HG23	2.01	0.43
8:H:281:ARG:NH1	8:H:283:ASP:OD2	2.52	0.43
11:K:84:THR:HG23	11:K:85:TYR:CD2	2.54	0.43
12:L:357:ARG:NH1	39:n:28:SER:OG	2.52	0.43
13:M:95:TYR:OH	13:M:226:ALA:HB3	2.17	0.43
13:M:126:LEU:O	13:M:129:THR:N	2.51	0.43
13:M:216:LEU:HB3	13:M:217:PRO:HD3	2.00	0.43
13:M:318:ALA:HB2	13:M:373:ILE:HG13	2.01	0.43
14:N:325:MET:O	14:N:329:LEU:HG	2.18	0.43
34:i:109:ILE:HB	34:i:113:GLY:HA3	2.01	0.43
37:l:8:LEU:O	37:l:25:LYS:NZ	2.49	0.43
39:n:161:ASP:OD1	39:n:162:LEU:N	2.51	0.43
9:I:67:HIS:ND1	9:I:115:MET:SD	2.89	0.43
12:L:221:THR:HG21	12:L:280:LEU:HD21	1.98	0.43
14:N:130:LEU:O	14:N:135:LYS:NZ	2.51	0.43
29:d:31:LEU:HD12	29:d:69:VAL:HG13	2.01	0.43
29:d:93:TYR:HD2	33:h:114:MET:HE3	1.80	0.43
5:E:14:GLU:OE1	5:E:14:GLU:N	2.51	0.43
5:E:106:THR:HB	5:E:107:PRO:HD3	2.01	0.43
6:F:394:GLU:OE1	7:G:129:ARG:NH1	2.48	0.43
7:G:432:ILE:O	7:G:435:GLY:N	2.52	0.43
8:H:172:MET:HE3	8:H:172:MET:HB3	1.93	0.43
11:K:12:PHE:CE2	11:K:40:LEU:HD21	2.53	0.43
12:L:245:ALA:O	12:L:249:SER:N	2.51	0.43
12:L:452:ASN:N	12:L:453:PRO:CD	2.82	0.43
13:M:231:LEU:O	13:M:236:LEU:HD13	2.19	0.43
14:N:88:GLN:N	14:N:89:GLN:OE1	2.52	0.43
14:N:118:VAL:HG12	14:N:122:ILE:HD11	2.01	0.43
20:T:13:ASP:O	20:T:16:LEU:HG	2.18	0.43
37:l:125:GLN:O	37:l:127:VAL:N	2.49	0.43
38:m:83:PRO:O	38:m:84:LYS:HB3	2.18	0.43
40:o:76:PHE:O	40:o:77:LEU:HB2	2.18	0.43
2:B:148:ARG:O	16:P:61:LEU:HD13	2.19	0.43
6:F:389:ILE:HG21	6:F:423:ARG:HH11	1.84	0.43
12:L:152:PHE:C	12:L:152:PHE:CD2	2.97	0.43
12:L:208:ASP:O	12:L:209:ASN:OD1	2.36	0.43
12:L:505:ASN:HA	12:L:508:THR:HG23	2.00	0.43
13:M:23:THR:O	13:M:27:VAL:HG12	2.19	0.43
14:N:46:ASN:OD1	14:N:47:LYS:N	2.50	0.43
14:N:291:PHE:C	14:N:291:PHE:CD2	2.97	0.43
20:T:11:ILE:N	20:T:13:ASP:OD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:r:56:ARG:O	43:r:57:ASP:C	2.62	0.43
6:F:120:GLU:OE2	6:F:236:ARG:NH2	2.52	0.43
6:F:268:VAL:HG12	6:F:269:GLU:N	2.34	0.43
8:H:148:ILE:HG21	8:H:297:THR:HG22	2.00	0.43
12:L:417:SER:HB2	12:L:493:ILE:HG12	2.01	0.43
14:N:337:LEU:N	14:N:338:PRO:CD	2.82	0.43
15:O:138:MET:CB	15:O:144:ILE:HD12	2.48	0.43
20:T:47:GLN:O	20:T:51:ILE:HG12	2.19	0.43
40:o:18:PRO:HA	40:o:21:ILE:HD11	2.01	0.43
8:H:100:LEU:CB	10:J:53:LEU:HD13	2.49	0.42
8:H:125:SER:HG	8:H:128:SER:CB	2.29	0.42
13:M:186:LEU:HD12	13:M:186:LEU:N	2.34	0.42
14:N:226:THR:HG22	14:N:227:ILE:N	2.34	0.42
14:N:298:TYR:O	14:N:303:THR:HG22	2.18	0.42
16:P:146:LEU:HD12	16:P:146:LEU:N	2.34	0.42
23:X:28:ALA:O	23:X:29:HIS:C	2.62	0.42
25:Z:97:MET:HE2	25:Z:103:TRP:CD2	2.53	0.42
1:A:78:ALA:HB2	10:J:142:ALA:HB1	2.01	0.42
4:D:165:THR:N	4:D:166:PRO:CD	2.83	0.42
6:F:263:ASN:ND2	6:F:286:GLY:O	2.52	0.42
6:F:273:SER:O	6:F:316:LEU:HD22	2.19	0.42
7:G:218:ARG:HH11	9:I:82:CYS:HA	1.85	0.42
12:L:167:ALA:HB2	12:L:235:SER:OG	2.19	0.42
32:g:53:VAL:O	32:g:56:MET:HG3	2.18	0.42
32:g:118:LEU:HD23	41:p:163:LEU:HD12	2.01	0.42
33:h:134:ASP:OD1	33:h:136:SER:N	2.47	0.42
39:n:100:GLU:O	39:n:103:LEU:HG	2.19	0.42
7:G:27:LEU:HD21	7:G:39:ARG:NH2	2.35	0.42
7:G:123:PHE:CD1	7:G:123:PHE:N	2.85	0.42
12:L:113:ASN:HB2	12:L:157:TRP:CZ2	2.54	0.42
12:L:332:HIS:NE2	12:L:336:LYS:HE3	2.34	0.42
1:A:68:GLU:HG2	1:A:98:LEU:HD22	2.01	0.42
1:A:106:TRP:C	1:A:106:TRP:CD1	2.97	0.42
7:G:402:ASN:O	7:G:403:ASP:C	2.62	0.42
11:K:1:FME:N	11:K:2:PRO:HD2	2.34	0.42
12:L:309:GLN:HE21	12:L:380:LEU:HD11	1.85	0.42
12:L:509:MET:O	12:L:510:LYS:HB3	2.20	0.42
12:L:589:MET:O	12:L:593:ILE:HG12	2.19	0.42
13:M:168:GLN:NE2	13:M:168:GLN:O	2.49	0.42
16:P:201:VAL:CG2	16:P:237:LEU:HD23	2.50	0.42
22:W:109:PHE:N	22:W:109:PHE:CD2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:29:SER:HB3	36:k:74:LYS:O	2.20	0.42
37:l:82:MET:HE3	37:l:83:TYR:OH	2.18	0.42
37:l:85:ARG:O	37:l:85:ARG:HG2	2.20	0.42
37:l:127:VAL:HG12	40:o:98:MET:CG	2.49	0.42
3:C:18:THR:HG22	3:C:22:LEU:HD12	2.01	0.42
4:D:323:ILE:HG13	4:D:324:LYS:N	2.35	0.42
5:E:140:ILE:HG22	5:E:141:GLU:N	2.34	0.42
7:G:680:ALA:O	7:G:681:SER:C	2.62	0.42
8:H:176:LEU:HB2	8:H:177:PRO:HD3	2.02	0.42
12:L:362:ILE:HA	12:L:365:ILE:CG2	2.50	0.42
12:L:441:ILE:HG23	12:L:443:ILE:HG12	2.02	0.42
14:N:40:ILE:O	14:N:41:ILE:C	2.61	0.42
16:P:334:THR:HG22	16:P:335:LYS:N	2.34	0.42
23:X:117:VAL:HG13	23:X:117:VAL:O	2.19	0.42
43:r:97:ALA:HB1	43:r:98:PRO:HD2	2.02	0.42
3:C:19:HIS:O	3:C:19:HIS:ND1	2.52	0.42
6:F:344:VAL:HG21	6:F:426:LEU:HD21	2.02	0.42
7:G:357:ASP:OD2	19:S:40:TYR:OH	2.37	0.42
12:L:532:ILE:HD11	37:l:104:LEU:CD2	2.49	0.42
2:B:69:MET:SD	2:B:97:ILE:HG21	2.60	0.42
2:B:85:VAL:HG12	2:B:86:PHE:N	2.35	0.42
3:C:195:ARG:NH2	9:I:94:ILE:O	2.49	0.42
4:D:93:TYR:OH	17:Q:82:MET:HE1	2.19	0.42
14:N:5:THR:HG22	14:N:9:ILE:HD12	2.02	0.42
14:N:59:TYR:CE1	14:N:63:GLN:NE2	2.87	0.42
14:N:89:GLN:OE1	14:N:89:GLN:N	2.52	0.42
17:Q:10:LEU:O	17:Q:11:ILE:HD13	2.19	0.42
20:T:32:VAL:HG12	20:T:74:GLN:HB2	2.02	0.42
23:X:128:THR:HG23	23:X:128:THR:O	2.19	0.42
37:l:114:MET:HE2	37:l:114:MET:HA	2.00	0.42
3:C:83:VAL:HG12	3:C:85:THR:HG22	2.02	0.42
4:D:132:PRO:O	4:D:136:TRP:HD1	2.03	0.42
10:J:75:THR:HG22	10:J:76:GLU:N	2.35	0.42
10:J:76:GLU:OE1	10:J:78:TYR:OH	2.37	0.42
12:L:17:SER:HB2	12:L:18:PRO:HD3	2.01	0.42
12:L:252:MET:HG2	12:L:252:MET:O	2.20	0.42
12:L:384:PRO:HB2	12:L:385:PHE:HD2	1.84	0.42
12:L:449:ASP:OD1	12:L:449:ASP:N	2.53	0.42
13:M:109:THR:HG23	13:M:110:PHE:N	2.34	0.42
14:N:221:LEU:HD22	14:N:240:MET:HE3	2.01	0.42
14:N:267:ILE:O	14:N:271:MET:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:79:LEU:HD11	15:O:83:TYR:CE2	2.54	0.42
20:U:9:ASP:OD1	20:U:10:GLY:N	2.50	0.42
37:l:95:VAL:HG12	37:l:96:SER:H	1.84	0.42
40:o:55:ARG:CG	40:o:55:ARG:O	2.68	0.42
9:I:16:MET:HE2	25:Z:32:TYR:OH	2.20	0.42
12:L:552:LEU:CD2	38:m:88:LEU:HD23	2.50	0.42
13:M:183:THR:O	13:M:184:HIS:ND1	2.53	0.42
14:N:139:LEU:O	14:N:143:ILE:HG12	2.19	0.42
15:O:253:ASP:OD1	15:O:253:ASP:N	2.50	0.42
15:O:308:TYR:OH	15:O:320:LYS:O	2.38	0.42
21:V:61:GLU:OE1	21:V:63:ASP:N	2.50	0.42
23:X:146:ARG:NH1	30:e:58:GLU:OE2	2.53	0.42
37:l:16:PRO:HA	37:l:19:ARG:HB2	2.02	0.42
40:o:73:PHE:HB3	40:o:74:PRO:HD3	2.02	0.42
3:C:119:SER:OG	3:C:120:ILE:N	2.53	0.42
3:C:178:ASP:OD1	3:C:179:GLU:N	2.53	0.42
6:F:221:THR:HG22	6:F:222:VAL:N	2.34	0.42
8:H:132:ALA:O	8:H:136:VAL:HG23	2.19	0.42
8:H:165:LEU:HD23	8:H:241:ILE:HA	2.02	0.42
11:K:10:MET:O	11:K:14:LEU:HG	2.20	0.42
14:N:37:LEU:HD12	14:N:63:GLN:HB3	2.01	0.42
14:N:324:LEU:N	14:N:324:LEU:HD12	2.34	0.42
15:O:93:SER:HB2	15:O:144:ILE:HD11	2.01	0.42
17:Q:74:SER:O	17:Q:75:THR:HG23	2.20	0.42
1:A:65:PHE:O	1:A:69:ILE:HG12	2.19	0.41
6:F:362:CYS:SG	6:F:404:ILE:HD12	2.60	0.41
7:G:150:MET:HE2	7:G:208:LEU:HD21	2.02	0.41
7:G:349:PHE:O	7:G:350:PRO:C	2.63	0.41
7:G:359:ARG:NH1	7:G:629:ASN:OD1	2.53	0.41
7:G:399:TRP:HA	7:G:404:LEU:HB3	2.02	0.41
12:L:152:PHE:HB2	12:L:172:ILE:HD11	2.02	0.41
23:X:8:THR:O	23:X:11:GLU:HG2	2.19	0.41
25:Z:18:ILE:HG22	25:Z:19:ASP:N	2.35	0.41
32:g:118:LEU:HD21	41:p:162:MET:HE3	2.01	0.41
37:l:114:MET:HE2	37:l:114:MET:CA	2.50	0.41
1:A:93:ILE:O	1:A:97:ILE:HG23	2.19	0.41
2:B:107:ALA:HB3	2:B:108:PRO:CD	2.48	0.41
7:G:326:GLU:N	7:G:326:GLU:OE1	2.53	0.41
8:H:69:SER:O	8:H:73:ILE:HG12	2.20	0.41
9:I:152:ASN:OD1	9:I:152:ASN:C	2.63	0.41
10:J:134:MET:HE3	30:e:26:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:16:LEU:HA	11:K:36:MET:HE3	2.02	0.41
12:L:211:ILE:N	12:L:212:PRO:HD2	2.35	0.41
12:L:309:GLN:NE2	12:L:380:LEU:HD11	2.36	0.41
13:M:204:LEU:O	13:M:207:MET:O	2.39	0.41
13:M:367:LEU:C	13:M:367:LEU:HD12	2.45	0.41
13:M:441:MET:O	13:M:444:LEU:N	2.51	0.41
16:P:71:LEU:HD12	16:P:72:GLU:N	2.35	0.41
16:P:153:GLU:OE1	16:P:167:ARG:NH1	2.50	0.41
18:R:11:ILE:HG22	18:R:12:THR:O	2.20	0.41
21:V:89:LEU:HD11	21:V:93:MET:SD	2.60	0.41
32:g:60:PHE:O	32:g:64:PHE:N	2.52	0.41
37:l:90:THR:HB	38:m:10:LEU:O	2.20	0.41
3:C:51:CYS:HB3	21:V:111:TRP:CH2	2.55	0.41
4:D:80:ILE:HD11	4:D:399:LEU:CD1	2.50	0.41
8:H:87:VAL:HB	8:H:88:PRO:HD3	2.02	0.41
10:J:33:ILE:HG12	10:J:64:LEU:HD23	2.02	0.41
12:L:534:HIS:CD2	12:L:534:HIS:N	2.89	0.41
16:P:2:HIS:O	16:P:6:ILE:HG12	2.20	0.41
16:P:295:THR:O	16:P:296:ASP:OD1	2.39	0.41
17:Q:32:THR:O	17:Q:32:THR:HG22	2.20	0.41
19:S:39:ARG:O	19:S:42:GLU:N	2.49	0.41
21:V:75:GLU:O	21:V:79:VAL:HG23	2.20	0.41
36:k:65:ASN:O	36:k:67:THR:HG23	2.20	0.41
39:n:80:ILE:HG21	39:n:87:GLY:N	2.36	0.41
3:C:104:ARG:NH1	4:D:373:GLU:OE2	2.50	0.41
48:F:501:FMN:H9	48:F:501:FMN:C2'	2.51	0.41
7:G:241:SER:OG	7:G:249:ARG:HG2	2.20	0.41
7:G:328:LEU:HD11	7:G:498:SER:OG	2.20	0.41
9:I:54:PHE:CZ	42:q:30:ALA:HB2	2.55	0.41
12:L:260:LEU:HD13	12:L:277:MET:HE2	2.01	0.41
12:L:529:PHE:HB3	12:L:530:PRO:HD3	2.02	0.41
12:L:546:LEU:HD13	38:m:71:ARG:HH21	1.84	0.41
13:M:200:MET:HE2	13:M:250:LEU:CD1	2.50	0.41
13:M:210:TYR:HB2	13:M:268:GLY:HA3	2.03	0.41
13:M:229:MET:HE2	13:M:328:CYS:SG	2.61	0.41
13:M:290:SER:OG	13:M:319:HIS:NE2	2.49	0.41
14:N:26:LEU:HD12	14:N:84:TRP:O	2.20	0.41
15:O:31:ILE:HA	15:O:126:ARG:HH22	1.86	0.41
20:T:26:ASP:N	20:T:27:PRO:CD	2.84	0.41
37:l:4:THR:HG22	37:l:5:LYS:N	2.35	0.41
42:q:29:ARG:NH2	42:q:73:THR:O	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:ILE:HG22	2:B:155:TYR:N	2.36	0.41
4:D:62:LEU:HD21	4:D:418:ILE:HD13	2.02	0.41
4:D:116:GLN:NE2	4:D:276:ASP:OD2	2.53	0.41
4:D:169:TRP:CE2	9:I:42:TYR:HD2	2.38	0.41
4:D:381:ASP:O	4:D:383:SER:N	2.47	0.41
7:G:338:VAL:O	7:G:338:VAL:HG12	2.21	0.41
9:I:76:GLU:OE2	9:I:101:ARG:NH1	2.53	0.41
10:J:92:LEU:HD23	10:J:92:LEU:O	2.20	0.41
22:W:56:ILE:HD13	22:W:109:PHE:CE1	2.56	0.41
24:Y:63:THR:O	24:Y:67:ILE:HG12	2.21	0.41
34:i:83:TYR:CD2	34:i:83:TYR:C	2.99	0.41
1:A:16:THR:O	1:A:20:VAL:HG23	2.21	0.41
2:B:79:MET:HG2	2:B:84:VAL:HB	2.03	0.41
4:D:416:ALA:O	4:D:420:THR:HG23	2.19	0.41
5:E:47:VAL:O	5:E:51:LEU:HD13	2.20	0.41
6:F:137:TYR:CD1	6:F:137:TYR:C	2.99	0.41
12:L:27:ILE:HG22	12:L:115:ASN:ND2	2.35	0.41
12:L:319:MET:SD	12:L:399:ILE:HA	2.61	0.41
13:M:42:LEU:HD13	13:M:453:LEU:CD2	2.51	0.41
13:M:75:LEU:HD23	13:M:440:HIS:CD2	2.55	0.41
14:N:122:ILE:HG22	14:N:123:PRO:O	2.21	0.41
42:q:117:VAL:O	42:q:117:VAL:HG23	2.21	0.41
5:E:89:MET:HE1	6:F:140:GLY:HA3	2.02	0.41
7:G:311:GLU:N	7:G:311:GLU:OE1	2.54	0.41
7:G:477:ILE:O	7:G:480:THR:OG1	2.25	0.41
9:I:161:ASP:OD2	18:R:36:ASN:ND2	2.49	0.41
10:J:99:GLU:OE1	11:K:10:MET:HE1	2.21	0.41
12:L:103:PHE:CD1	12:L:341:MET:HG3	2.55	0.41
12:L:405:ASN:OD1	12:L:406:ALA:N	2.52	0.41
13:M:2:LEU:HB3	13:M:6:LEU:HD23	2.01	0.41
13:M:61:LEU:HD22	13:M:244:ILE:HG21	2.02	0.41
14:N:289:ASN:HA	14:N:292:PHE:CE1	2.55	0.41
15:O:25:ILE:HG22	15:O:26:THR:N	2.35	0.41
19:S:72:GLN:OE1	19:S:72:GLN:N	2.47	0.41
20:T:52:MET:HE1	22:W:42:TYR:CB	2.50	0.41
22:W:55:ASP:OD2	22:W:56:ILE:N	2.54	0.41
25:Z:9:MET:O	25:Z:9:MET:HG3	2.21	0.41
41:p:23:THR:HG23	41:p:25:LEU:H	1.84	0.41
5:E:12:THR:HB	5:E:13:PRO:HD2	2.02	0.41
8:H:228:TYR:CD1	8:H:231:ILE:HD12	2.56	0.41
8:H:291:LYS:O	8:H:292:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:113:ILE:CG2	9:I:114:ASP:N	2.83	0.41
13:M:30:TYR:O	13:M:34:ILE:HG12	2.21	0.41
13:M:300:SER:HB3	13:M:381:ILE:HG23	2.03	0.41
14:N:176:ARG:NH1	14:N:225:MET:SD	2.94	0.41
16:P:97:ARG:HG3	16:P:99:TRP:O	2.21	0.41
17:Q:105:VAL:CG1	17:Q:106:GLU:N	2.84	0.41
18:R:4:VAL:HG12	18:R:5:SER:N	2.36	0.41
23:X:93:MET:SD	26:a:40:ARG:NH2	2.86	0.41
30:e:2:PHE:C	30:e:2:PHE:CD2	2.99	0.41
36:k:41:LEU:O	36:k:46:LEU:N	2.51	0.41
1:A:89:ILE:O	1:A:93:ILE:HG12	2.20	0.41
4:D:265:ILE:HG22	4:D:266:GLN:N	2.36	0.41
5:E:70:ALA:HA	5:E:75:VAL:HG12	2.03	0.41
8:H:167:THR:OG1	23:X:97:ARG:NH2	2.54	0.41
8:H:172:MET:SD	8:H:173:TRP:N	2.94	0.41
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.55	0.41
8:H:234:MET:O	8:H:238:THR:HG23	2.20	0.41
8:H:251:LEU:N	8:H:252:PRO:HD3	2.35	0.41
10:J:78:TYR:O	10:J:80:GLU:N	2.47	0.41
12:L:424:MET:CE	12:L:502:LEU:HD21	2.51	0.41
12:L:462:ILE:HG22	12:L:463:PHE:CD1	2.56	0.41
12:L:556:ILE:HD11	38:m:75:ILE:CG2	2.51	0.41
13:M:354:LEU:O	13:M:355:MET:C	2.64	0.41
14:N:338:PRO:C	14:N:339:LEU:HD23	2.46	0.41
30:e:81:GLN:NE2	30:e:85:LEU:HD21	2.36	0.41
38:m:53:PRO:HG3	39:n:128:ARG:HE	1.84	0.41
39:n:57:MET:SD	39:n:58:ARG:N	2.94	0.41
41:p:39:VAL:HG13	41:p:40:VAL:HG23	2.02	0.41
42:q:66:THR:O	42:q:73:THR:OG1	2.11	0.41
7:G:524:LEU:HD12	7:G:524:LEU:O	2.21	0.41
8:H:139:THR:HG23	8:H:192:GLU:OE1	2.20	0.41
8:H:264:LEU:HD22	26:a:12:MET:HE2	2.02	0.41
10:J:37:PHE:O	10:J:41:LEU:HG	2.21	0.41
12:L:161:ARG:NH1	12:L:238:GLU:OE1	2.54	0.41
12:L:256:GLY:O	12:L:260:LEU:HG	2.21	0.41
12:L:386:LEU:HD21	35:j:36:ILE:HD11	2.02	0.41
12:L:409:LEU:O	12:L:413:LEU:HG	2.20	0.41
12:L:562:ILE:HB	12:L:563:PRO:CD	2.51	0.41
13:M:160:LEU:O	13:M:164:LEU:HG	2.20	0.41
15:O:5:LEU:HD12	15:O:257:HIS:CE1	2.56	0.41
37:l:95:VAL:HG12	37:l:96:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:q:30:ALA:O	42:q:32:ASP:N	2.49	0.41
4:D:395:GLY:HA3	4:D:428:ILE:HD11	2.03	0.40
5:E:63:ILE:HG23	5:E:64:SER:N	2.36	0.40
5:E:199:LEU:HD11	6:F:28:ARG:HH22	1.85	0.40
6:F:372:MET:O	6:F:376:MET:HG2	2.21	0.40
12:L:161:ARG:O	12:L:162:THR:C	2.63	0.40
13:M:17:LEU:HD11	31:f:11:VAL:HG12	2.01	0.40
13:M:78:MET:HE2	13:M:436:LEU:HD21	2.03	0.40
13:M:263:LEU:CD1	38:m:100:TRP:HB2	2.51	0.40
13:M:348:LEU:O	13:M:349:GLN:HB3	2.20	0.40
16:P:29:PHE:HE1	16:P:174:ARG:O	2.04	0.40
16:P:54:TYR:HA	16:P:57:MET:HG2	2.04	0.40
16:P:111:VAL:HG22	16:P:152:GLY:CA	2.52	0.40
16:P:121:SER:OG	16:P:126:VAL:HG21	2.21	0.40
50:d:201:CDL:O1	31:f:29:ASP:OD1	2.38	0.40
3:C:114:LEU:HD11	17:Q:19:ILE:CG2	2.51	0.40
3:C:179:GLU:HG2	3:C:180:VAL:HG13	2.03	0.40
4:D:68:LEU:HD23	4:D:72:MET:O	2.21	0.40
4:D:80:ILE:HG22	4:D:81:GLY:N	2.35	0.40
6:F:304:THR:HG21	6:F:328:GLY:O	2.20	0.40
8:H:186:PHE:O	8:H:186:PHE:CG	2.73	0.40
12:L:32:PHE:N	12:L:33:PRO:CD	2.84	0.40
12:L:292:ALA:O	12:L:422:TYR:HB3	2.20	0.40
13:M:369:LEU:HD23	13:M:370:PRO:O	2.22	0.40
15:O:214:MET:HB3	15:O:218:CYS:SG	2.61	0.40
20:T:48:VAL:HG13	22:W:39:ARG:HE	1.86	0.40
32:g:90:GLU:O	32:g:94:LEU:HD23	2.21	0.40
32:g:118:LEU:HD23	41:p:163:LEU:CD1	2.51	0.40
41:p:81:VAL:HG23	41:p:82:LEU:N	2.37	0.40
42:q:58:ARG:O	42:q:58:ARG:CG	2.69	0.40
2:B:62:LEU:HD13	2:B:101:THR:O	2.21	0.40
2:B:70:MET:HB3	4:D:171:PHE:HE2	1.86	0.40
5:E:19:THR:HG23	5:E:20:PRO:HD2	2.04	0.40
7:G:450:MET:HE3	7:G:491:ASN:OD1	2.21	0.40
8:H:75:PRO:HB2	8:H:222:LEU:HD12	2.04	0.40
12:L:285:THR:O	12:L:415:ALA:HB2	2.21	0.40
13:M:403:THR:HA	13:M:406:TYR:CE1	2.57	0.40
15:O:6:LEU:O	15:O:10:LEU:HG	2.22	0.40
42:q:8:LYS:HA	42:q:11:VAL:HG22	2.02	0.40
43:r:42:VAL:HB	43:r:46:HIS:CD2	2.56	0.40
43:r:95:THR:HB	43:r:96:PRO:HD2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:128:ASN:HA	3:C:145:HIS:HE2	1.86	0.40
3:C:202:PRO:HB2	17:Q:48:GLY:HA3	2.03	0.40
4:D:391:ILE:HG22	4:D:392:LYS:N	2.36	0.40
6:F:306:LEU:H	6:F:306:LEU:HD23	1.87	0.40
7:G:191:PHE:O	7:G:191:PHE:CG	2.73	0.40
12:L:83:ASP:O	12:L:84:PHE:C	2.64	0.40
13:M:209:LEU:CD2	13:M:298:ILE:HD13	2.51	0.40
13:M:277:LEU:HD23	13:M:406:TYR:HB3	2.03	0.40
14:N:49:ASN:O	14:N:53:THR:HG23	2.22	0.40
15:O:104:ARG:NH2	15:O:131:ASP:OD1	2.49	0.40
15:O:154:GLU:OE2	15:O:158:LEU:HD11	2.21	0.40
16:P:57:MET:HE1	16:P:60:ARG:NE	2.36	0.40
22:W:44:GLU:O	22:W:45:VAL:C	2.63	0.40
23:X:19:VAL:HG13	26:a:65:GLY:O	2.21	0.40
26:a:18:ILE:N	26:a:19:PRO:CD	2.84	0.40
33:h:36:VAL:O	33:h:40:ILE:HG12	2.22	0.40
33:h:138:LYS:O	33:h:139:ALA:HB3	2.20	0.40
35:j:18:THR:HG22	35:j:19:ARG:N	2.36	0.40
35:j:18:THR:HG22	35:j:19:ARG:H	1.87	0.40
43:r:51:ASN:O	43:r:51:ASN:CG	2.65	0.40
5:E:145:LEU:HD12	5:E:153:MET:SD	2.61	0.40
6:F:367:GLU:OE1	7:G:100:ASN:ND2	2.55	0.40
7:G:323:VAL:HG12	7:G:324:ASP:N	2.37	0.40
7:G:476:LYS:O	7:G:479:VAL:HG22	2.22	0.40
8:H:96:ILE:HG22	8:H:98:LEU:CG	2.51	0.40
9:I:2:TYR:CZ	43:r:105:LEU:HD23	2.57	0.40
12:L:313:MET:SD	12:L:329:ILE:HG13	2.62	0.40
14:N:328:THR:HA	29:d:41:THR:HG21	2.03	0.40
16:P:64:ASP:OD1	16:P:65:LEU:N	2.39	0.40
23:X:69:PHE:CZ	23:X:73:ILE:HD11	2.56	0.40
25:Z:8:ASP:OD1	25:Z:8:ASP:N	2.54	0.40
26:a:45:TRP:CZ3	26:a:48:MET:HE2	2.57	0.40
39:n:19:TYR:CE2	39:n:23:LEU:HD11	2.57	0.40
43:r:8:GLN:O	43:r:12:ASN:ND2	2.55	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	89/115 (77%)	83 (93%)	6 (7%)	0	100	100
2	B	153/224 (68%)	136 (89%)	17 (11%)	0	100	100
3	C	205/263 (78%)	181 (88%)	24 (12%)	0	100	100
4	D	410/463 (89%)	379 (92%)	30 (7%)	1 (0%)	43	73
5	E	208/248 (84%)	180 (86%)	28 (14%)	0	100	100
6	F	426/464 (92%)	385 (90%)	41 (10%)	0	100	100
7	G	684/727 (94%)	617 (90%)	67 (10%)	0	100	100
8	H	299/318 (94%)	267 (89%)	32 (11%)	0	100	100
9	I	176/212 (83%)	157 (89%)	19 (11%)	0	100	100
10	J	169/172 (98%)	154 (91%)	15 (9%)	0	100	100
11	K	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
12	L	604/607 (100%)	544 (90%)	60 (10%)	0	100	100
13	M	457/459 (100%)	411 (90%)	46 (10%)	0	100	100
14	N	342/345 (99%)	316 (92%)	26 (8%)	0	100	100
15	O	317/355 (89%)	283 (89%)	34 (11%)	0	100	100
16	P	280/377 (74%)	244 (87%)	36 (13%)	0	100	100
17	Q	123/175 (70%)	111 (90%)	12 (10%)	0	100	100
18	R	92/116 (79%)	84 (91%)	8 (9%)	0	100	100
19	S	80/99 (81%)	76 (95%)	4 (5%)	0	100	100
20	T	70/156 (45%)	62 (89%)	8 (11%)	0	100	100
20	U	86/156 (55%)	75 (87%)	11 (13%)	0	100	100
21	V	110/116 (95%)	99 (90%)	11 (10%)	0	100	100
22	W	112/131 (86%)	103 (92%)	9 (8%)	0	100	100
23	X	169/172 (98%)	153 (90%)	15 (9%)	1 (1%)	21	55
24	Y	138/143 (96%)	129 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	Z	137/144 (95%)	126 (92%)	11 (8%)	0	100	100
26	a	66/68 (97%)	62 (94%)	4 (6%)	0	100	100
27	b	80/84 (95%)	69 (86%)	11 (14%)	0	100	100
28	c	44/76 (58%)	41 (93%)	3 (7%)	0	100	100
29	d	117/120 (98%)	109 (93%)	8 (7%)	0	100	100
30	e	102/106 (96%)	87 (85%)	15 (15%)	0	100	100
31	f	49/57 (86%)	41 (84%)	8 (16%)	0	100	100
32	g	100/151 (66%)	88 (88%)	12 (12%)	0	100	100
33	h	135/189 (71%)	121 (90%)	14 (10%)	0	100	100
34	i	91/128 (71%)	71 (78%)	20 (22%)	0	100	100
35	j	60/105 (57%)	55 (92%)	5 (8%)	0	100	100
36	k	75/104 (72%)	69 (92%)	6 (8%)	0	100	100
37	l	154/186 (83%)	132 (86%)	22 (14%)	0	100	100
38	m	123/129 (95%)	114 (93%)	9 (7%)	0	100	100
39	n	174/179 (97%)	162 (93%)	12 (7%)	0	100	100
40	o	112/137 (82%)	95 (85%)	17 (15%)	0	100	100
41	p	166/176 (94%)	151 (91%)	15 (9%)	0	100	100
42	q	141/145 (97%)	122 (86%)	19 (14%)	0	100	100
43	r	92/112 (82%)	80 (87%)	12 (13%)	0	100	100
44	s	37/104 (36%)	34 (92%)	3 (8%)	0	100	100
All	All	7950/9211 (86%)	7148 (90%)	800 (10%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
23	X	168	PHE
4	D	86	GLY

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	84/103 (82%)	84 (100%)	0	100	100
2	B	131/185 (71%)	131 (100%)	0	100	100
3	C	189/227 (83%)	189 (100%)	0	100	100
4	D	361/394 (92%)	361 (100%)	0	100	100
5	E	183/206 (89%)	183 (100%)	0	100	100
6	F	343/370 (93%)	343 (100%)	0	100	100
7	G	578/610 (95%)	578 (100%)	0	100	100
8	H	267/279 (96%)	267 (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	283/309 (92%)	283 (100%)	0	100	100
16	P	249/325 (77%)	249 (100%)	0	100	100
17	Q	112/153 (73%)	112 (100%)	0	100	100
18	R	79/96 (82%)	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	72/73 (99%)	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
31	f	47/53 (89%)	47 (100%)	0	100	100
32	g	93/129 (72%)	93 (100%)	0	100	100
33	h	122/162 (75%)	122 (100%)	0	100	100
34	i	90/120 (75%)	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
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	7060/7946 (89%)	7060 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
2	B	172	GLN
3	C	41	GLN
3	C	67	HIS
3	C	88	ASN
4	D	347	HIS
5	E	15	ASN
5	E	27	ASN
5	E	37	ASN
5	E	101	GLN
5	E	155	GLN
6	F	96	ASN
6	F	437	HIS
7	G	179	ASN
7	G	336	ASN
7	G	365	ASN

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Mol	Chain	Res	Type
7	G	546	GLN
7	G	682	GLN
8	H	235	ASN
8	H	258	ASN
8	H	304	HIS
9	I	92	GLN
9	I	172	GLN
10	J	3	ASN
11	K	92	ASN
12	L	29	HIS
12	L	135	ASN
12	L	321	GLN
12	L	328	HIS
12	L	354	GLN
12	L	400	ASN
12	L	471	ASN
12	L	506	ASN
12	L	534	HIS
12	L	572	ASN
12	L	594	ASN
13	M	81	GLN
13	M	138	ASN
13	M	170	HIS
13	M	338	HIS
13	M	422	HIS
14	N	87	GLN
14	N	88	GLN
14	N	172	GLN
14	N	174	GLN
15	O	19	HIS
15	O	50	HIS
15	O	57	GLN
15	O	114	HIS
15	O	120	GLN
15	O	141	GLN
15	O	180	GLN
15	O	184	GLN
15	O	204	ASN
15	O	287	HIS
16	P	2	HIS
16	P	3	HIS
16	P	58	HIS

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Mol	Chain	Res	Type
16	P	131	HIS
16	P	134	HIS
16	P	240	HIS
18	R	3	GLN
18	R	68	HIS
20	U	74	GLN
22	W	47	ASN
23	X	30	HIS
23	X	34	GLN
23	X	101	GLN
23	X	102	GLN
23	X	108	GLN
23	X	142	HIS
24	Y	18	GLN
25	Z	89	ASN
25	Z	102	ASN
25	Z	134	ASN
26	a	68	ASN
27	b	51	ASN
33	h	44	ASN
33	h	135	HIS
34	i	12	GLN
37	l	2	HIS
37	l	51	ASN
37	l	77	HIS
37	l	125	GLN
37	l	154	HIS
38	m	74	ASN
38	m	116	GLN
38	m	125	ASN
39	n	73	ASN
40	o	81	HIS
40	o	84	HIS
40	o	109	GLN
41	p	90	GLN
41	p	139	GLN
42	q	12	GLN
42	q	13	GLN
42	q	91	HIS
42	q	112	ASN
42	q	123	GLN
43	r	12	ASN

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Mol	Chain	Res	Type
43	r	46	HIS
43	r	109	GLN
44	s	38	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

9 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	$\#\|Z\| > 2$
11	FME	K	1	11	8,9,10	0.94	0	7,9,11	1.35	1 (14%)
4	2MR	D	85	4	10,12,13	2.46	2 (20%)	5,13,15	1.72	2 (40%)
12	FME	L	1	12	8,9,10	0.95	0	7,9,11	0.93	0
13	FME	M	1	13	8,9,10	0.95	0	7,9,11	0.67	0
14	FME	N	1	14	8,9,10	0.89	0	7,9,11	1.22	1 (14%)
43	AYA	r	1	43	6,7,8	1.29	1 (16%)	5,8,10	1.26	1 (20%)
8	FME	H	1	8	8,9,10	0.93	0	7,9,11	1.13	1 (14%)
10	FME	J	1	10	8,9,10	0.92	0	7,9,11	0.85	0
1	FME	A	1	1	8,9,10	0.89	0	7,9,11	1.46	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
11	FME	K	1	11	-	3/7/9/11	-
4	2MR	D	85	4	-	3/10/13/15	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	FME	L	1	12	-	3/7/9/11	-
13	FME	M	1	13	-	1/7/9/11	-
14	FME	N	1	14	-	4/7/9/11	-
43	AYA	r	1	43	-	1/4/6/8	-
8	FME	H	1	8	-	2/7/9/11	-
10	FME	J	1	10	-	1/7/9/11	-
1	FME	A	1	1	-	4/7/9/11	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	85	2MR	CZ-NE	5.31	1.45	1.34
4	D	85	2MR	CZ-NH2	4.94	1.44	1.33
43	r	1	AYA	CA-N	-2.54	1.43	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	FME	C-CA-N	3.12	115.36	109.73
11	K	1	FME	C-CA-N	2.90	114.97	109.73
4	D	85	2MR	CD-NE-CZ	2.87	128.79	123.41
43	r	1	AYA	CB-CA-N	2.50	112.39	109.61
4	D	85	2MR	NE-CZ-NH2	-2.46	117.23	119.48
8	H	1	FME	C-CA-N	2.38	114.04	109.73
14	N	1	FME	CA-N-CN	2.09	126.04	122.82

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O-C-CA-CB
8	H	1	FME	CB-CA-N-CN
8	H	1	FME	CA-CB-CG-SD
11	K	1	FME	N-CA-CB-CG
12	L	1	FME	O-C-CA-CB
12	L	1	FME	CA-CB-CG-SD
13	M	1	FME	O-C-CA-CB
14	N	1	FME	CB-CA-N-CN
14	N	1	FME	C-CA-CB-CG
14	N	1	FME	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	D	85	2MR	NE-CD-CG-CB
12	L	1	FME	CB-CG-SD-CE
1	A	1	FME	N-CA-CB-CG
14	N	1	FME	N-CA-CB-CG
1	A	1	FME	CB-CG-SD-CE
10	J	1	FME	CB-CG-SD-CE
43	r	1	AYA	C-CA-N-CT
11	K	1	FME	CB-CG-SD-CE
11	K	1	FME	C-CA-CB-CG
4	D	85	2MR	CA-CB-CG-CD
1	A	1	FME	CB-CA-N-CN
4	D	85	2MR	N-CA-CB-CG

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	K	1	FME	3	0
4	D	85	2MR	1	0
14	N	1	FME	3	0
1	A	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\#\|Z\| > 2$
49	3PE	L	701	-	44,44,50	0.90	4 (9%)	47,49,55	1.12	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	3PE	M	501	-	37,37,50	0.99	4 (10%)	40,42,55	1.10	2 (5%)
45	SF4	G	802	7	0,12,12	-	-	-		
48	FMN	F	501	-	33,33,33	1.09	2 (6%)	48,50,50	1.25	9 (18%)
54	EHZ	T	201	20	29,36,37	1.69	5 (17%)	35,44,47	1.53	4 (11%)
54	EHZ	U	201	20	29,36,37	1.72	5 (17%)	35,44,47	1.55	6 (17%)
47	FES	G	803	7	0,4,4	-	-	-		
45	SF4	B	201	2	0,12,12	-	-	-		
45	SF4	F	502	6	0,12,12	-	-	-		
49	3PE	H	401	-	41,41,50	0.95	4 (9%)	44,46,55	1.26	4 (9%)
45	SF4	I	201	9	0,12,12	-	-	-		
45	SF4	G	801	7	0,12,12	-	-	-		
46	PC1	B	202	-	25,25,53	1.36	4 (16%)	31,33,61	1.10	2 (6%)
50	CDL	L	702	-	53,53,99	1.18	8 (15%)	59,65,111	1.13	4 (6%)
50	CDL	d	201	-	49,49,99	1.22	7 (14%)	55,61,111	1.35	5 (9%)
52	NDP	P	501	-	49,52,52	2.18	6 (12%)	66,80,80	1.68	11 (16%)
47	FES	E	301	5	0,4,4	-	-	-		
49	3PE	J	401	-	37,37,50	0.99	4 (10%)	40,42,55	1.11	2 (5%)
51	ATP	O	401	-	29,33,33	1.28	4 (13%)	44,52,52	2.14	12 (27%)
45	SF4	I	202	9	0,12,12	-	-	-		

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
49	3PE	L	701	-	-	25/48/48/54	-
49	3PE	M	501	-	-	23/41/41/54	-
48	FMN	F	501	-	-	10/18/18/18	0/3/3/3
54	EHZ	T	201	20	-	15/42/44/45	-
45	SF4	G	802	7	-	-	0/6/5/5
54	EHZ	U	201	20	-	24/42/44/45	-
45	SF4	B	201	2	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
45	SF4	F	502	6	-	-	0/6/5/5
49	3PE	H	401	-	-	13/45/45/54	-
45	SF4	I	201	9	-	-	0/6/5/5
45	SF4	G	801	7	-	-	0/6/5/5
46	PC1	B	202	-	-	15/29/29/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	CDL	L	702	-	-	25/64/64/110	-
50	CDL	d	201	-	-	22/59/59/110	-
52	NDP	P	501	-	-	9/34/77/77	0/5/5/5
49	3PE	J	401	-	-	18/41/41/54	-
51	ATP	O	401	-	-	5/22/38/38	0/3/3/3
47	FES	E	301	5	-	-	0/1/1/1
45	SF4	I	202	9	-	-	0/6/5/5

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	P	501	NDP	P2B-O2B	12.32	1.82	1.59
54	U	201	EHZ	C15-N2	5.60	1.45	1.33
54	T	201	EHZ	C15-N2	5.51	1.45	1.33
54	U	201	EHZ	C12-N1	5.38	1.45	1.33
54	T	201	EHZ	C12-N1	5.28	1.45	1.33
51	O	401	ATP	C5-C4	4.30	1.47	1.39
52	P	501	NDP	PN-O5D	4.09	1.75	1.59
48	F	501	FMN	C4A-N5	3.70	1.37	1.30
52	P	501	NDP	O2B-C2B	-3.14	1.32	1.44
50	d	201	CDL	OA6-CA4	-2.65	1.40	1.46
50	L	702	CDL	OB6-CB4	-2.63	1.40	1.46
50	L	702	CDL	OA6-CA4	-2.61	1.40	1.46
49	J	401	3PE	O21-C2	-2.57	1.40	1.46
49	M	501	3PE	O21-C2	-2.55	1.40	1.46
48	F	501	FMN	C10-N1	2.55	1.38	1.33
50	L	702	CDL	OB8-CB7	2.52	1.40	1.33
46	B	202	PC1	O21-C2	-2.51	1.40	1.46
50	d	201	CDL	OA8-CA7	2.50	1.40	1.33
50	d	201	CDL	OB8-CB7	2.49	1.40	1.33
50	L	702	CDL	OA8-CA7	2.46	1.40	1.33
51	O	401	ATP	C5-C6	2.46	1.47	1.41
54	U	201	EHZ	C9-S1	2.45	1.82	1.76
49	H	401	3PE	O31-C31	2.40	1.40	1.33
51	O	401	ATP	C8-N7	2.39	1.36	1.31
49	H	401	3PE	O21-C2	-2.39	1.40	1.46
49	M	501	3PE	O31-C31	2.35	1.40	1.33
54	T	201	EHZ	C9-S1	2.34	1.81	1.76
52	P	501	NDP	C5A-C4A	2.33	1.43	1.39
54	U	201	EHZ	O4-C15	-2.30	1.18	1.23
50	d	201	CDL	OB6-CB5	2.29	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	T	201	EHZ	O4-C15	-2.28	1.18	1.23
46	B	202	PC1	O31-C31	2.27	1.40	1.33
49	L	701	3PE	O31-C31	2.27	1.40	1.33
51	O	401	ATP	C5-N7	-2.26	1.34	1.39
46	B	202	PC1	O31-C3	-2.26	1.40	1.45
49	L	701	3PE	O21-C21	2.25	1.40	1.34
49	J	401	3PE	O31-C31	2.25	1.39	1.33
49	J	401	3PE	O31-C3	-2.24	1.40	1.45
50	d	201	CDL	OB6-CB4	-2.24	1.41	1.46
49	L	701	3PE	O31-C3	-2.21	1.40	1.45
54	U	201	EHZ	O3-C12	-2.20	1.18	1.23
50	d	201	CDL	OA6-CA5	2.20	1.40	1.35
54	T	201	EHZ	O3-C12	-2.19	1.18	1.23
52	P	501	NDP	O5D-C5D	-2.17	1.36	1.44
49	H	401	3PE	O21-C21	2.17	1.40	1.34
49	M	501	3PE	O31-C3	-2.16	1.40	1.45
46	B	202	PC1	O21-C21	2.15	1.40	1.34
52	P	501	NDP	C7N-N7N	2.15	1.39	1.33
50	L	702	CDL	OA6-CA5	2.14	1.40	1.34
50	d	201	CDL	OB8-CB6	-2.14	1.40	1.45
49	L	701	3PE	O21-C2	-2.11	1.41	1.46
50	L	702	CDL	OB6-CB5	2.11	1.40	1.34
49	J	401	3PE	O21-C21	2.09	1.40	1.34
50	L	702	CDL	OA8-CA6	-2.09	1.40	1.45
49	M	501	3PE	O21-C21	2.06	1.40	1.34
49	H	401	3PE	O31-C3	-2.05	1.40	1.45
50	L	702	CDL	OB8-CB6	-2.04	1.40	1.45

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	PN-O3-PA	-7.51	107.07	132.83
51	O	401	ATP	C5-C4-N3	-6.28	118.56	126.75
54	T	201	EHZ	C8-C9-S1	5.46	120.39	113.63
54	U	201	EHZ	C8-C9-S1	5.36	120.26	113.63
51	O	401	ATP	N3-C4-N9	5.02	135.36	127.08
50	d	201	CDL	OA6-CA5-C11	4.75	119.83	111.09
49	L	701	3PE	O21-C21-C22	4.64	121.51	111.50
51	O	401	ATP	PA-O3A-PB	-4.55	117.21	132.83
50	d	201	CDL	OB6-CB5-C51	4.30	120.78	111.50
51	O	401	ATP	C2-N3-C4	4.05	121.32	111.75
51	O	401	ATP	PB-O3B-PG	-4.00	119.11	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	J	401	3PE	O21-C21-C22	3.98	120.07	111.50
50	L	702	CDL	OB6-CB5-C51	3.81	119.72	111.50
49	M	501	3PE	O21-C21-C22	3.77	119.62	111.50
46	B	202	PC1	O21-C21-C22	3.70	119.47	111.50
49	H	401	3PE	O21-C21-C22	3.64	119.34	111.50
51	O	401	ATP	N3-C2-N1	-3.56	123.03	128.60
50	L	702	CDL	OA6-CA5-C11	3.33	120.08	110.80
48	F	501	FMN	C4-N3-C2	-3.21	119.71	125.64
52	P	501	NDP	O2B-P2B-O1X	-3.18	97.13	109.39
52	P	501	NDP	PA-O5B-C5B	-3.16	103.15	121.68
49	H	401	3PE	O31-C31-C32	3.13	121.72	111.91
51	O	401	ATP	C4-C5-N7	-3.10	106.84	110.62
50	d	201	CDL	OB8-CB7-C71	3.00	121.33	111.91
51	O	401	ATP	C4-N9-C8	2.86	108.82	105.73
51	O	401	ATP	C5-N7-C8	2.81	107.50	103.51
52	P	501	NDP	PN-O5D-C5D	-2.78	105.38	121.68
49	M	501	3PE	O31-C31-C32	2.70	120.37	111.91
48	F	501	FMN	C4A-C4-N3	2.68	120.00	113.19
54	U	201	EHZ	C18-C17-C16	2.66	113.43	108.82
49	H	401	3PE	C2-O21-C21	-2.65	111.26	117.79
48	F	501	FMN	O4-C4-C4A	-2.64	119.60	126.60
50	d	201	CDL	OA8-CA7-C31	2.64	120.19	111.91
49	H	401	3PE	C24-C23-C22	-2.53	104.10	113.19
52	P	501	NDP	N3A-C4A-N9A	2.52	131.23	127.08
50	L	702	CDL	OA8-CA7-C31	2.51	119.80	111.91
52	P	501	NDP	O3X-P2B-O2X	2.51	117.24	107.64
50	d	201	CDL	CA4-OA6-CA5	-2.50	113.23	117.90
54	T	201	EHZ	O2-C9-S1	-2.49	119.39	122.61
46	B	202	PC1	O31-C31-C32	2.48	119.68	111.91
50	L	702	CDL	OB8-CB7-C71	2.47	119.67	111.91
54	U	201	EHZ	C10-S1-C9	2.47	109.57	101.87
54	U	201	EHZ	C16-C15-N2	2.45	121.46	116.58
48	F	501	FMN	C4A-C10-N1	-2.43	119.10	124.73
49	J	401	3PE	O31-C31-C32	2.42	119.51	111.91
49	L	701	3PE	O31-C31-C32	2.37	119.36	111.91
51	O	401	ATP	C3'-C2'-C1'	2.37	105.92	101.43
52	P	501	NDP	C2A-N1A-C6A	-2.36	114.72	118.77
48	F	501	FMN	C4A-C10-N10	2.32	119.88	116.48
51	O	401	ATP	N9-C8-N7	-2.31	110.76	113.91
52	P	501	NDP	C5A-C4A-N3A	-2.27	123.79	126.75
54	U	201	EHZ	O2-C9-S1	-2.24	119.71	122.61
48	F	501	FMN	C9A-C5A-N5	-2.18	120.06	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	P	501	NDP	O2N-PN-O1N	2.17	122.96	112.24
52	P	501	NDP	C4B-O4B-C1B	-2.16	104.70	109.47
48	F	501	FMN	C5A-C9A-N10	2.16	120.18	117.95
51	O	401	ATP	C6-C5-N7	2.15	136.02	132.02
52	P	501	NDP	O4B-C4B-C3B	2.12	109.32	105.11
48	F	501	FMN	C4-C4A-C10	2.12	120.35	116.79
48	F	501	FMN	C10-C4A-N5	-2.08	120.44	124.86
54	T	201	EHZ	C13-C12-N1	2.05	119.87	116.42
54	U	201	EHZ	C7-C8-C9	-2.03	109.27	113.89
54	T	201	EHZ	C10-S1-C9	2.00	108.10	101.87

There are no chirality outliers.

All (204) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	B	202	PC1	C1-O11-P-O12
46	B	202	PC1	C1-O11-P-O14
46	B	202	PC1	O13-C11-C12-N
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C2'-C3'-C4'-O4'
48	F	501	FMN	C2'-C3'-C4'-C5'
48	F	501	FMN	O3'-C3'-C4'-O4'
49	H	401	3PE	C1-O11-P-O12
49	H	401	3PE	C1-O11-P-O13
49	H	401	3PE	C1-O11-P-O14
49	H	401	3PE	C22-C21-O21-C2
49	J	401	3PE	O11-C1-C2-O21
49	J	401	3PE	O22-C21-O21-C2
49	L	701	3PE	C1-O11-P-O12
49	L	701	3PE	C11-O13-P-O12
49	L	701	3PE	C11-O13-P-O14
49	L	701	3PE	O13-C11-C12-N
49	L	701	3PE	O22-C21-O21-C2
49	M	501	3PE	C1-O11-P-O12
49	M	501	3PE	C1-O11-P-O14
49	M	501	3PE	O13-C11-C12-N
49	M	501	3PE	C22-C21-O21-C2
50	L	702	CDL	C51-CB5-OB6-CB4
50	d	201	CDL	O1-C1-CB2-OB2
50	d	201	CDL	OB7-CB5-OB6-CB4
50	d	201	CDL	C71-CB7-OB8-CB6

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Mol	Chain	Res	Type	Atoms
51	O	401	ATP	PB-O3B-PG-O3G
51	O	401	ATP	C5'-O5'-PA-O1A
51	O	401	ATP	C5'-O5'-PA-O2A
52	P	501	NDP	C5D-O5D-PN-O1N
54	T	201	EHZ	C11-C10-S1-C9
54	T	201	EHZ	N2-C15-C16-C17
54	T	201	EHZ	N2-C15-C16-O5
54	T	201	EHZ	O4-C15-C16-C17
54	T	201	EHZ	O2-C9-S1-C10
54	T	201	EHZ	C8-C9-S1-C10
54	U	201	EHZ	O1-C7-C8-C9
54	U	201	EHZ	C7-C8-C9-S1
54	U	201	EHZ	N2-C15-C16-C17
54	U	201	EHZ	N2-C15-C16-O5
54	U	201	EHZ	O4-C15-C16-C17
54	U	201	EHZ	O4-C15-C16-O5
54	U	201	EHZ	C15-C16-C17-C18
54	U	201	EHZ	C15-C16-C17-C19
54	U	201	EHZ	C15-C16-C17-C20
54	U	201	EHZ	O5-C16-C17-C18
54	U	201	EHZ	O5-C16-C17-C19
54	U	201	EHZ	O5-C16-C17-C20
54	U	201	EHZ	O2-C9-S1-C10
54	U	201	EHZ	C8-C9-S1-C10
50	d	201	CDL	C11-CA5-OA6-CA4
46	B	202	PC1	O32-C31-O31-C3
50	d	201	CDL	OB9-CB7-OB8-CB6
49	J	401	3PE	O32-C31-O31-C3
50	d	201	CDL	OA7-CA5-OA6-CA4
49	H	401	3PE	O22-C21-O21-C2
49	M	501	3PE	O22-C21-O21-C2
50	L	702	CDL	OB7-CB5-OB6-CB4
46	B	202	PC1	C32-C31-O31-C3
49	J	401	3PE	C22-C21-O21-C2
49	L	701	3PE	C22-C21-O21-C2
50	d	201	CDL	C51-CB5-OB6-CB4
49	J	401	3PE	C32-C31-O31-C3
49	M	501	3PE	C32-C31-O31-C3
49	M	501	3PE	O32-C31-O31-C3
52	P	501	NDP	O4D-C1D-N1N-C6N
50	L	702	CDL	O1-C1-CB2-OB2
48	F	501	FMN	O3'-C3'-C4'-C5'

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Mol	Chain	Res	Type	Atoms
54	T	201	EHZ	C13-C14-N2-C15
50	L	702	CDL	CA2-C1-CB2-OB2
49	J	401	3PE	C31-C32-C33-C34
49	M	501	3PE	C21-C22-C23-C24
46	B	202	PC1	C11-O13-P-O11
46	B	202	PC1	C1-O11-P-O13
49	J	401	3PE	C11-O13-P-O11
49	L	701	3PE	C1-O11-P-O13
49	L	701	3PE	C11-O13-P-O11
49	M	501	3PE	C1-O11-P-O13
50	L	702	CDL	CA2-OA2-PA1-OA5
50	d	201	CDL	CA2-C1-CB2-OB2
50	L	702	CDL	C11-CA5-OA6-CA4
50	L	702	CDL	C74-C75-C76-C77
49	L	701	3PE	C3-C2-O21-C21
50	L	702	CDL	OA7-CA5-OA6-CA4
49	M	501	3PE	C35-C36-C37-C38
49	L	701	3PE	C2A-C2B-C2C-C2D
49	L	701	3PE	C22-C23-C24-C25
49	L	701	3PE	C35-C36-C37-C38
54	T	201	EHZ	C3-C4-C5-C6
49	J	401	3PE	C23-C24-C25-C26
50	L	702	CDL	C52-C53-C54-C55
54	U	201	EHZ	S1-C10-C11-N1
49	M	501	3PE	C3E-C3F-C3G-C3H
50	L	702	CDL	C71-C72-C73-C74
50	d	201	CDL	CA7-C31-C32-C33
49	L	701	3PE	C33-C34-C35-C36
54	U	201	EHZ	C2-C3-C4-C5
54	T	201	EHZ	C1-C21-C22-C23
54	U	201	EHZ	C13-C14-N2-C15
50	d	201	CDL	OA5-CA3-CA4-OA6
54	U	201	EHZ	C21-C22-C23-C24
49	M	501	3PE	C3A-C3B-C3C-C3D
49	J	401	3PE	C22-C23-C24-C25
48	F	501	FMN	O2'-C2'-C3'-C4'
49	M	501	3PE	C39-C3A-C3B-C3C
49	L	701	3PE	C1-C2-C3-O31
49	H	401	3PE	C33-C34-C35-C36
49	J	401	3PE	C34-C35-C36-C37
50	L	702	CDL	C76-C77-C78-C79
54	T	201	EHZ	O4-C15-C16-O5

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Mol	Chain	Res	Type	Atoms
49	L	701	3PE	C21-C22-C23-C24
50	d	201	CDL	OB6-CB4-CB6-OB8
50	d	201	CDL	C56-C57-C58-C59
54	U	201	EHZ	C5-C6-C7-C8
49	J	401	3PE	O11-C1-C2-C3
49	M	501	3PE	O11-C1-C2-C3
50	d	201	CDL	OA5-CA3-CA4-CA6
49	H	401	3PE	C3B-C3C-C3D-C3E
49	M	501	3PE	C3C-C3D-C3E-C3F
46	B	202	PC1	C2-C1-O11-P
50	L	702	CDL	C51-C52-C53-C54
49	M	501	3PE	C32-C33-C34-C35
50	d	201	CDL	CB3-CB4-CB6-OB8
54	U	201	EHZ	C7-C8-C9-O2
49	M	501	3PE	C36-C37-C38-C39
54	U	201	EHZ	C5-C6-C7-O1
49	M	501	3PE	C33-C34-C35-C36
49	L	701	3PE	C28-C29-C2A-C2B
49	L	701	3PE	C34-C35-C36-C37
50	L	702	CDL	C72-C73-C74-C75
49	J	401	3PE	C3-C2-O21-C21
54	T	201	EHZ	C12-C13-C14-N2
50	L	702	CDL	C1-CA2-OA2-PA1
50	L	702	CDL	CA4-CA3-OA5-PA1
49	M	501	3PE	O11-C1-C2-O21
49	H	401	3PE	C35-C36-C37-C38
54	T	201	EHZ	O1-C7-C8-C9
49	H	401	3PE	C28-C29-C2A-C2B
52	P	501	NDP	C5D-O5D-PN-O3
52	P	501	NDP	PN-O3-PA-O2A
50	d	201	CDL	C52-C53-C54-C55
50	L	702	CDL	C31-CA7-OA8-CA6
46	B	202	PC1	C11-O13-P-O12
46	B	202	PC1	C11-O13-P-O14
49	J	401	3PE	C11-O13-P-O12
49	J	401	3PE	C11-O13-P-O14
49	L	701	3PE	C1-O11-P-O14
50	L	702	CDL	CA2-OA2-PA1-OA4
52	P	501	NDP	C5D-O5D-PN-O2N
54	U	201	EHZ	C6-C7-C8-C9
49	J	401	3PE	O13-C11-C12-N
48	F	501	FMN	C1'-C2'-C3'-O3'

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Mol	Chain	Res	Type	Atoms
54	U	201	EHZ	C1-C2-C3-C4
50	L	702	CDL	OA9-CA7-OA8-CA6
54	U	201	EHZ	C21-C1-C2-C3
49	H	401	3PE	C3A-C3B-C3C-C3D
50	d	201	CDL	CB3-CB4-OB6-CB5
49	L	701	3PE	C37-C38-C39-C3A
49	M	501	3PE	C2-C1-O11-P
49	M	501	3PE	C3F-C3G-C3H-C3I
49	L	701	3PE	O21-C2-C3-O31
50	L	702	CDL	CA3-OA5-PA1-OA2
50	L	702	CDL	CB2-OB2-PB2-OB5
50	d	201	CDL	CA3-OA5-PA1-OA2
50	d	201	CDL	CB3-OB5-PB2-OB2
49	L	701	3PE	C3A-C3B-C3C-C3D
50	d	201	CDL	C54-C55-C56-C57
54	T	201	EHZ	C1-C2-C3-C4
49	L	701	3PE	C26-C27-C28-C29
54	T	201	EHZ	S1-C10-C11-N1
49	H	401	3PE	C24-C25-C26-C27
49	M	501	3PE	C3D-C3E-C3F-C3G
52	P	501	NDP	C1B-C2B-O2B-P2B
49	L	701	3PE	C2B-C2C-C2D-C2E
46	B	202	PC1	O22-C21-O21-C2
54	T	201	EHZ	C2-C1-C21-C22
49	H	401	3PE	C36-C37-C38-C39
49	H	401	3PE	C2A-C2B-C2C-C2D
50	L	702	CDL	OB6-CB4-CB6-OB8
50	d	201	CDL	C1-CB2-OB2-PB2
49	J	401	3PE	O31-C31-C32-C33
46	B	202	PC1	O21-C21-C22-C23
51	O	401	ATP	C5'-O5'-PA-O3A
52	P	501	NDP	O4D-C4D-C5D-O5D
52	P	501	NDP	PN-O3-PA-O1A
46	B	202	PC1	C22-C21-O21-C2
49	L	701	3PE	C24-C25-C26-C27
49	J	401	3PE	O32-C31-C32-C33
48	F	501	FMN	O2'-C2'-C3'-O3'
49	L	701	3PE	C36-C37-C38-C39
51	O	401	ATP	O4'-C4'-C5'-O5'
46	B	202	PC1	O22-C21-C22-C23
50	L	702	CDL	CB5-C51-C52-C53
46	B	202	PC1	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
49	M	501	3PE	C12-C11-O13-P
50	d	201	CDL	C55-C56-C57-C58
52	P	501	NDP	C3B-C2B-O2B-P2B
50	L	702	CDL	OB5-CB3-CB4-OB6
49	J	401	3PE	C37-C38-C39-C3A
50	L	702	CDL	C52-C51-CB5-OB6
48	F	501	FMN	C2'-C1'-N10-C10
50	d	201	CDL	C32-C31-CA7-OA8
50	L	702	CDL	C52-C51-CB5-OB7

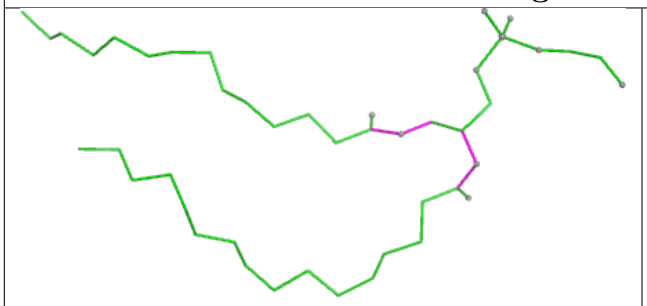
There are no ring outliers.

7 monomers are involved in 16 short contacts:

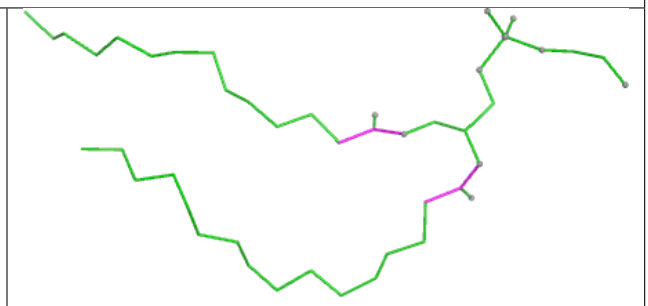
Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	M	501	3PE	2	0
48	F	501	FMN	5	0
46	B	202	PC1	1	0
50	L	702	CDL	1	0
50	d	201	CDL	1	0
52	P	501	NDP	4	0
51	O	401	ATP	2	0

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.

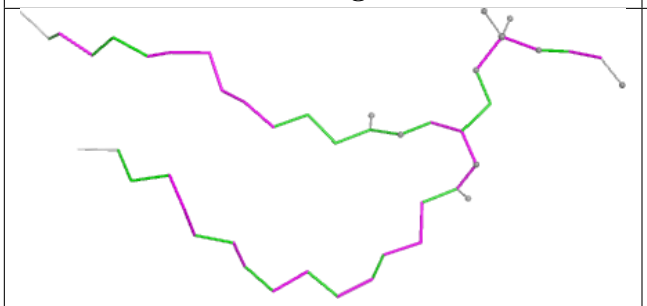
Ligand 3PE L 701



Bond lengths



Bond angles

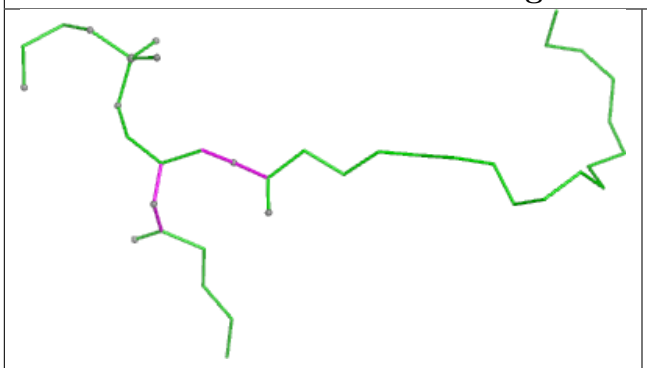


Torsions



Rings

Ligand 3PE M 501



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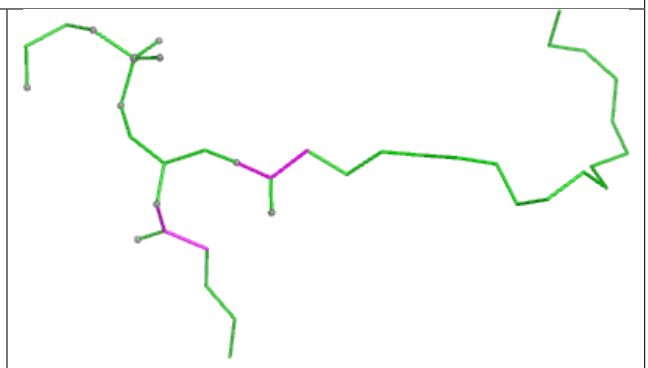

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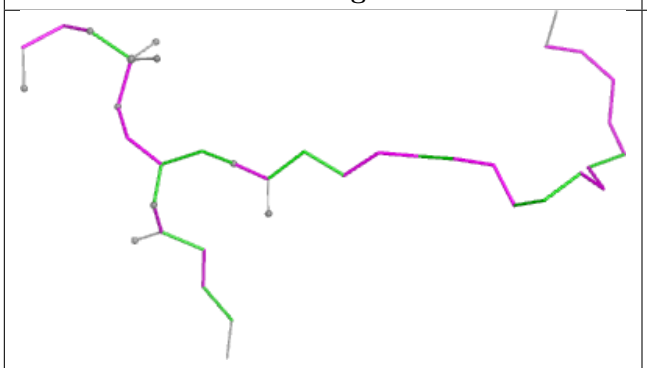
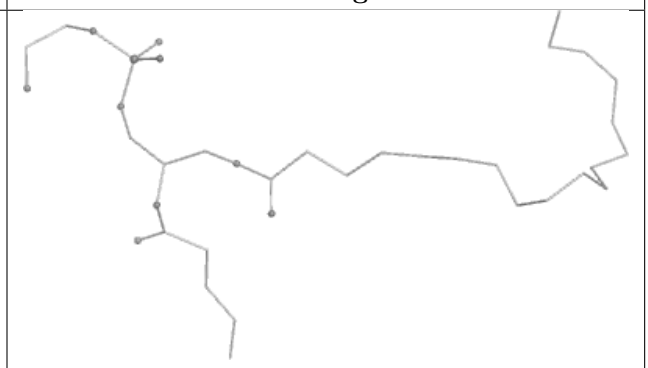
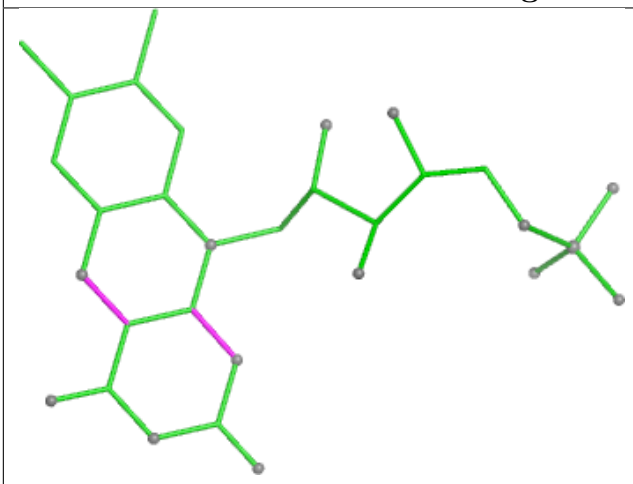


Torsions



Rings

Ligand FMN F 501



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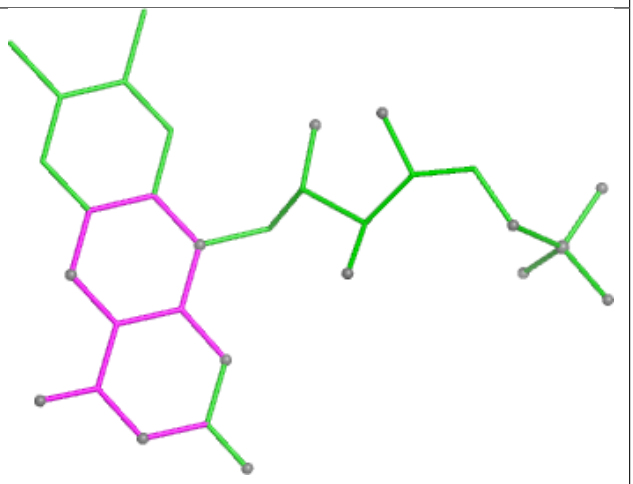

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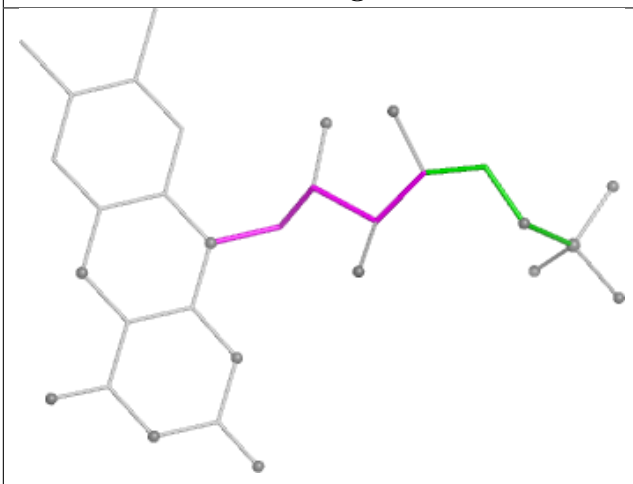

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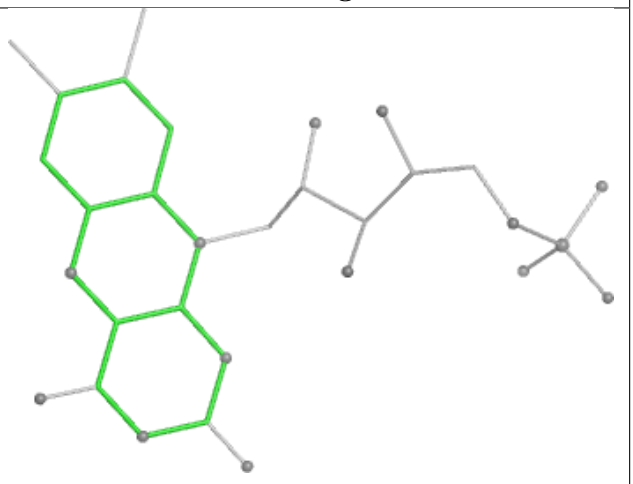
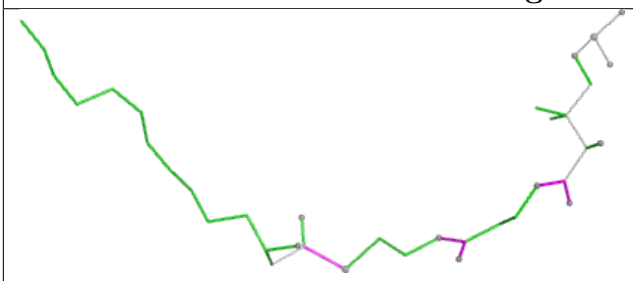


Rings

Ligand EHZ T 201



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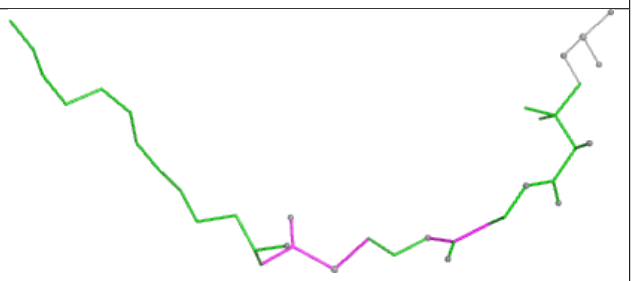

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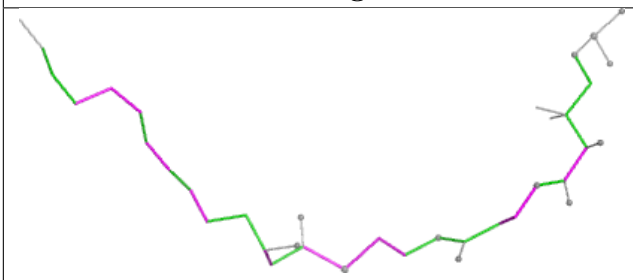

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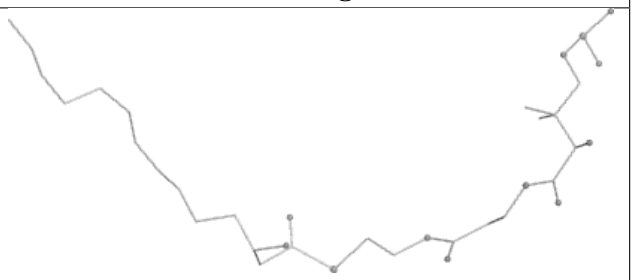
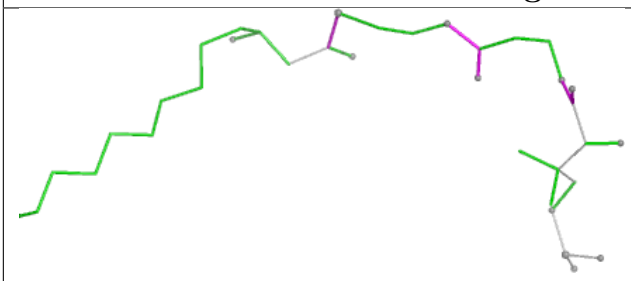


Rings

Ligand EHZ U 201



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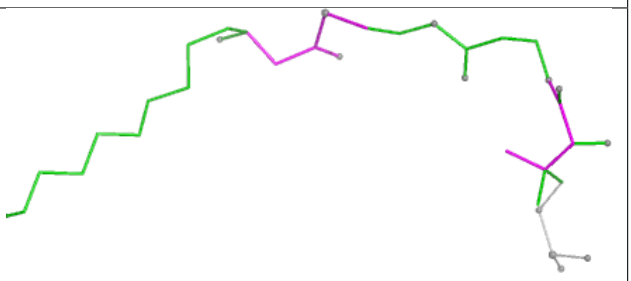
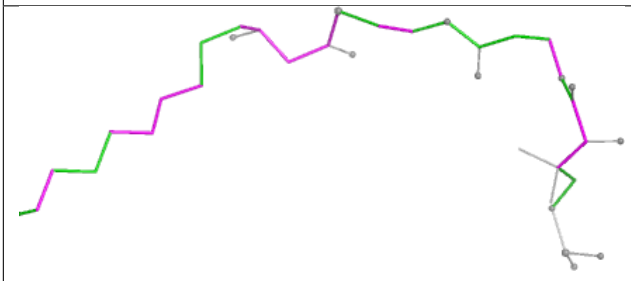


Bond angles



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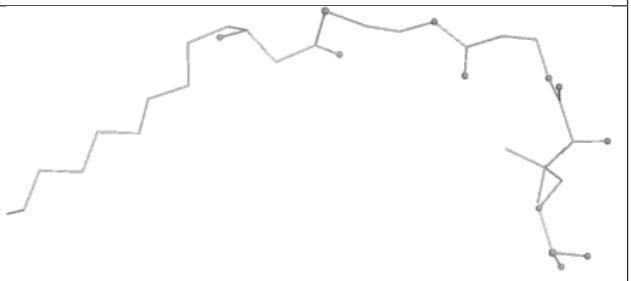
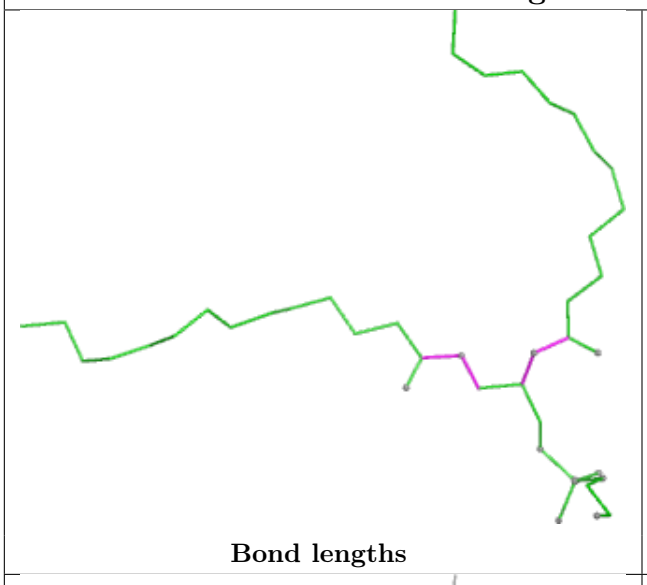


Rings

Ligand 3PE H 401



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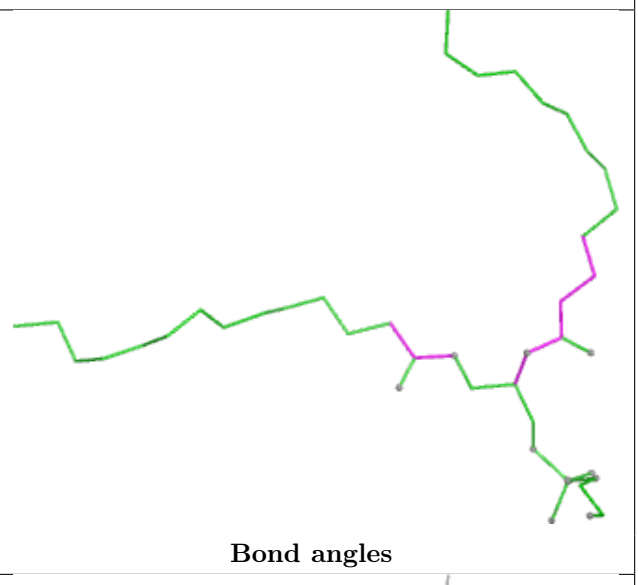

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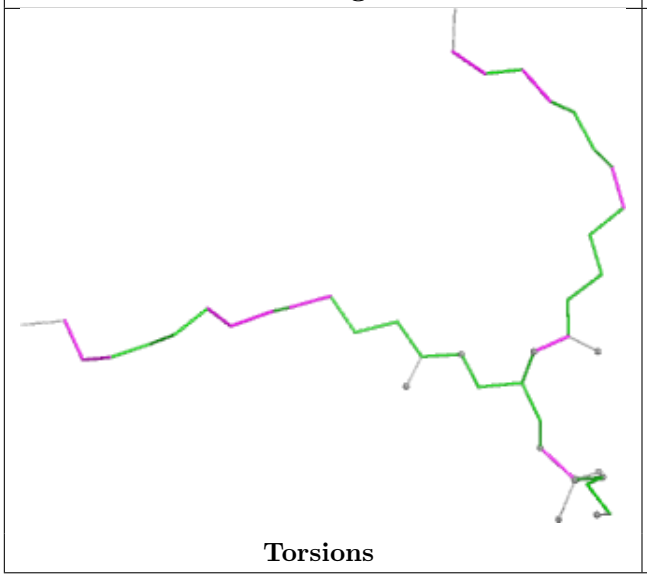

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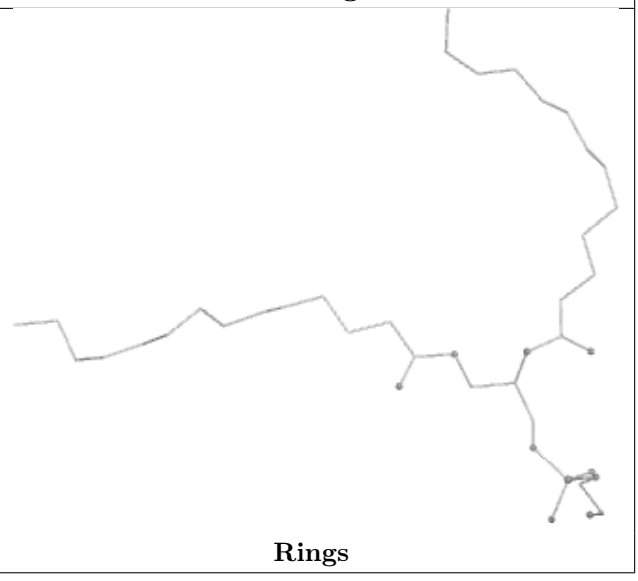
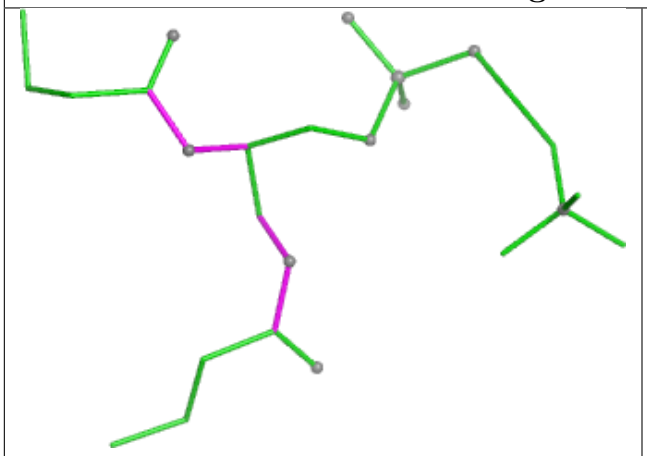


Rings

Ligand PC1 B 202



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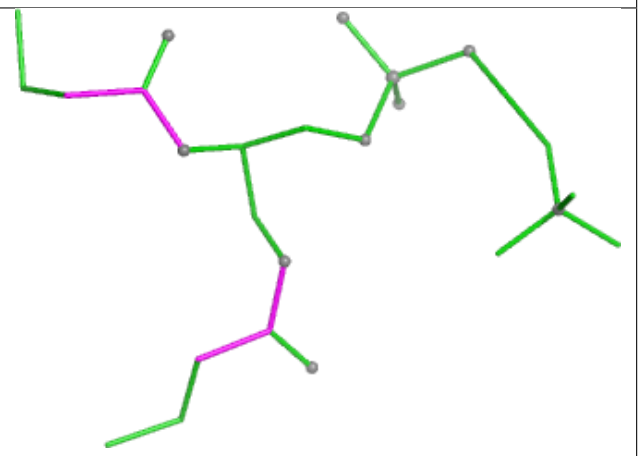

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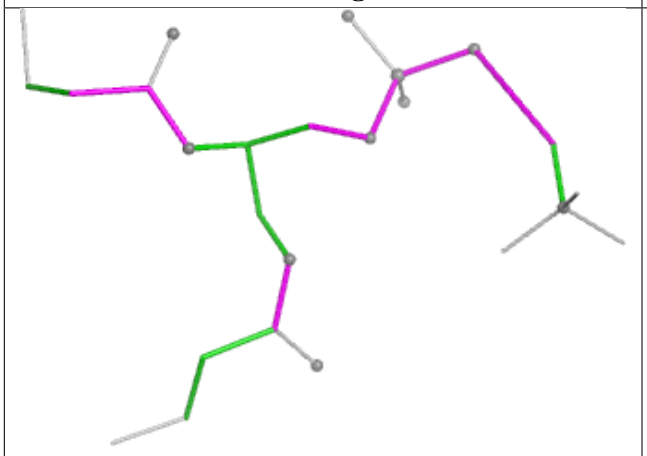

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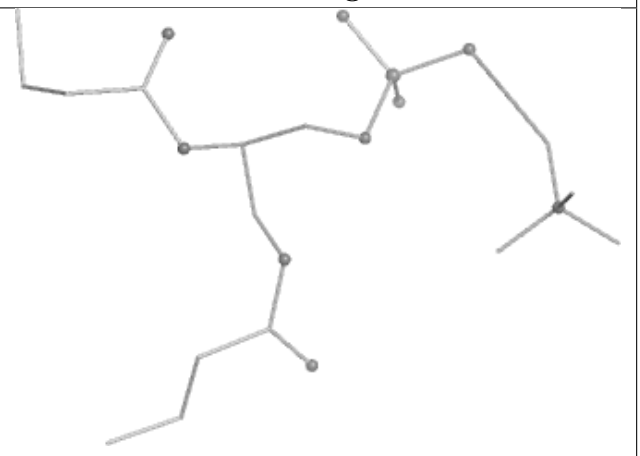
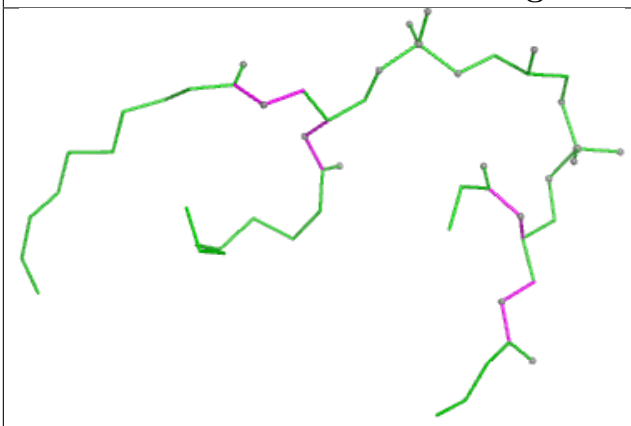


Rings

Ligand CDL L 702



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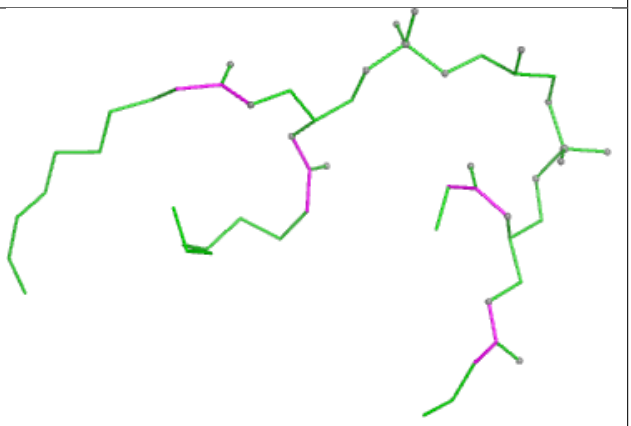

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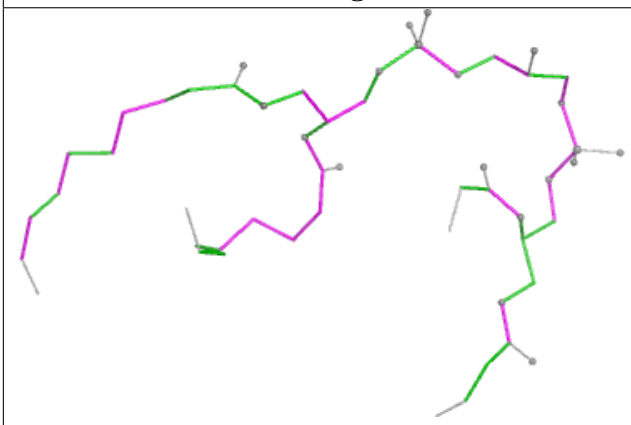

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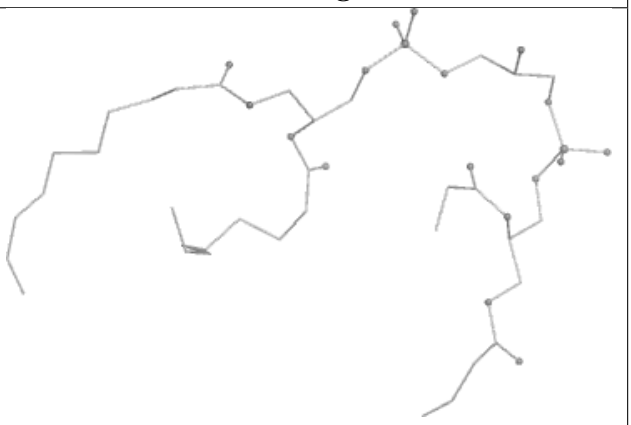
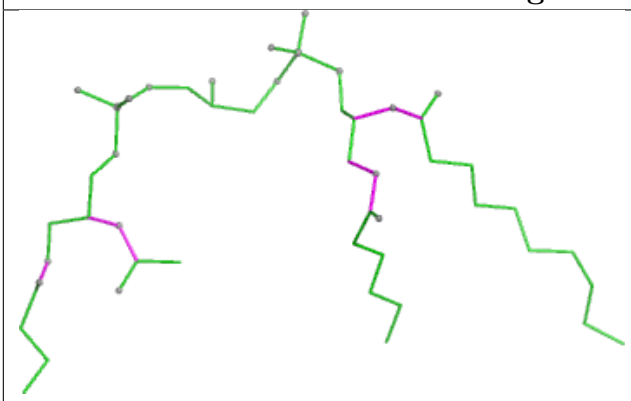


Rings

Ligand CDL d 201



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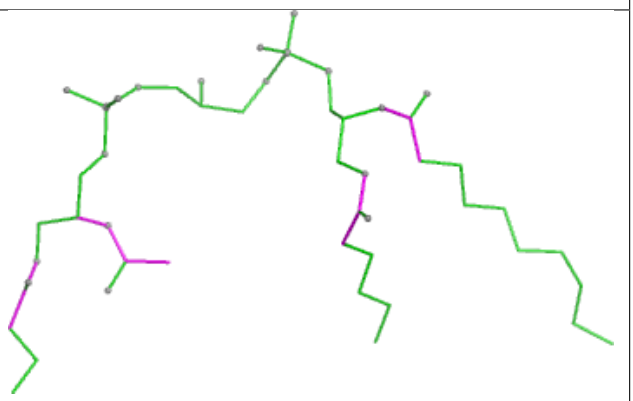

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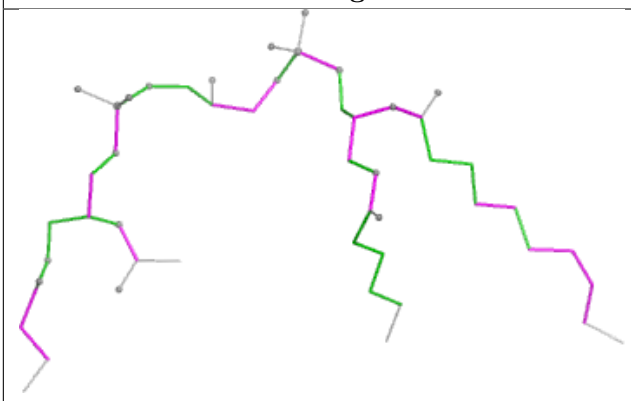

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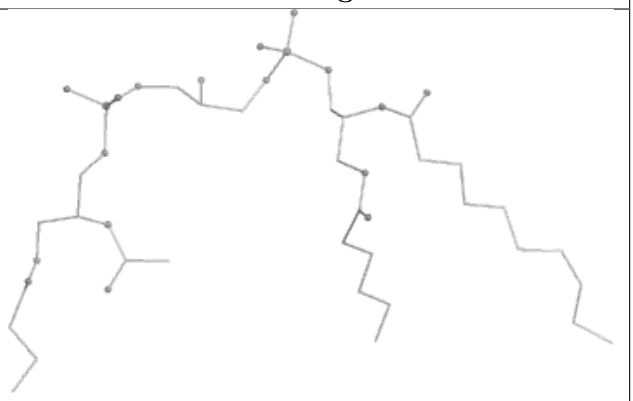
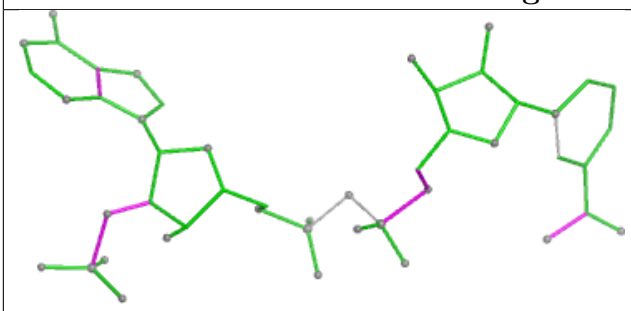


Rings

Ligand NDP P 501



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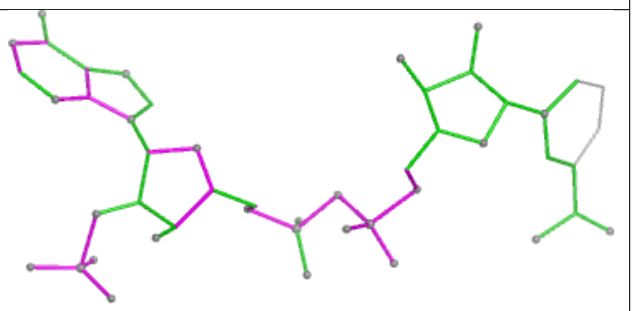
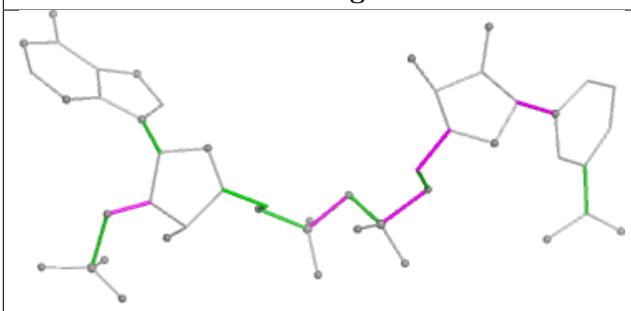
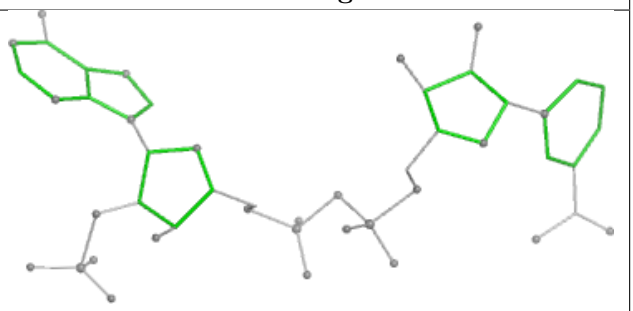


Bond angles

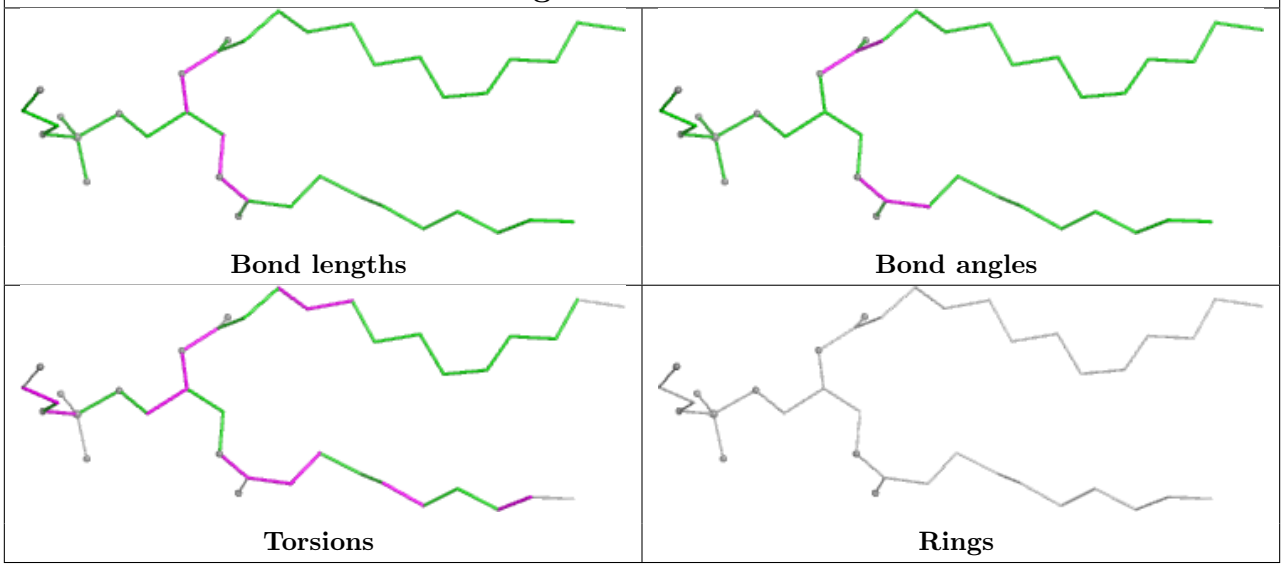


Torsions

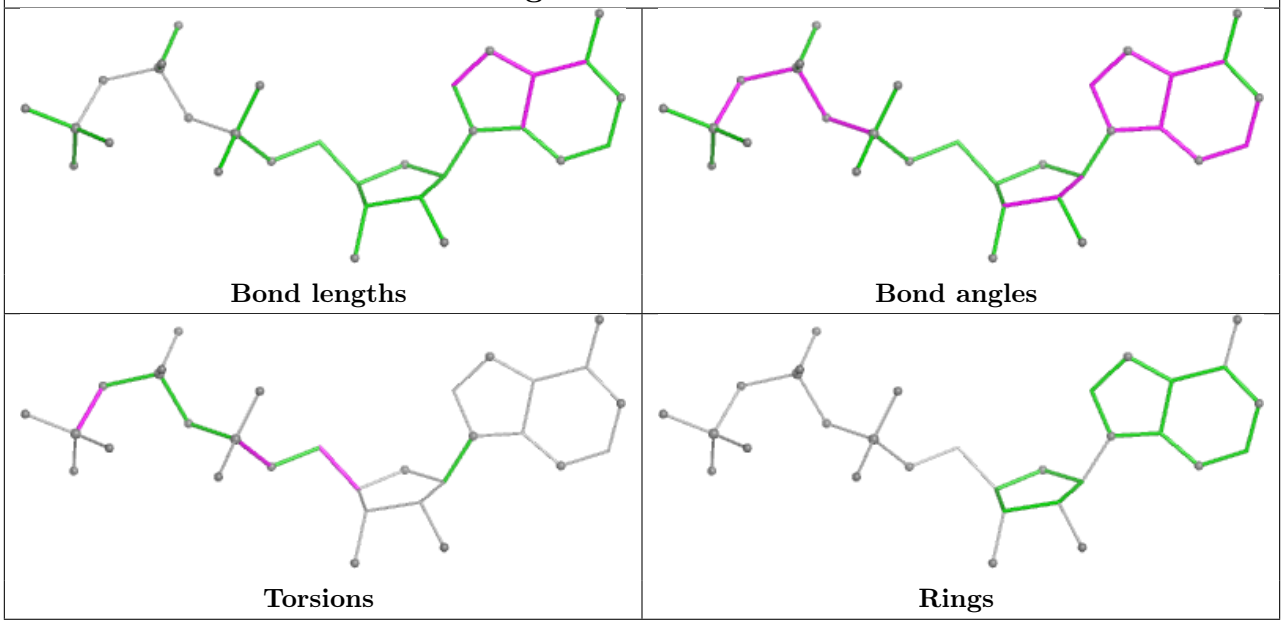


Rings

Ligand 3PE J 401



Ligand ATP O 401



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.

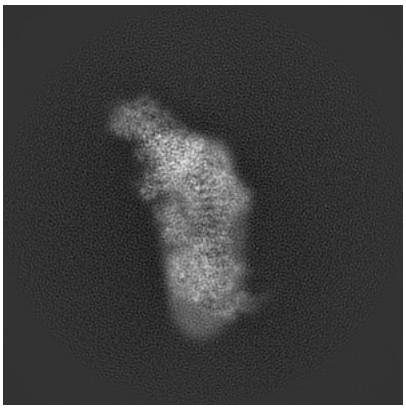
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-11811. These allow visual inspection of the internal detail of the map and identification of artifacts.

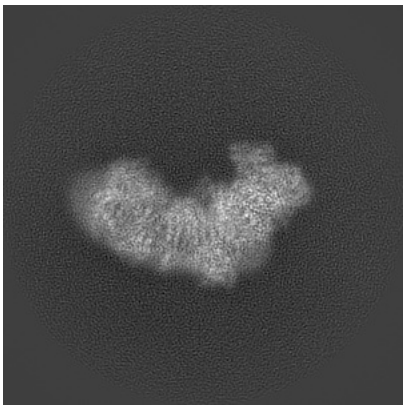
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

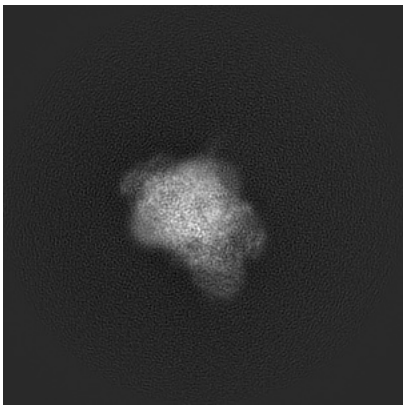
6.1.1 Primary map



X

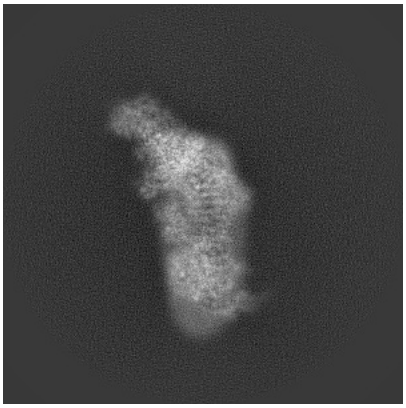


Y

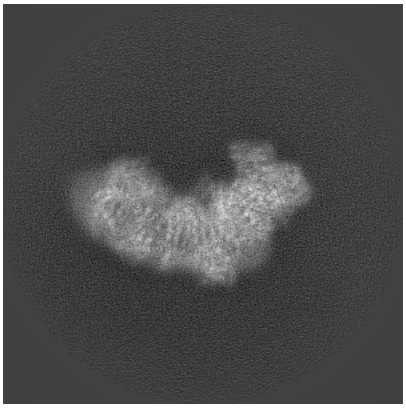


Z

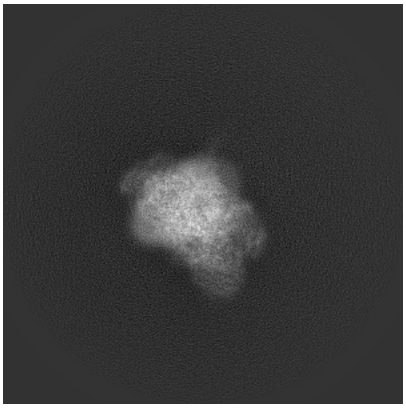
6.1.2 Raw map



X



Y

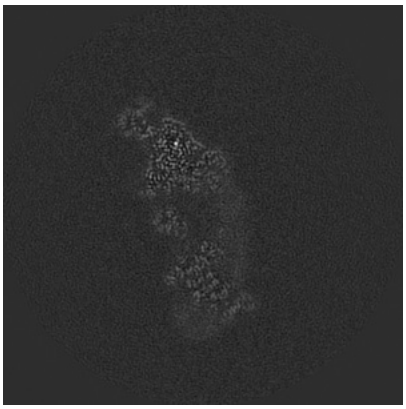


Z

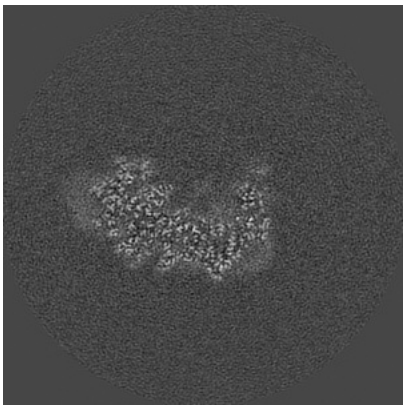
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

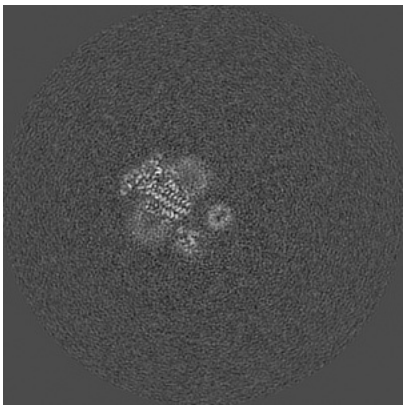
6.2.1 Primary map



X Index: 225

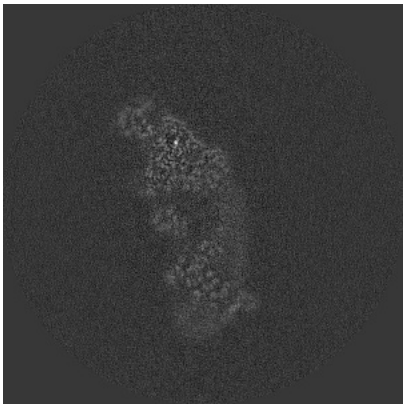


Y Index: 225

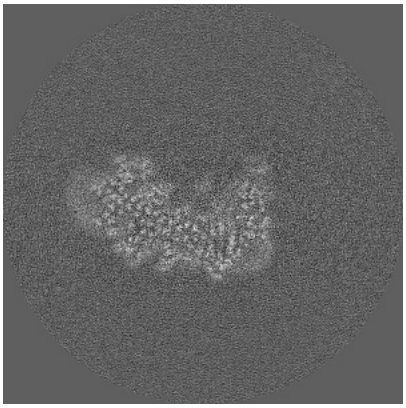


Z Index: 225

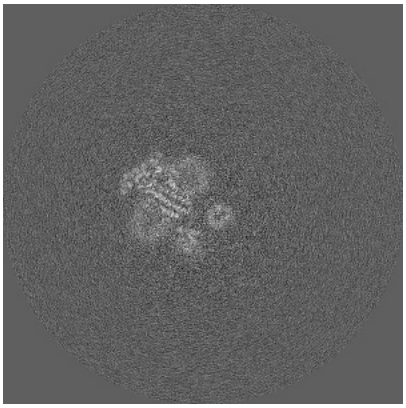
6.2.2 Raw map



X Index: 225



Y Index: 225

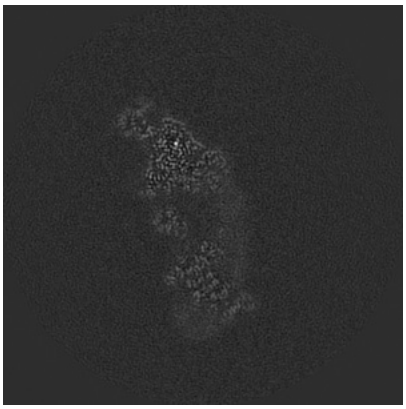


Z Index: 225

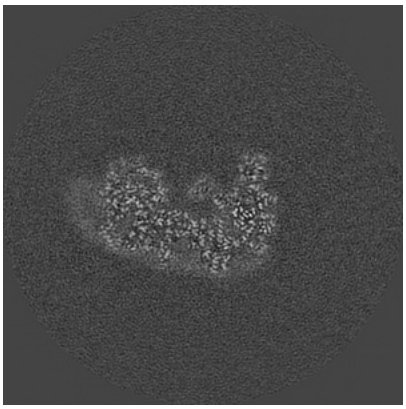
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

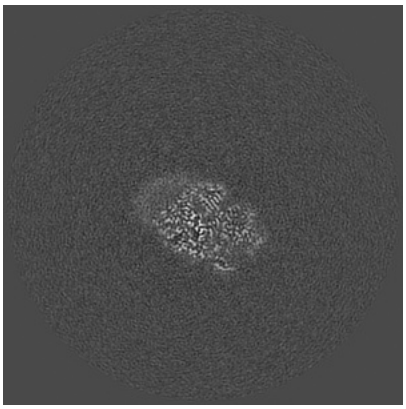
6.3.1 Primary map



X Index: 225

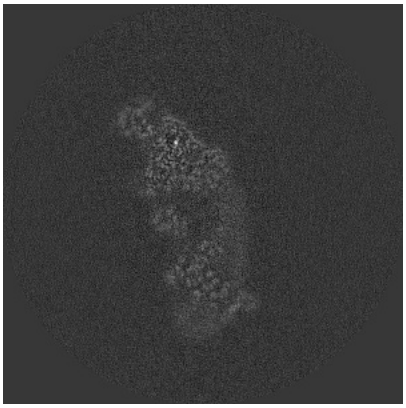


Y Index: 216

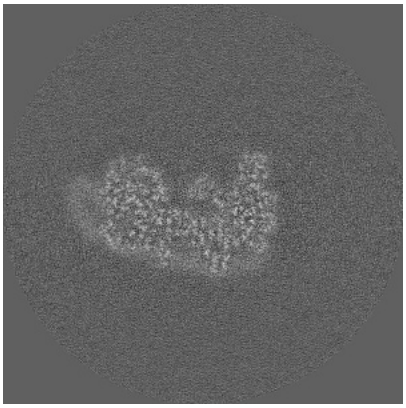


Z Index: 279

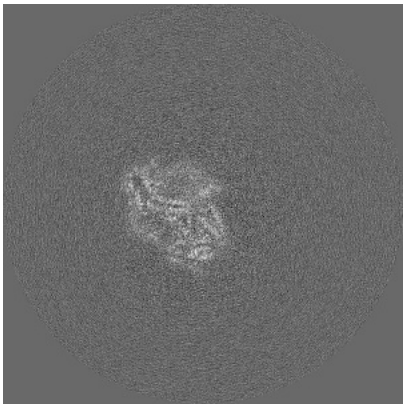
6.3.2 Raw map



X Index: 225



Y Index: 216

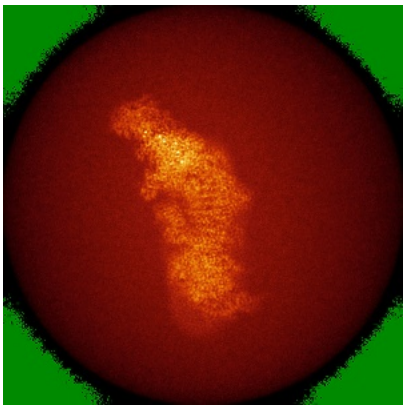


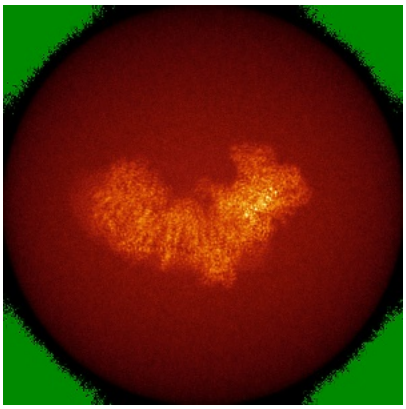
Z Index: 245

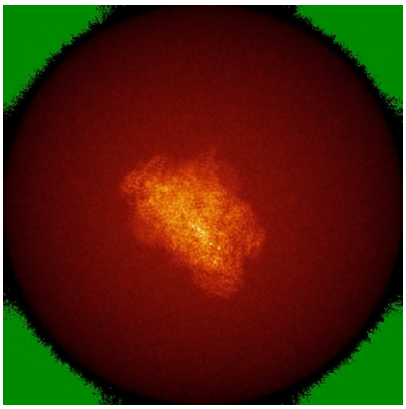
The images above show the largest variance slices of the map in three orthogonal directions.

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

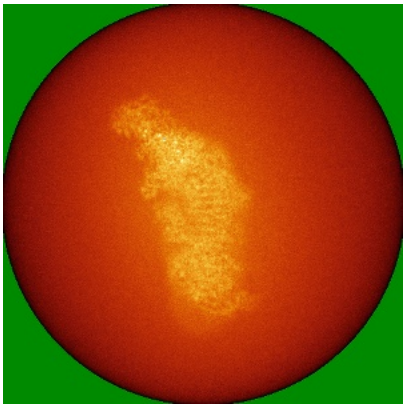
6.4.1 Primary map

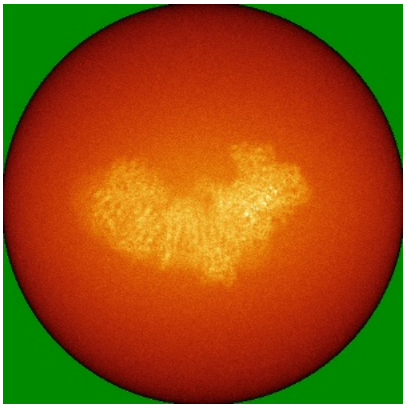

X

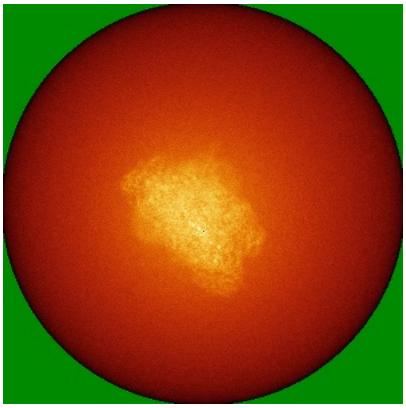

Y


Z

6.4.2 Raw map


X

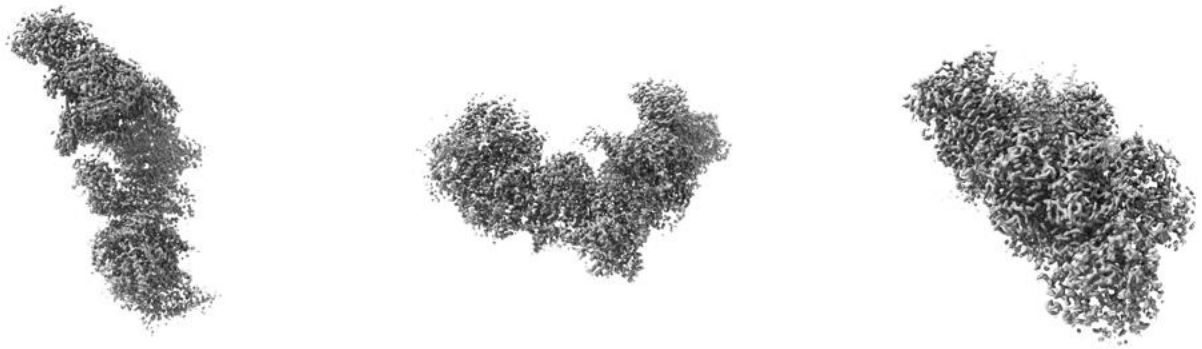

Y


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)

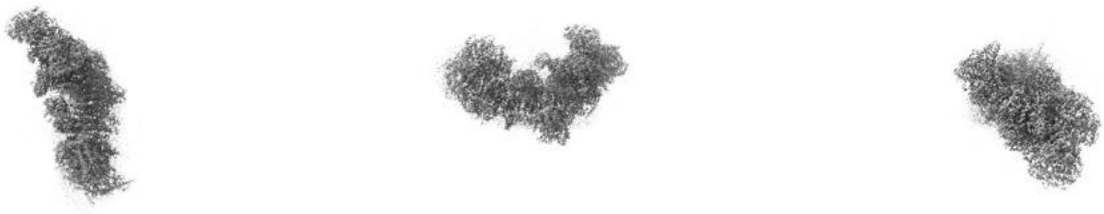
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0268. 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.

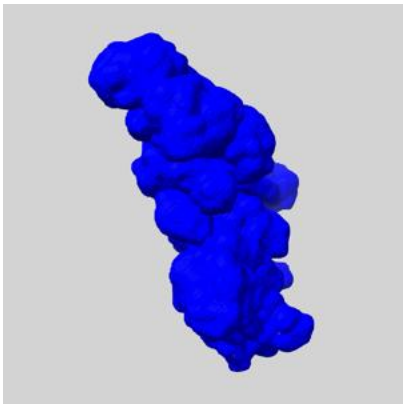
6.6 Mask visualisation

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

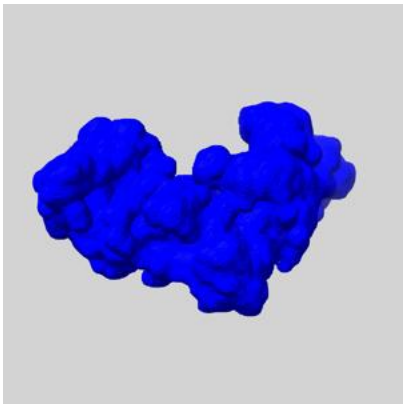
A mask typically either:

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

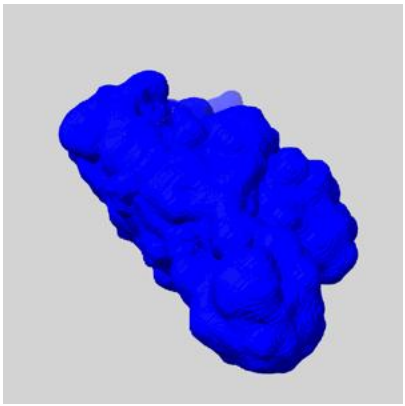
6.6.1 emd_11811_msk_1.map



X



Y

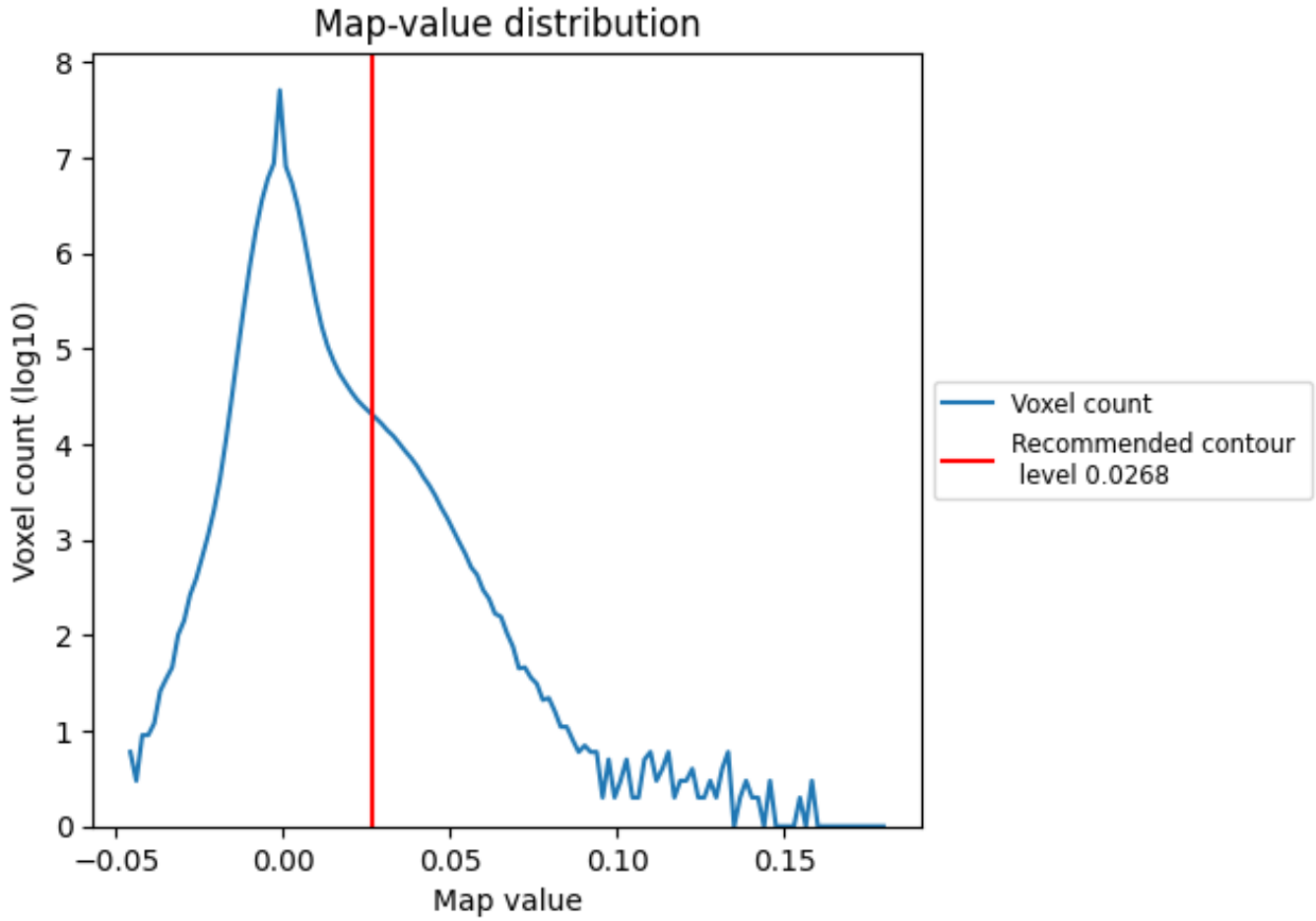


Z

7 Map analysis

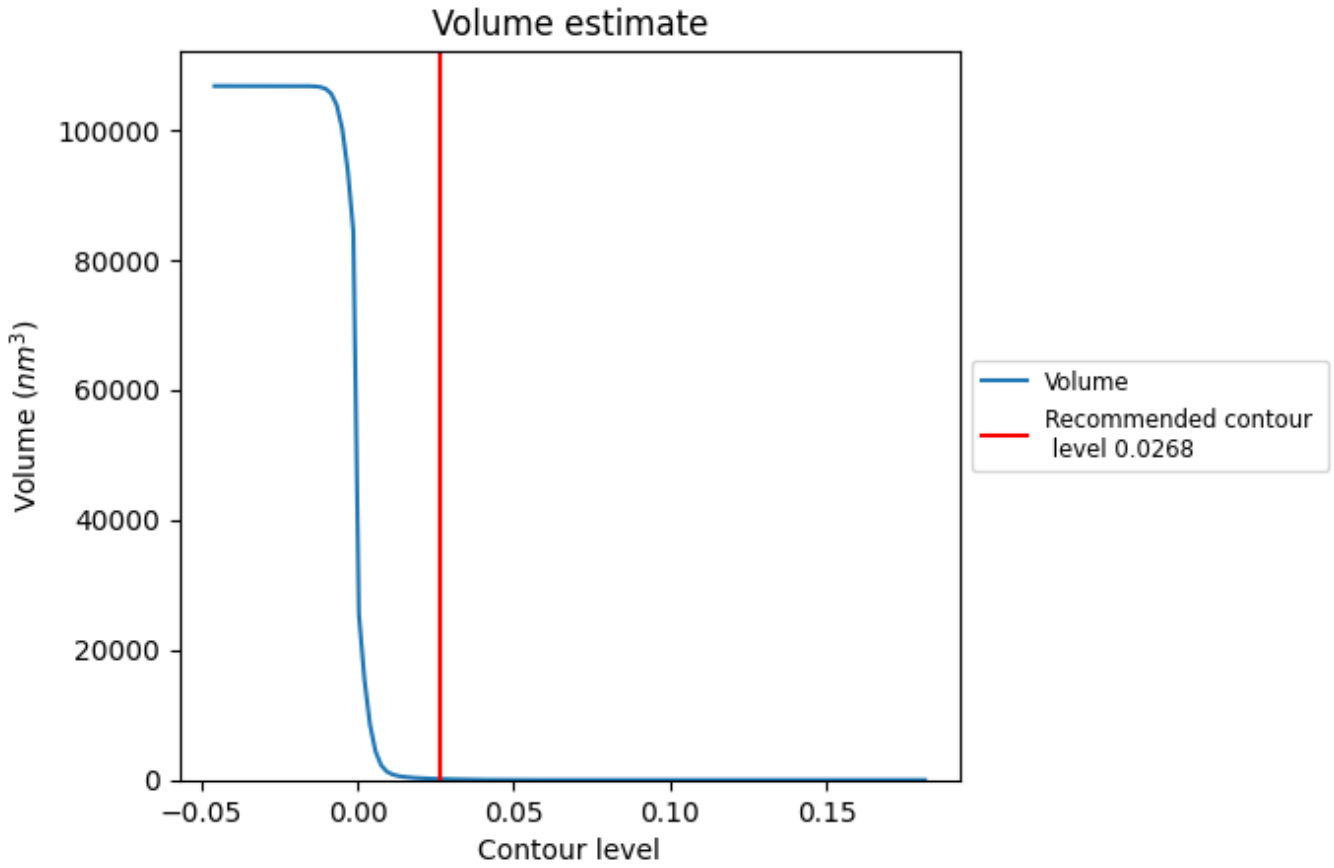
This section contains the results of statistical analysis of the map.

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.

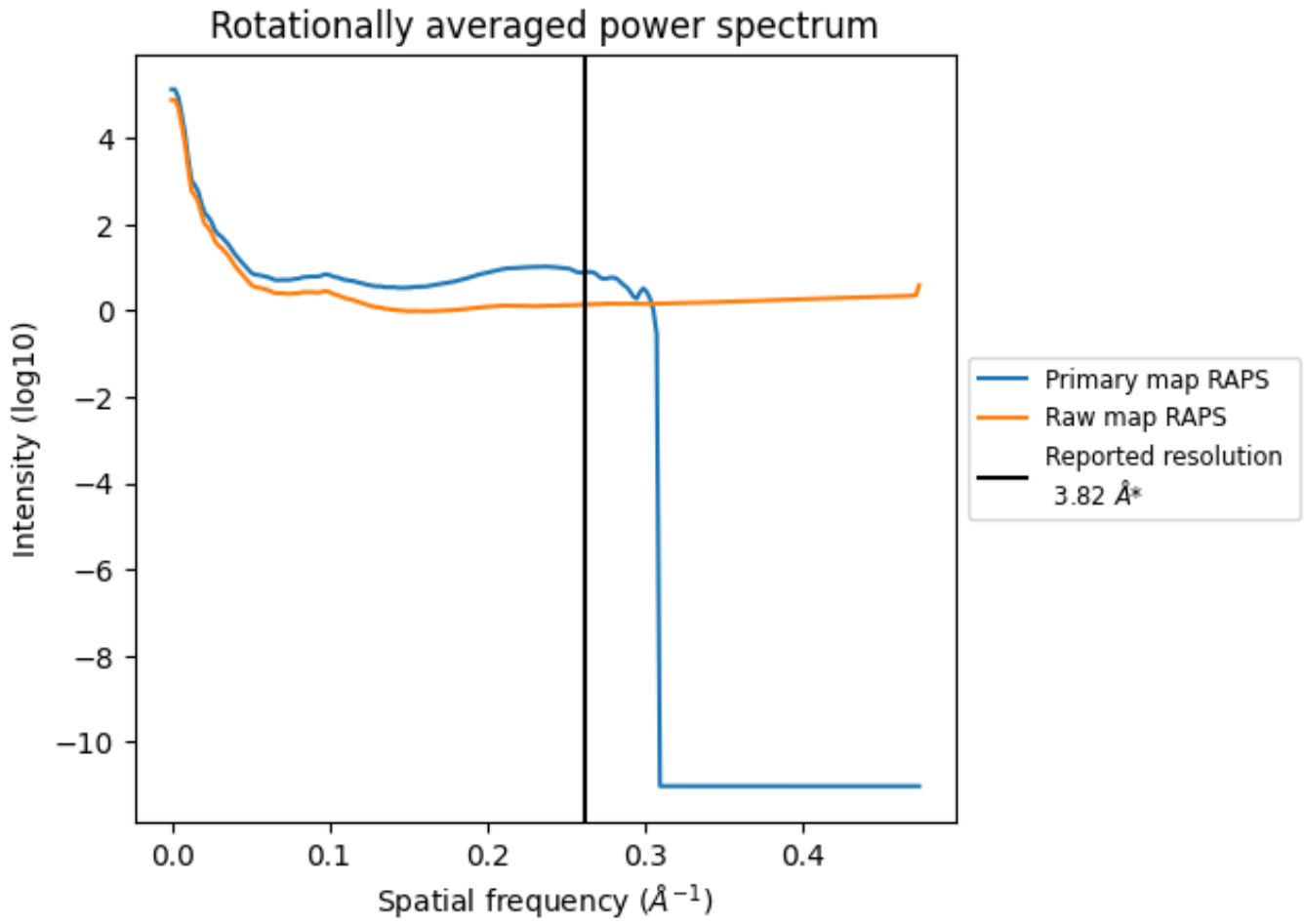
7.2 Volume estimate



The volume at the recommended contour level is 146 nm^3; this corresponds to an approximate mass of 132 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)

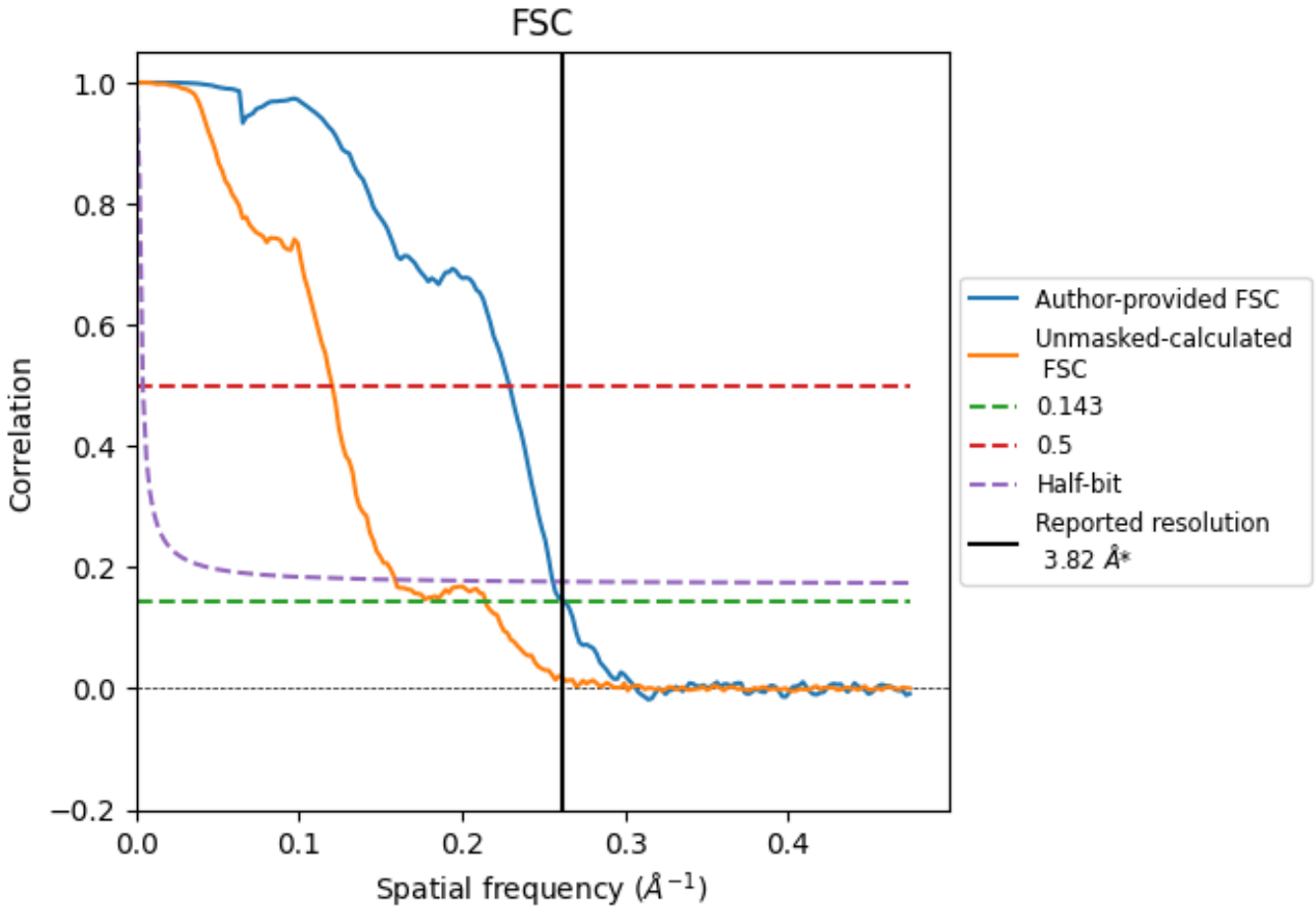


*Reported resolution corresponds to spatial frequency of 0.262 Å^{-1}

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 0.262 Å^{-1}

8.2 Resolution estimates (i)

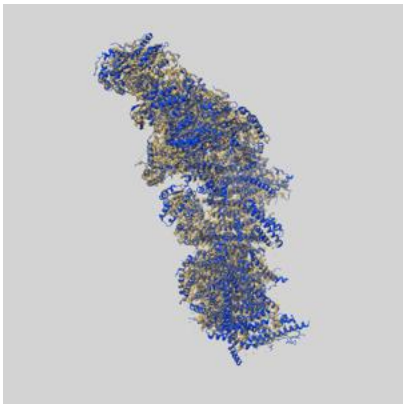
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.82	-	-
Author-provided FSC curve	3.80	4.37	3.91
Unmasked-calculated*	4.66	8.31	6.30

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.66 differs from the reported value 3.82 by more than 10 %

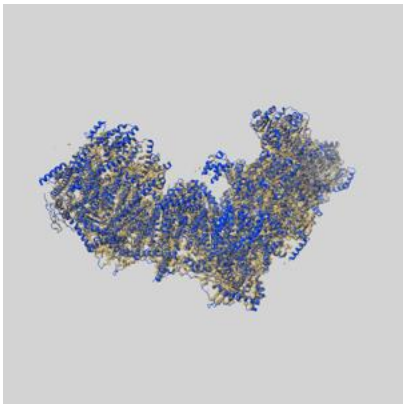
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-11811 and PDB model 7AK6. Per-residue inclusion information can be found in section 3 on page 18.

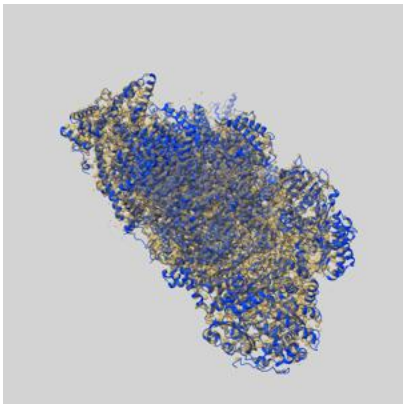
9.1 Map-model overlay



X



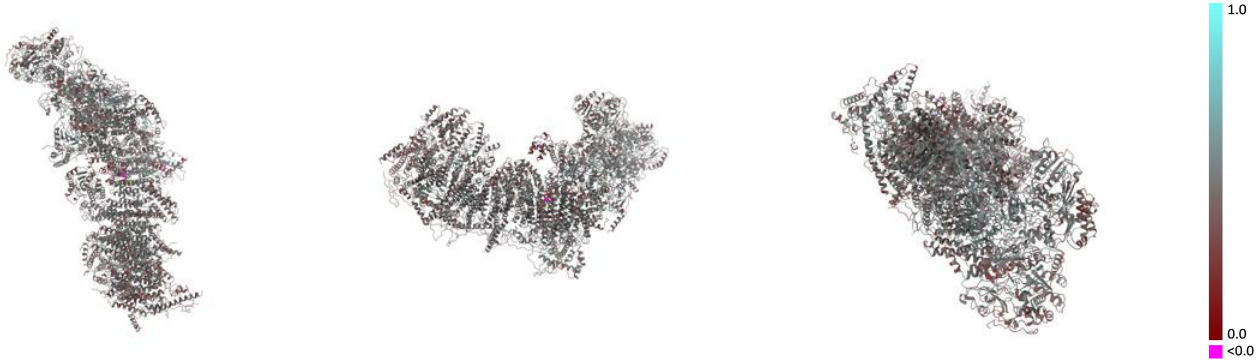
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0268 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.

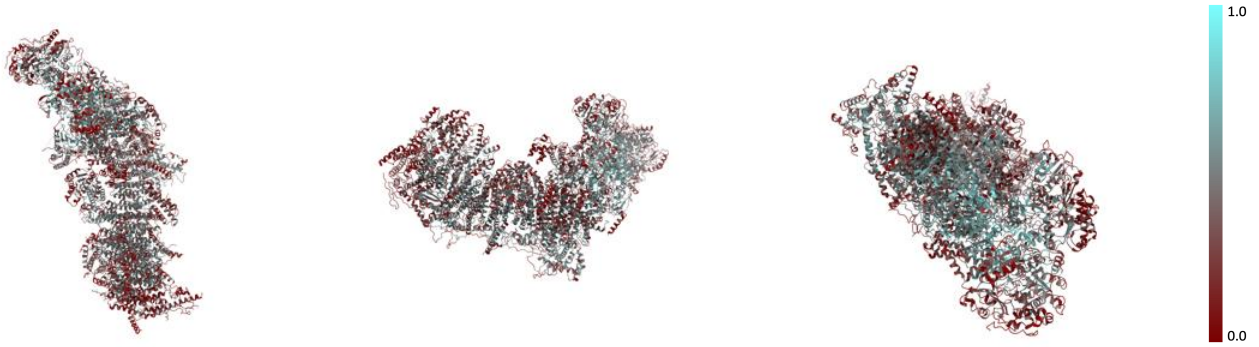
9.2 Q-score mapped to coordinate model



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.

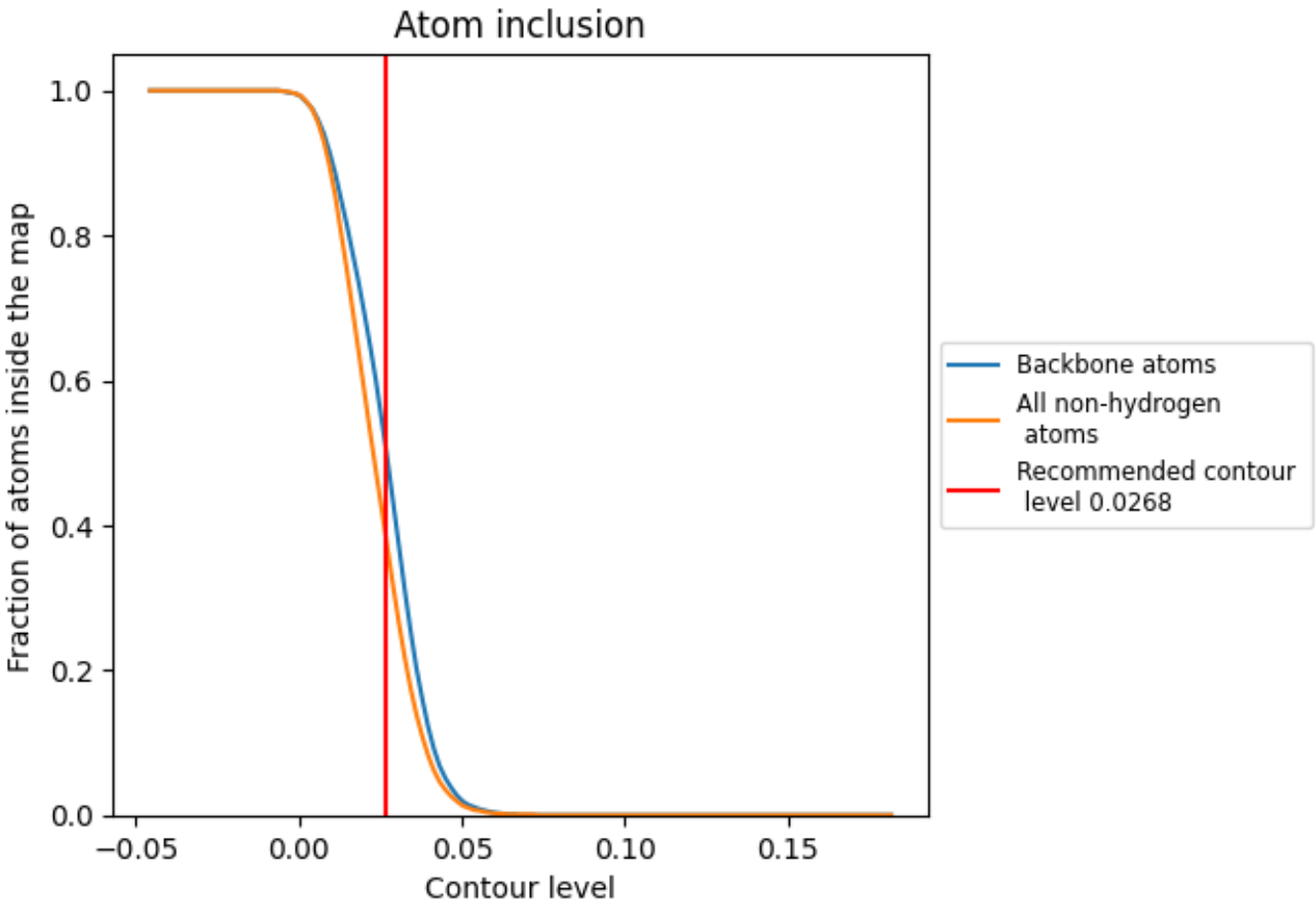
9.3 Atom inclusion mapped to coordinate model



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 (0.0268).

9.4 Atom inclusion (i)



At the recommended contour level, 50% of all backbone atoms, 38% 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 (0.0268) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3810	0.4470
A	0.3090	0.4300
B	0.5680	0.4850
C	0.5340	0.4930
D	0.5190	0.4770
E	0.3040	0.4230
F	0.3490	0.4430
G	0.4310	0.4570
H	0.4020	0.4510
I	0.5890	0.4930
J	0.2760	0.4190
K	0.3850	0.4600
L	0.3490	0.4400
M	0.4610	0.4670
N	0.4800	0.4640
O	0.3610	0.4480
P	0.3410	0.4350
Q	0.4420	0.4760
R	0.4400	0.4750
S	0.1920	0.3990
T	0.0760	0.3060
U	0.1930	0.3950
V	0.3270	0.4380
W	0.3420	0.4330
X	0.3480	0.4540
Y	0.2180	0.4140
Z	0.4400	0.4540
a	0.4260	0.4560
b	0.3340	0.4240
c	0.2810	0.4230
d	0.3780	0.4630
e	0.3950	0.4520
f	0.2800	0.4130
g	0.3510	0.4440
h	0.4250	0.4620



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.2660	0.4070
j	0.1650	0.3950
k	0.1680	0.4170
l	0.3220	0.4450
m	0.2950	0.4260
n	0.3130	0.4290
o	0.2060	0.3850
p	0.3540	0.4300
q	0.4260	0.4660
r	0.3950	0.4560
s	0.2250	0.4390