Full wwPDB EM Validation Report ⓘ

Mar 7, 2026 – 03:14 AM UTC

PDB ID	:	7W32 / pdb_00007w32
EMDB ID	:	EMD-32270
Title	:	Deactive state CI from DQ-NADH dataset, Subclass 2
Authors	:	Gu, J.K.; Yang, M.J.
Deposited on	:	2021-11-24
Resolution	:	2.90 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:

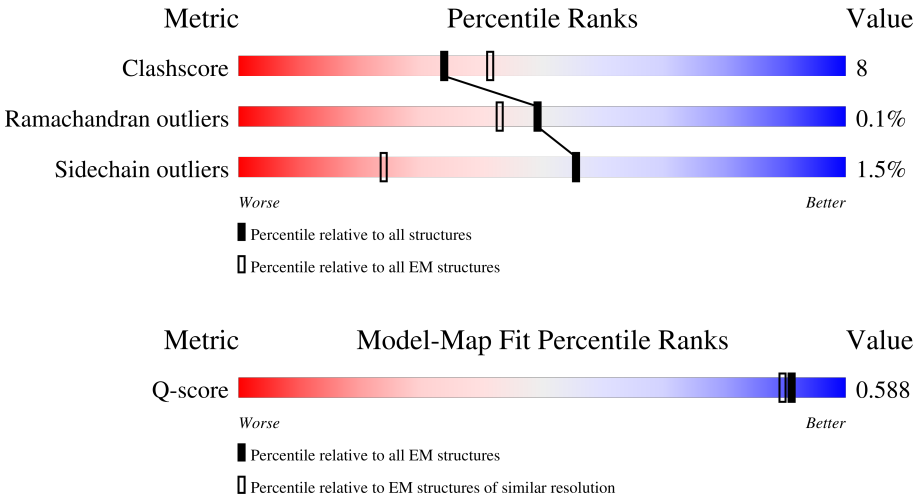
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.49

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 2.90 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.



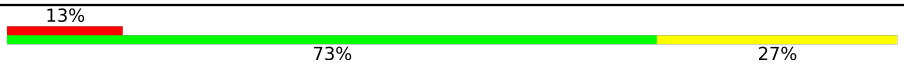
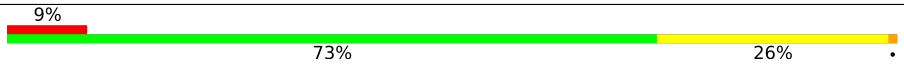
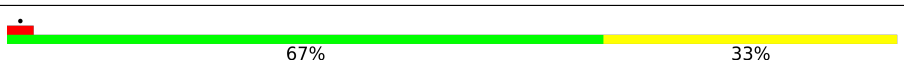
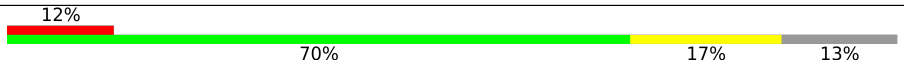
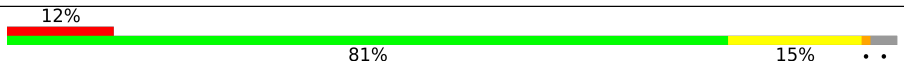
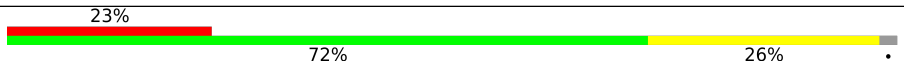
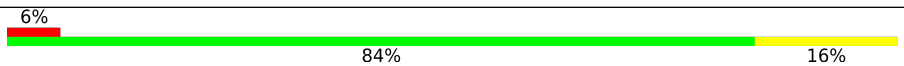
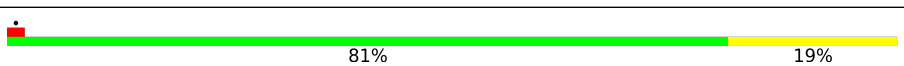
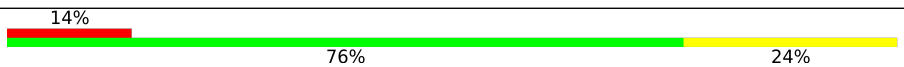
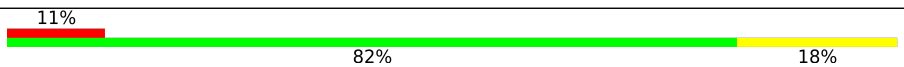
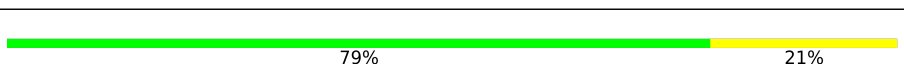
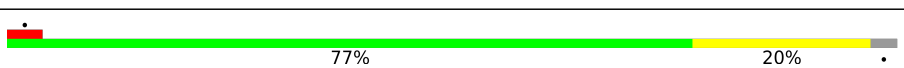
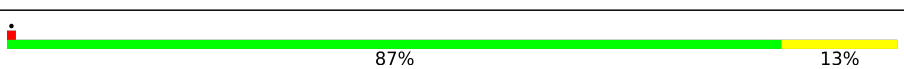
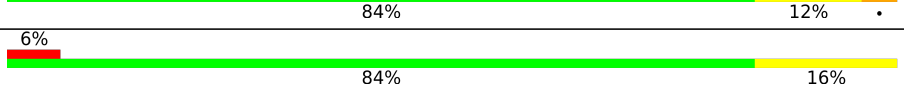
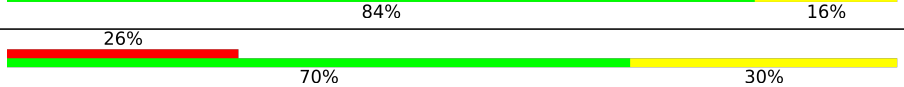
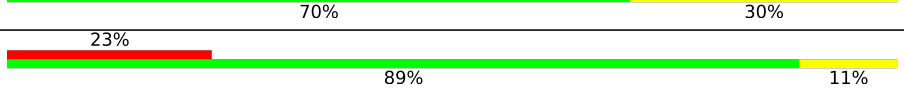
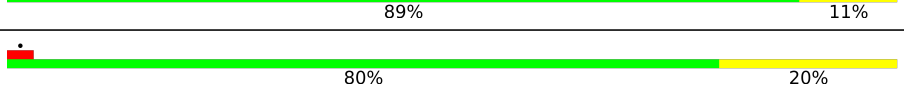
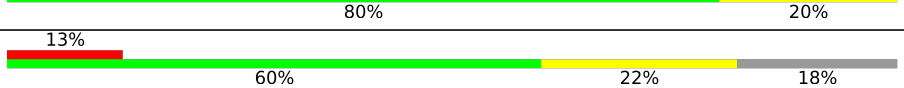
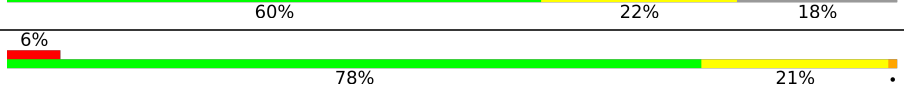
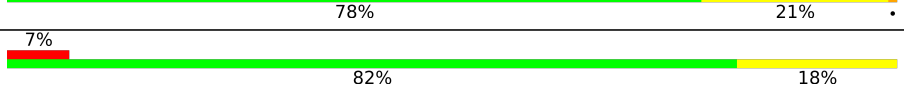
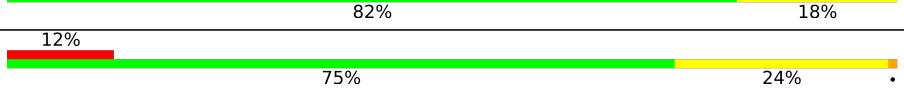
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

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

Mol	Chain	Length	Quality of chain
1	A	433	76% 24%
2	B	176	77% 22%
3	C	156	83% 16%
4	E	115	8% 83% 17%

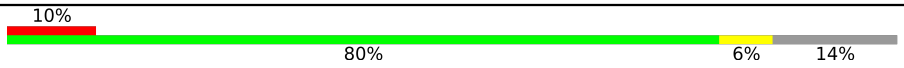
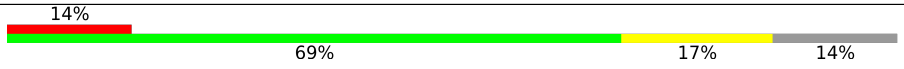
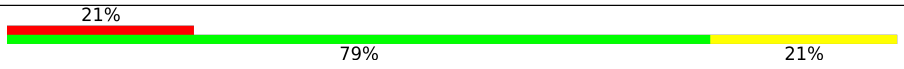
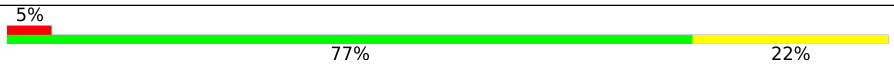
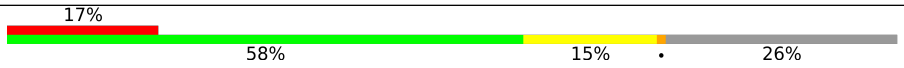
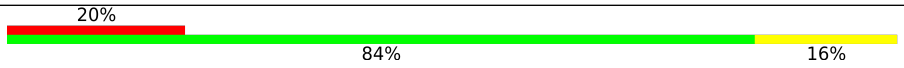
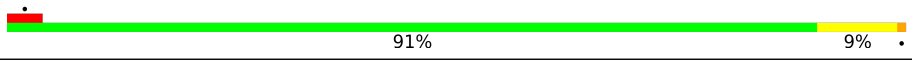
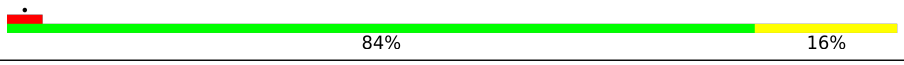
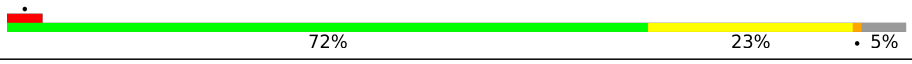
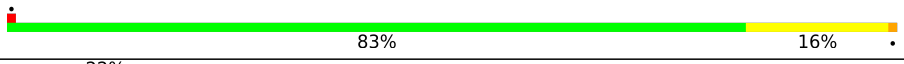
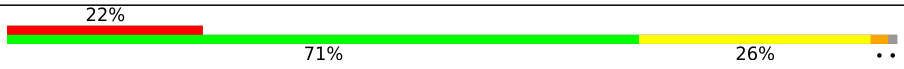
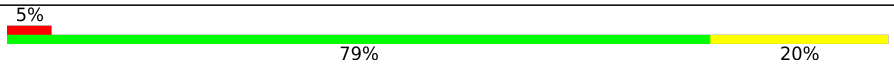
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	F	86	
6	G	88	
6	X	88	
7	H	112	
8	I	112	
9	J	342	
10	K	43	
11	L	125	
12	M	690	
13	N	144	
14	O	217	
15	P	208	
16	Q	430	
17	S	70	
18	T	96	
19	U	83	
20	V	140	
21	W	142	
22	Y	70	
23	Z	84	
24	a	140	
25	b	126	
26	c	156	
27	d	175	
28	e	107	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	f	49	
30	g	121	
31	h	105	
32	i	347	
33	j	115	
34	k	98	
35	l	606	
36	m	175	
37	n	56	
38	o	128	
39	p	178	
40	r	459	
41	s	318	
42	u	171	
43	v	125	
44	w	320	

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 66660 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	431	3318	2095	591	612	20	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	156	1248	794	227	213	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	115	971	619	179	168	5	0	0

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

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

- Molecule 6 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	88	Total	C	N	O	S	0	0
			673	435	102	131	5		
6	X	88	Total	C	N	O	S	0	0
			695	448	103	139	5		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	331	Total	C	N	O	S	0	0
			2613	1694	459	452	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	419	Total	C	N	O	S	0	0
			3377	2162	578	613	24		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			567	364	104	94	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1014	646	174	188	6		

- Molecule 21 is a protein called Complex I-B16.6.

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	103	Total	C	N	O	S	0	0
			878	573	158	146	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	156	Total	C	N	O	S	0	0
			1312	852	213	239	8		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	175	Total	C	N	O	S	0	0
			1458	915	264	271	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	107	Total	C	N	O	S	0	0
			886	566	145	171	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	603	Total	C	N	O	S	0	0
			4720	3118	739	814	49		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	129	Total	C	N	O	S	0	0
			919	614	137	160	8		

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	v	124	Total	C	N	O	S	0	0
			998	625	183	181	9		

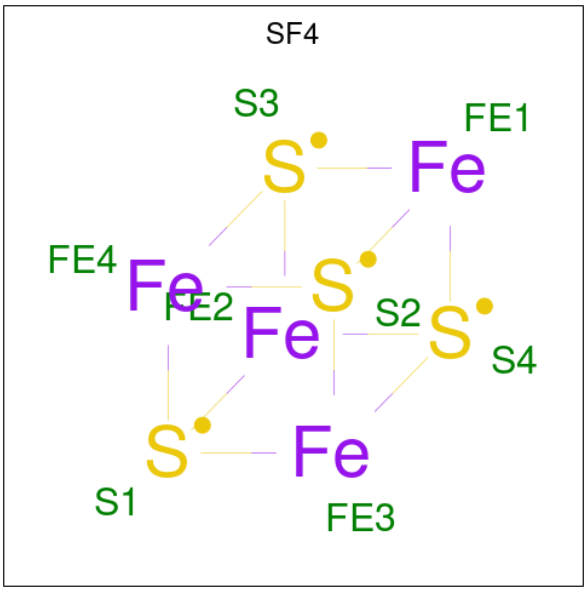
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	1	MYR	-	acetylation	UNP F1SCH1

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

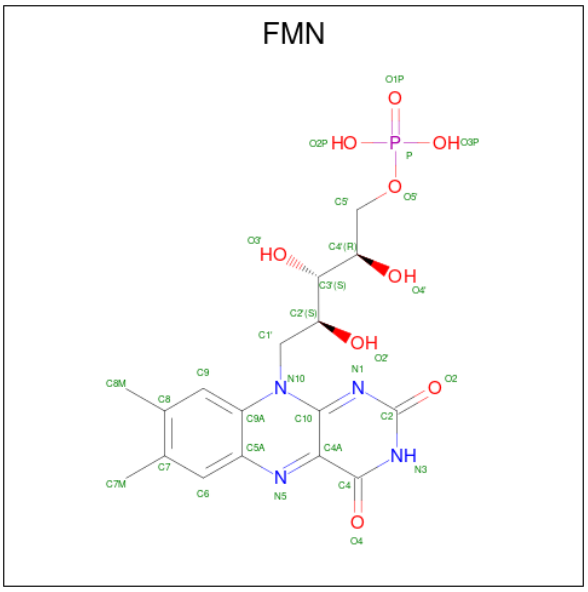
Mol	Chain	Residues	Atoms					AltConf	Trace
44	w	320	Total	C	N	O	S	0	0
			2579	1642	438	489	10		

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



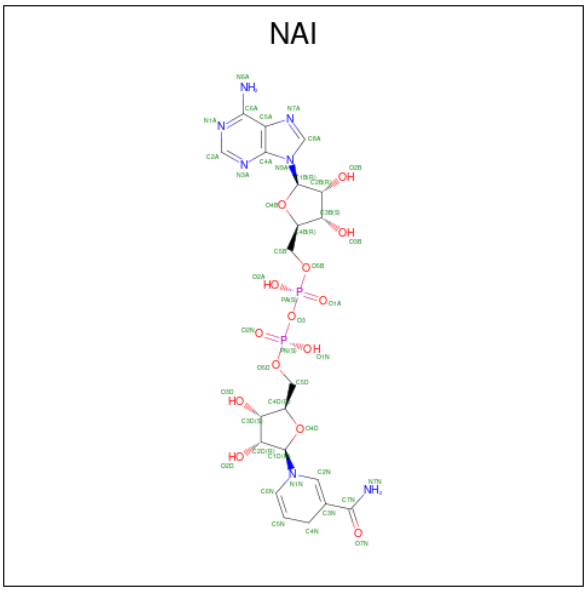
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



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

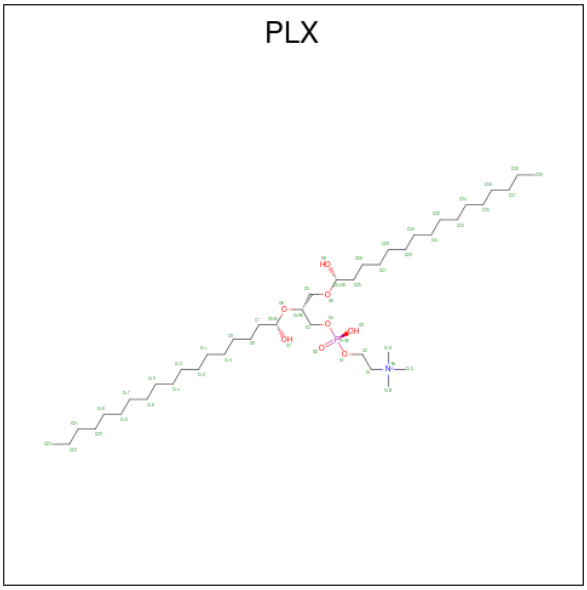
- Molecule 47 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



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

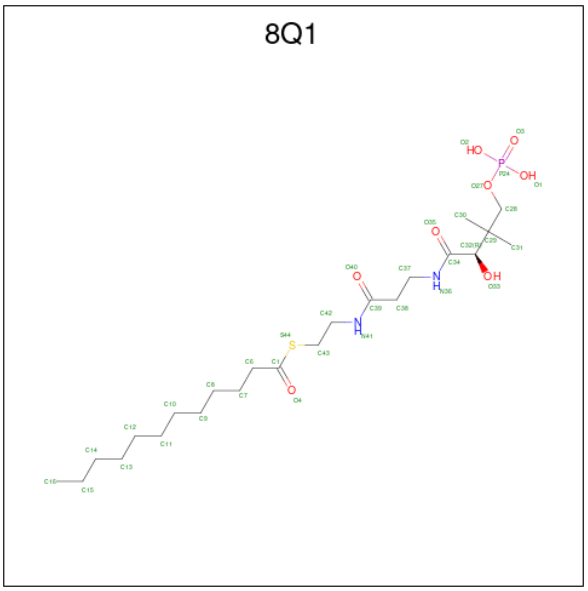
- Molecule 48 is (9R,11S)-9-({[(1S)-1-HYDROXYHEXADECYL]OXY}METHYL)-2,2-DIMETHYL-5,7,10-TRIOXA-2LAMBDA 5 -AZA-6LAMBDA 5 -PHOSPHAOCTACOSANE-6,6,

11-TRIOL (CCD ID: PLX) (formula: $C_{42}H_{89}NO_8P$).



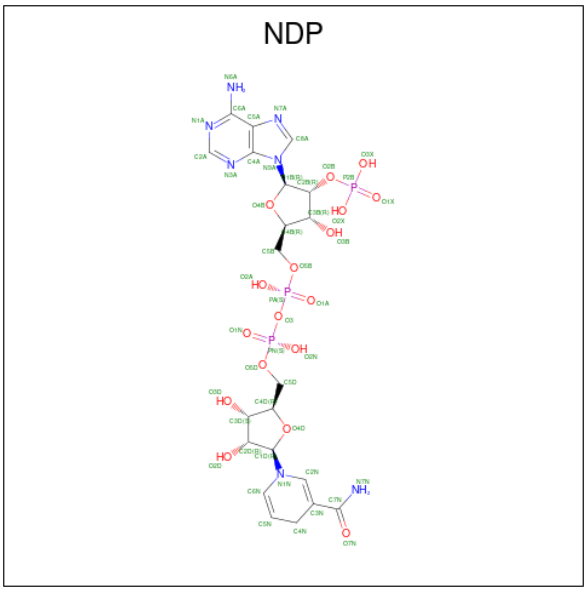
Mol	Chain	Residues	Atoms					AltConf
48	C	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	e	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	g	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	m	1	Total	C	N	O	P	0
			52	42	1	8	1	
48	r	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 49 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



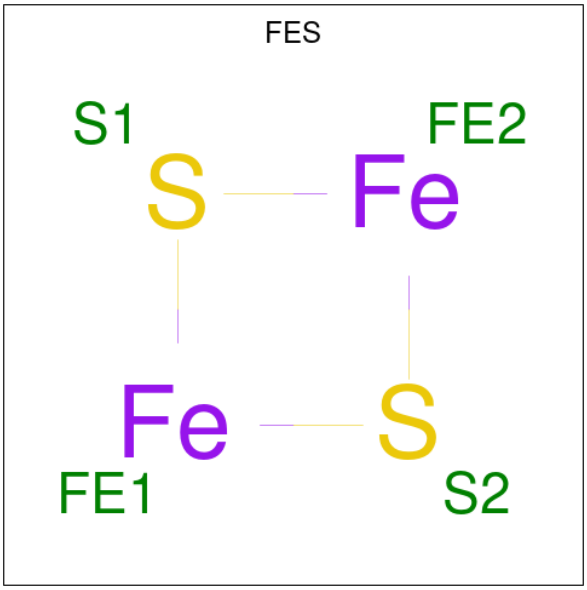
Mol	Chain	Residues	Atoms						AltConf
49	G	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
49	X	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

- Molecule 50 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



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

- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).

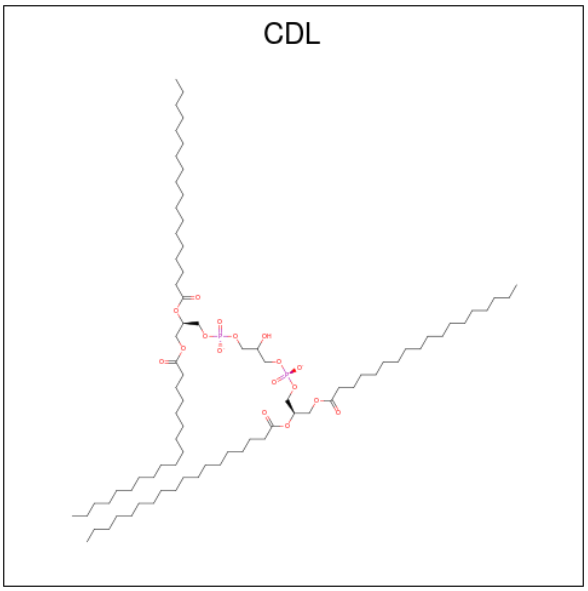


Mol	Chain	Residues	Atoms	AltConf
51	M	1	Total Fe S 4 2 2	0
51	O	1	Total Fe S 4 2 2	0

- Molecule 52 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

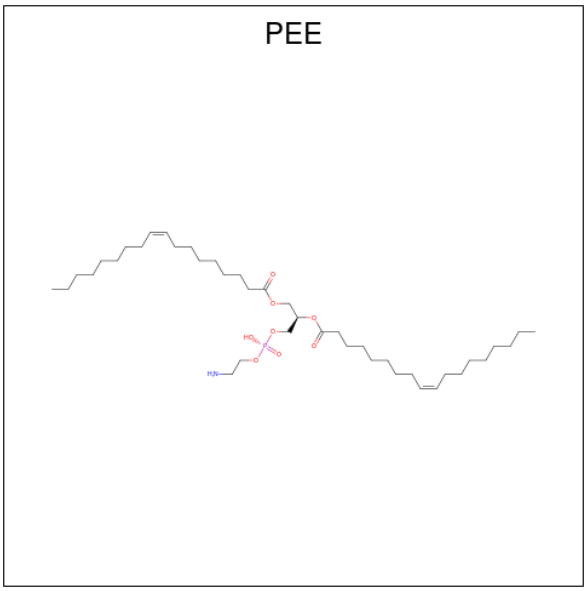
Mol	Chain	Residues	Atoms	AltConf
52	M	1	Total Mg 1 1	0

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	N	1	Total	C	O	P	0
			51	32	17	2	
53	a	1	Total	C	O	P	0
			91	72	17	2	
53	i	1	Total	C	O	P	0
			66	47	17	2	
53	l	1	Total	C	O	P	0
			100	81	17	2	
53	r	1	Total	C	O	P	0
			99	80	17	2	
53	r	1	Total	C	O	P	0
			100	81	17	2	

- Molecule 54 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (CCD ID: PEE) (formula: $C_{41}H_{78}NO_8P$).

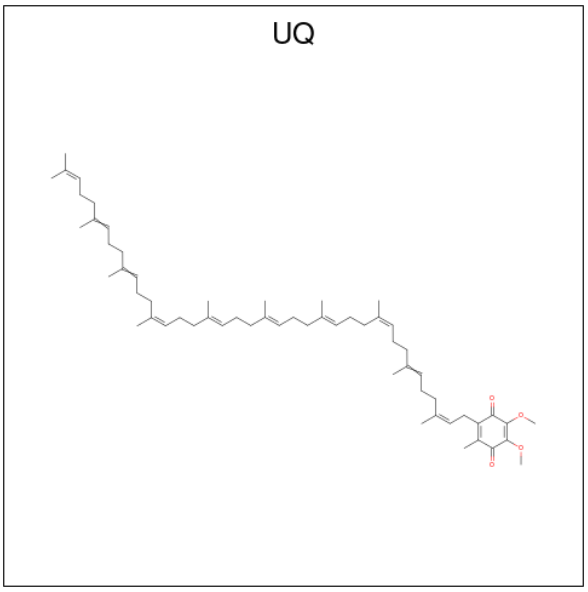


Mol	Chain	Residues	Atoms					AltConf
54	Q	1	Total	C	N	O	P	0
			51	41	1	8	1	
54	i	1	Total	C	N	O	P	0
			47	37	1	8	1	
54	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	l	1	Total	C	N	O	P	0
			46	36	1	8	1	
54	m	1	Total	C	N	O	P	0
			41	31	1	8	1	
54	r	1	Total	C	N	O	P	0
			51	41	1	8	1	
54	s	1	Total	C	N	O	P	0
			51	41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

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

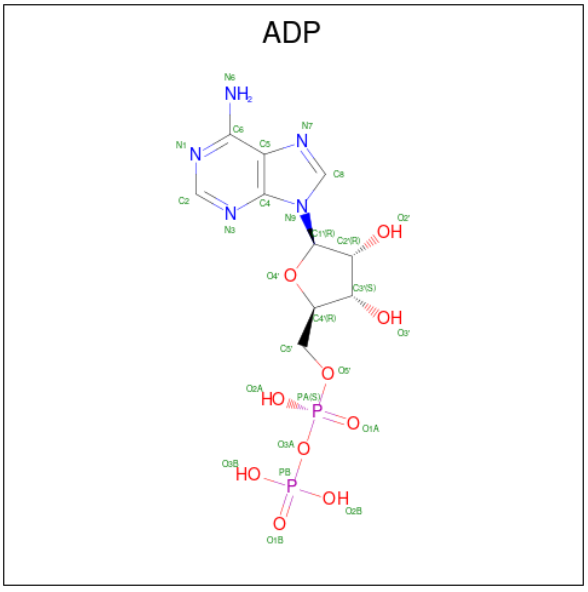
Mol	Chain	Residues	Atoms		AltConf
55	T	1	Total	Zn	0
			1	1	

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



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

- Molecule 57 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



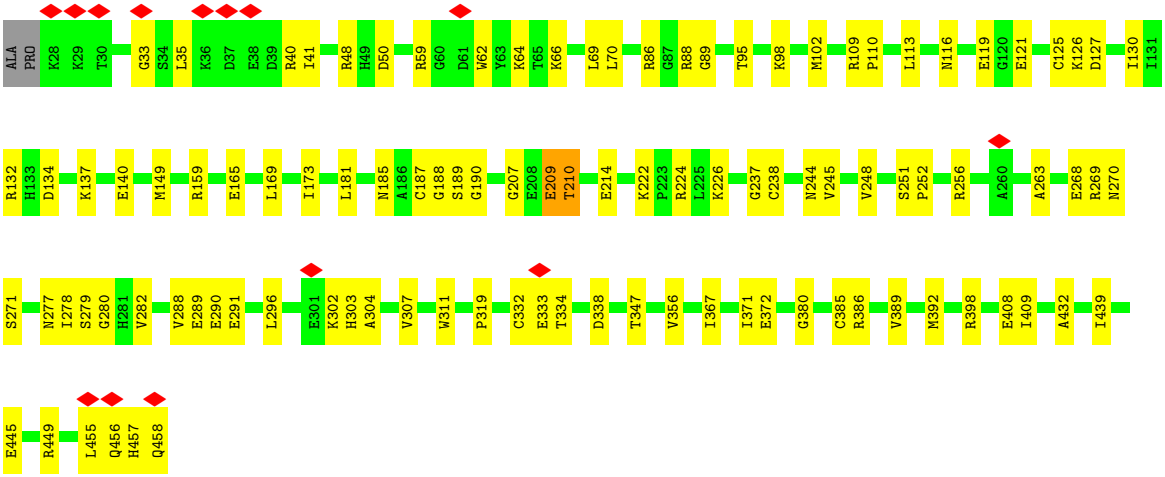
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
57	w	1	27	10	5	10	2	0

3 Residue-property plots (i)

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

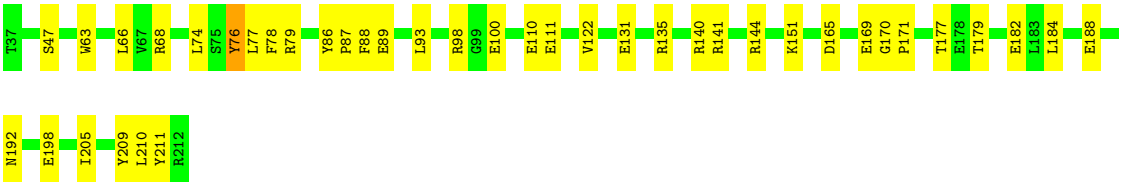
• Molecule 1: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain A:



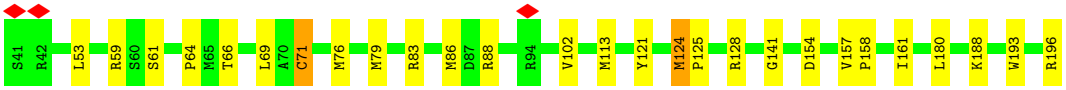
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain B:



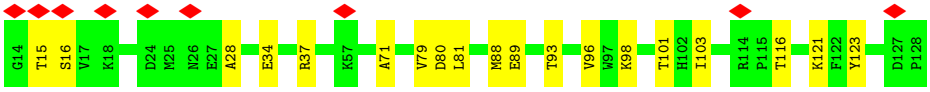
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain C:



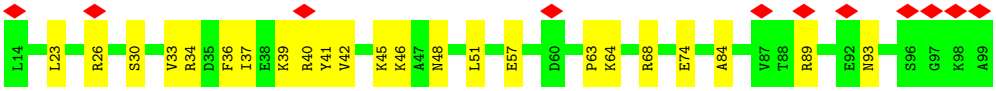
• Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E:



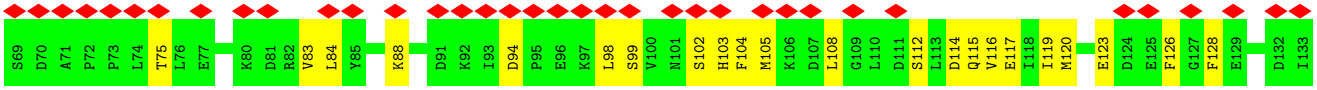
• Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

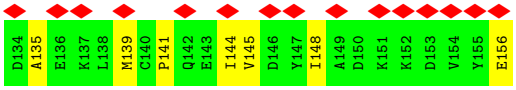
Chain F:



• Molecule 6: Acyl carrier protein

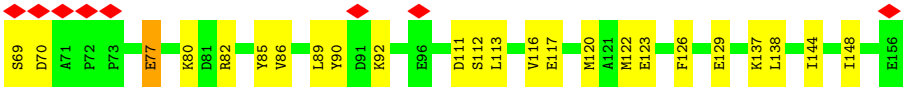
Chain G:





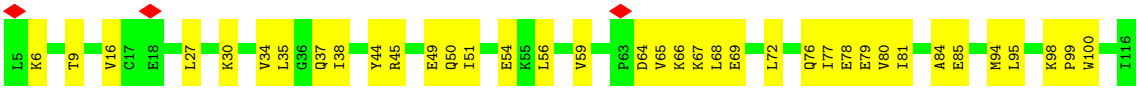
• Molecule 6: Acyl carrier protein

Chain X:



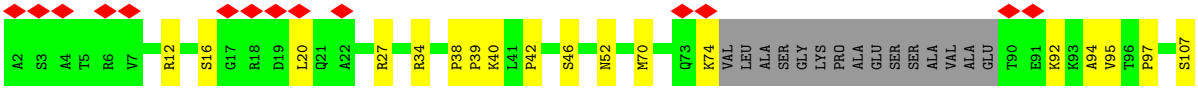
• Molecule 7: Complex I subunit B13

Chain H:



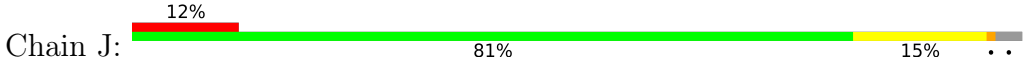
• Molecule 8: Complex I-B14.5a

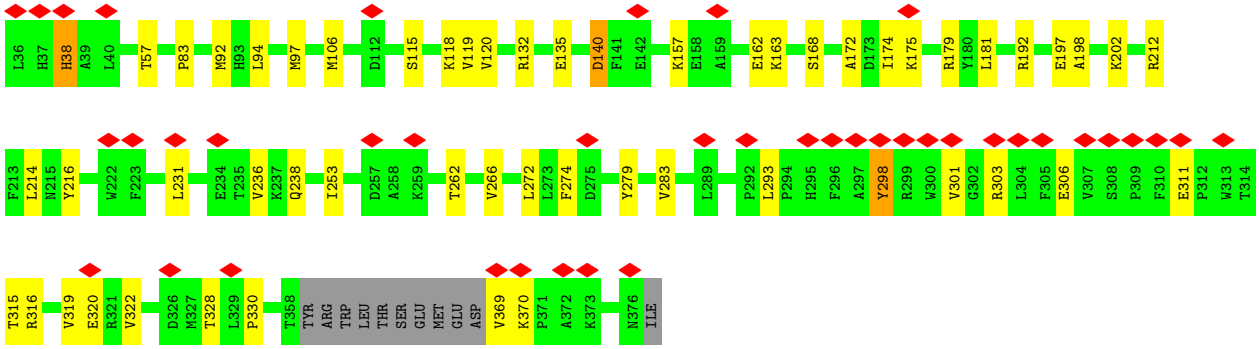
Chain I:



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

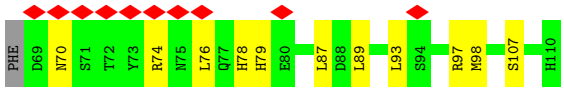
Chain J:





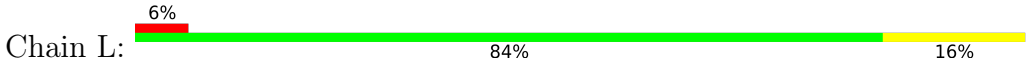
• Molecule 10: Complex I-9kD

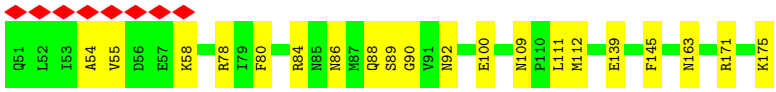
Chain K:



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

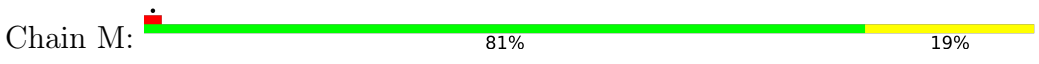
Chain L:

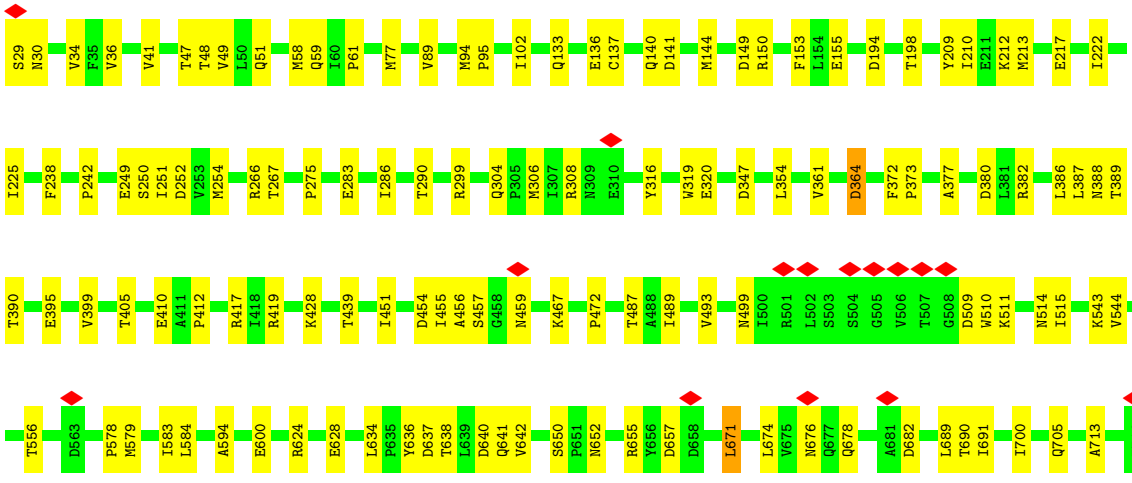




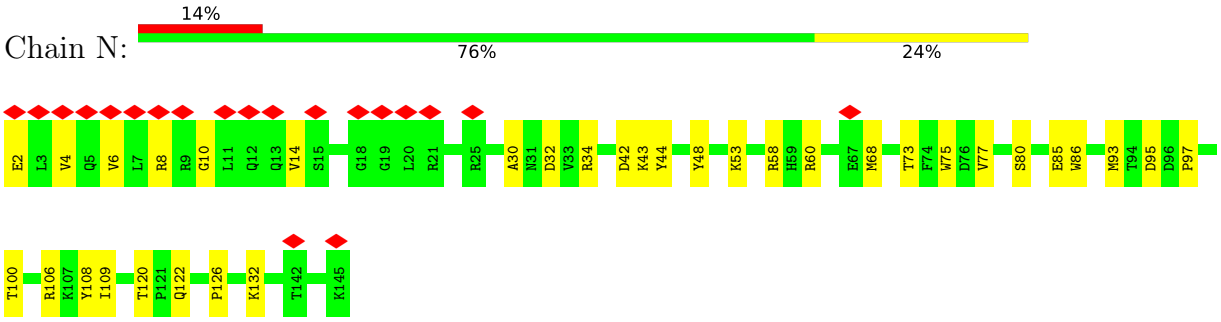
• Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain M:

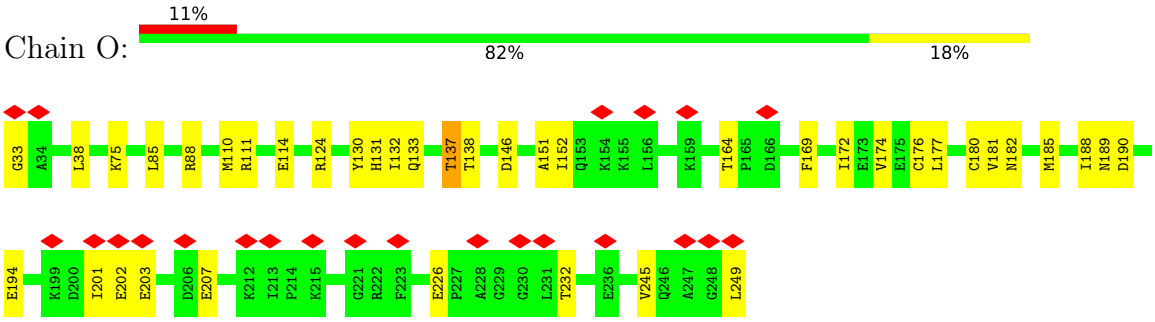




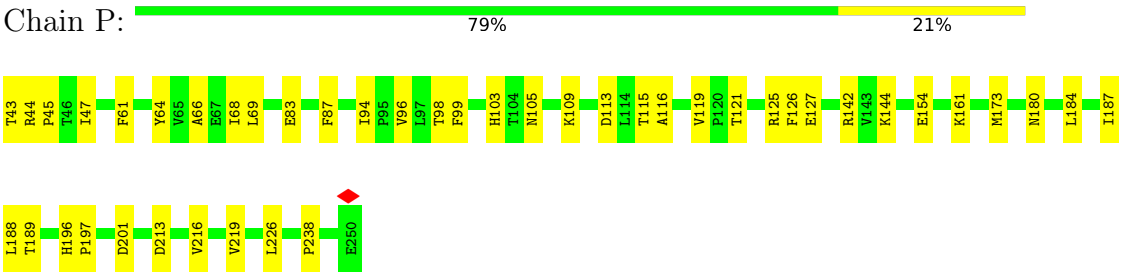
• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



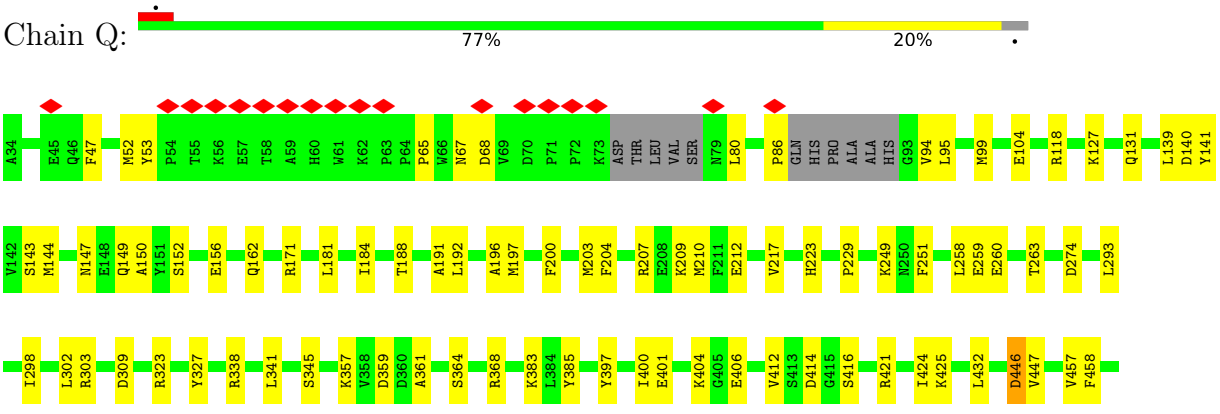
• Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



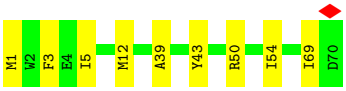
• Molecule 15: Complex I-30kD



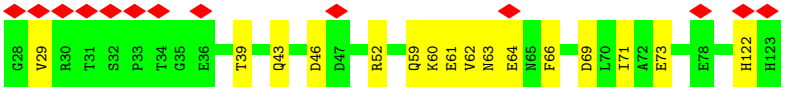
• Molecule 16: Complex I-49kD



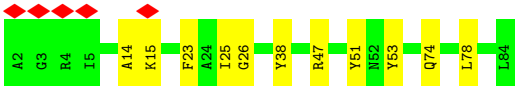
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



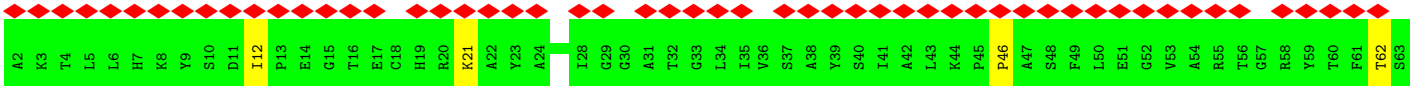
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

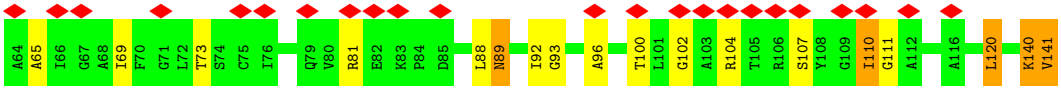


• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

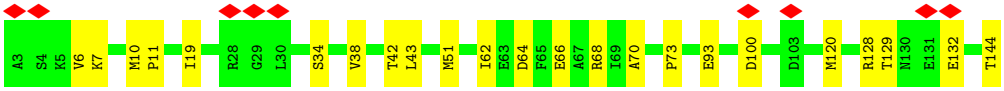


• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

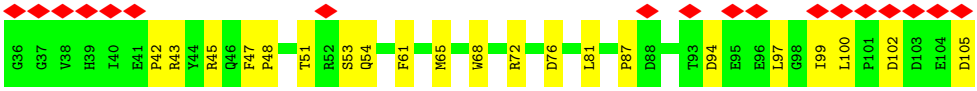




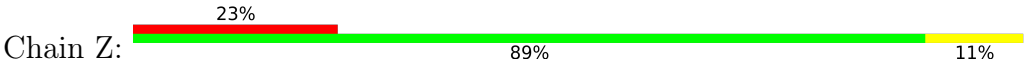
• Molecule 21: Complex I-B16.6

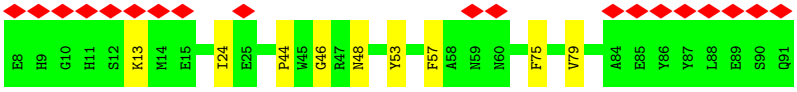


• Molecule 22: Complex I-AGGG

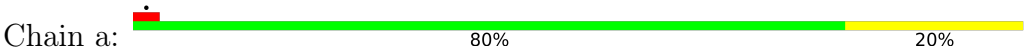


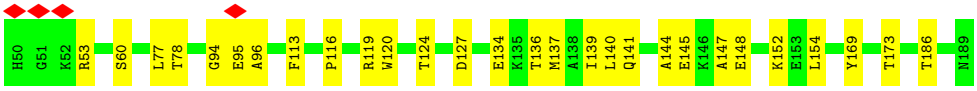
• Molecule 23: Complex I-B12



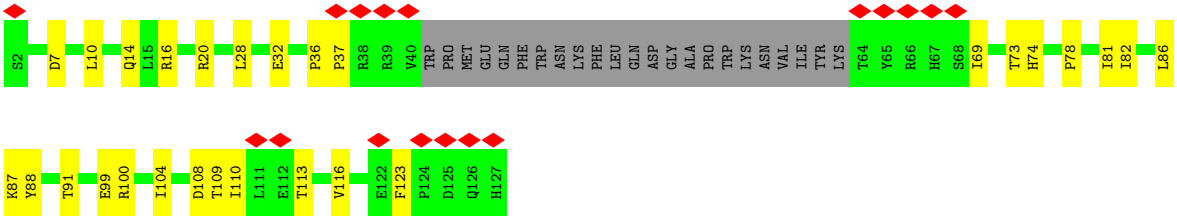


• Molecule 24: Complex I-SGDH

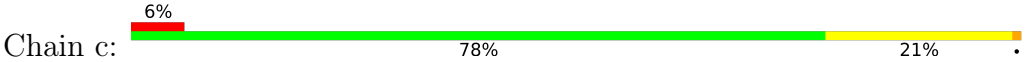


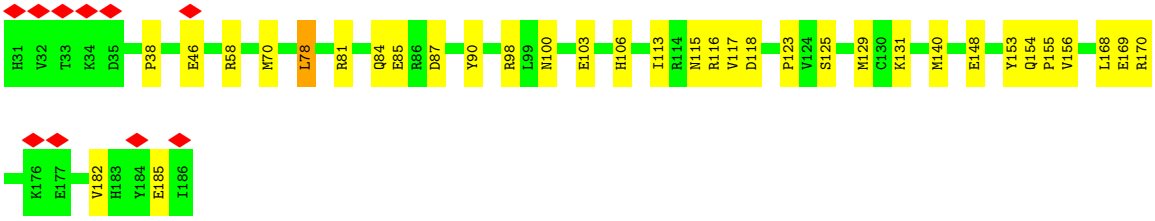


• Molecule 25: Complex I-B17

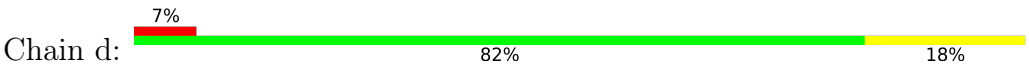


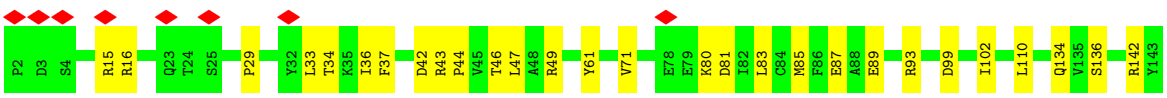
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

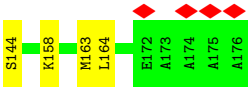




• Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10





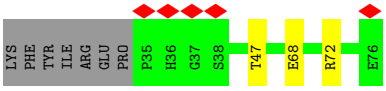


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e:

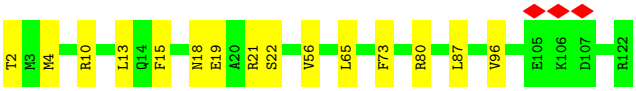
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f:



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

Chain g:

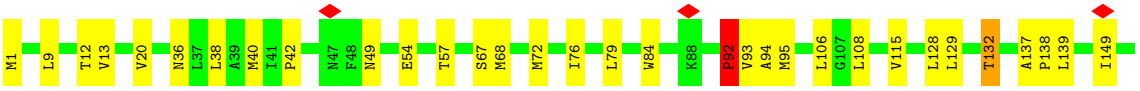


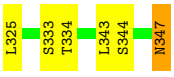
• Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h:

• Molecule 32: NADH-ubiquinone oxidoreductase chain 2

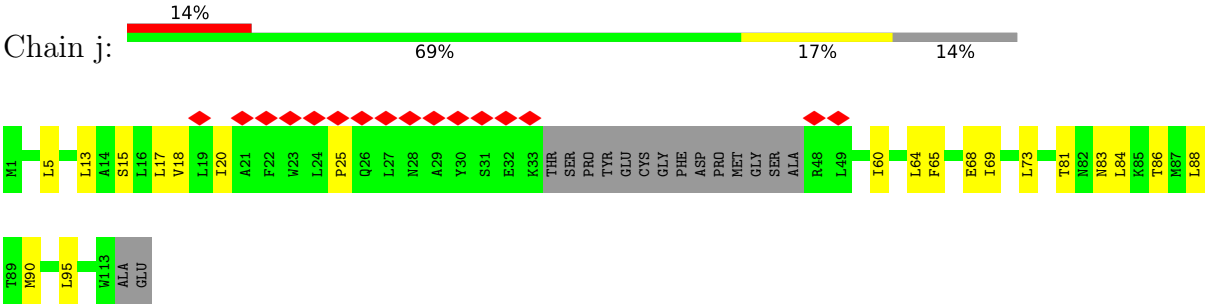
Chain i:





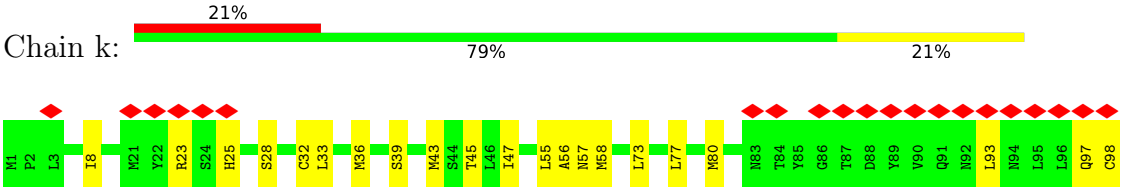
• Molecule 33: NADH-ubiquinone oxidoreductase chain 3

Chain j:



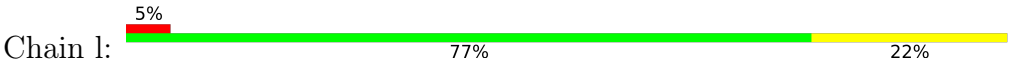
• Molecule 34: NADH-ubiquinone oxidoreductase chain 4L

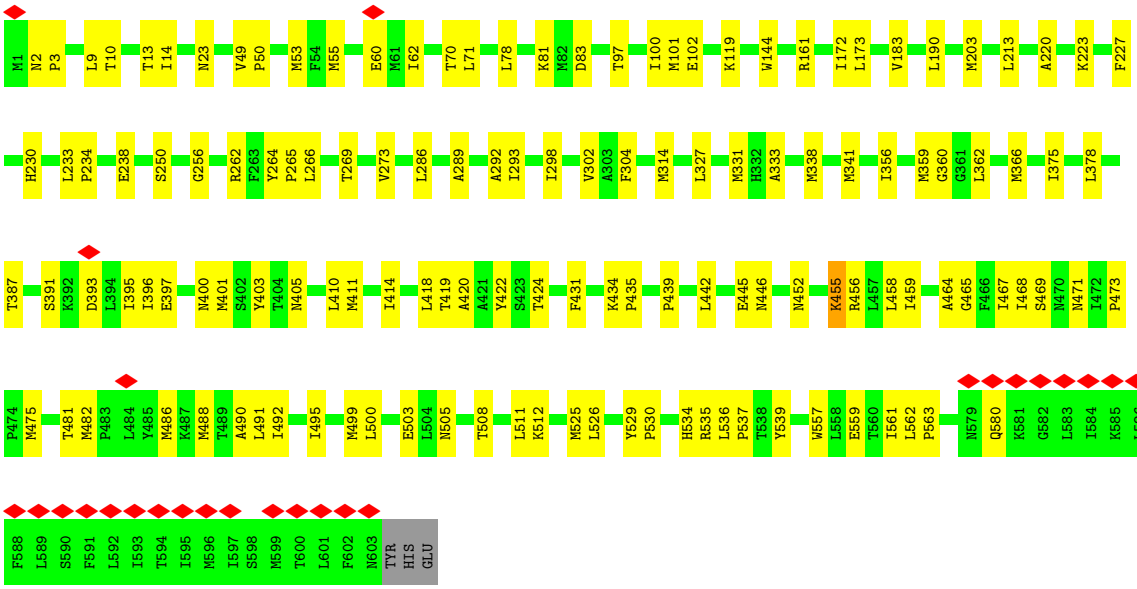
Chain k:



• Molecule 35: NADH-ubiquinone oxidoreductase chain 5

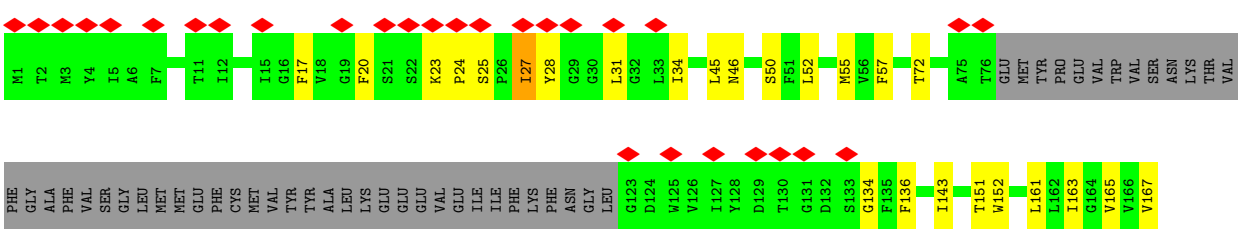
Chain l:

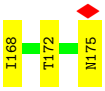




• Molecule 36: NADH-ubiquinone oxidoreductase chain 6

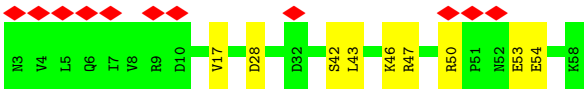
Chain m:





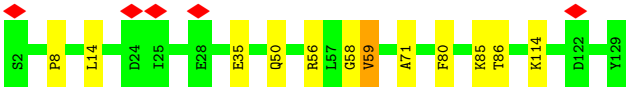
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n:



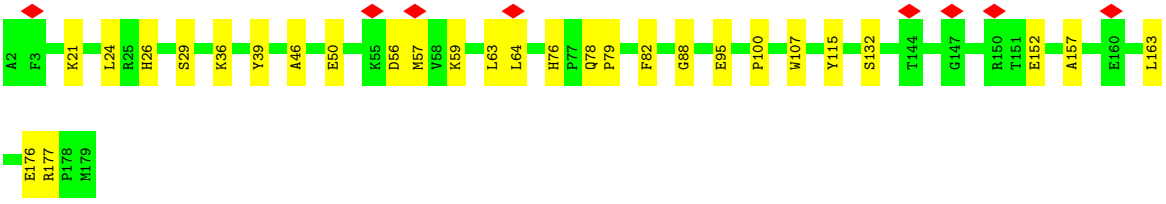
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o:



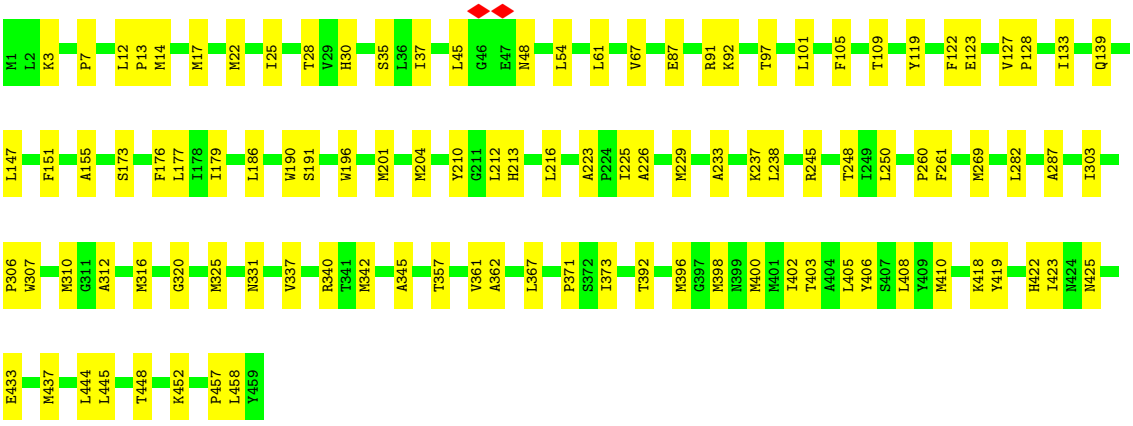
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p:



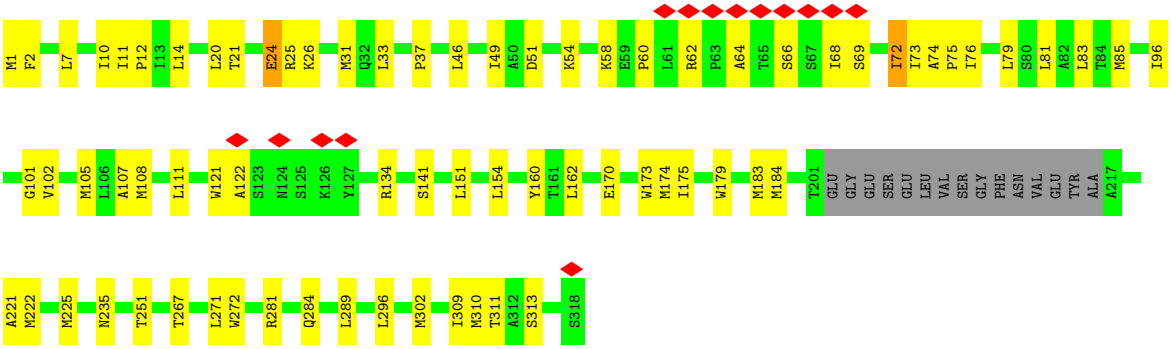
• Molecule 40: NADH-ubiquinone oxidoreductase chain 4

Chain r:

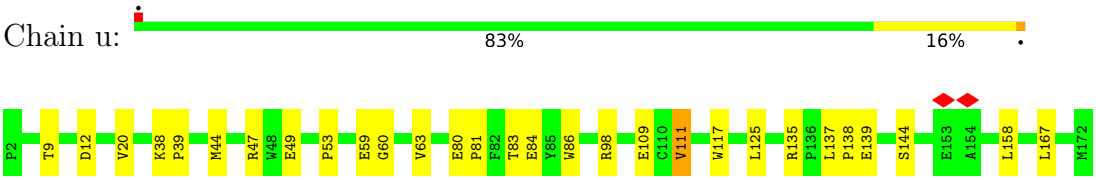


• Molecule 41: NADH-ubiquinone oxidoreductase chain 1

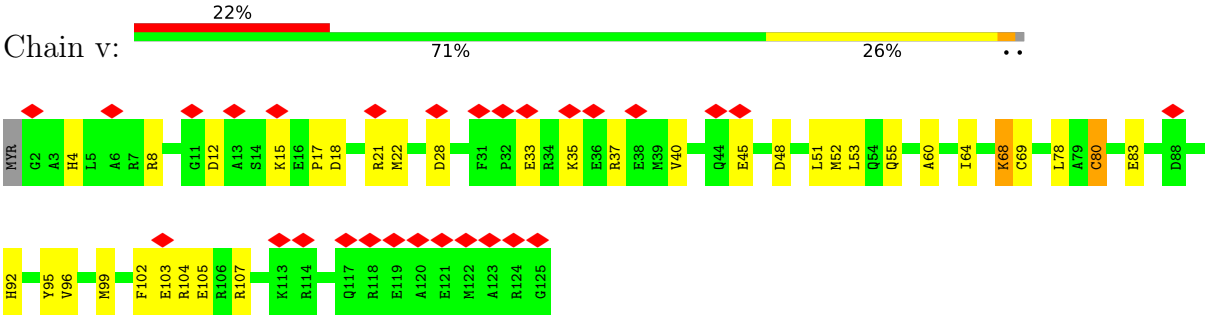
Chain s:



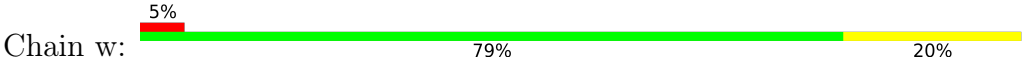
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

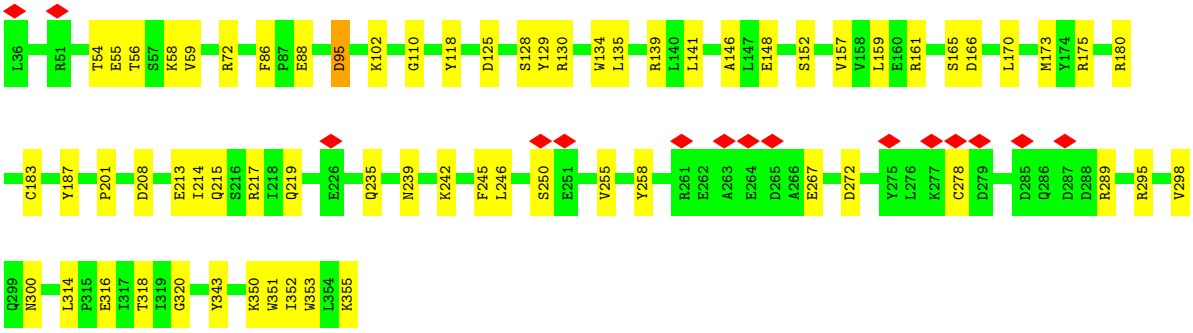


• Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



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





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	145530	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.113	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0254	Depositor
Map size (Å)	333.002, 333.002, 333.002	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0742, 1.0742, 1.0742	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.13	0/3393	0.34	1/4584 (0.0%)
2	B	0.12	0/1443	0.30	0/1952
3	C	0.16	0/1279	0.45	2/1730 (0.1%)
4	E	0.14	0/995	0.36	0/1340
5	F	0.16	0/702	0.42	0/945
6	G	0.20	0/684	0.53	0/929
6	X	0.13	0/707	0.35	0/958
7	H	0.12	0/929	0.33	0/1258
8	I	0.13	0/798	0.37	0/1079
9	J	0.11	0/2682	0.33	0/3636
10	K	0.09	0/365	0.29	0/493
11	L	0.11	0/1039	0.30	0/1403
12	M	0.12	0/5384	0.32	0/7295
13	N	0.11	0/1245	0.29	0/1694
14	O	0.12	0/1711	0.34	0/2328
15	P	0.13	0/1789	0.35	0/2436
16	Q	0.14	0/3451	0.33	0/4672
17	S	0.14	0/582	0.34	0/783
18	T	0.09	0/755	0.27	0/1018
19	U	0.11	0/664	0.27	0/912
20	V	0.19	0/1035	0.42	0/1402
21	W	0.12	0/1198	0.27	0/1617
22	Y	0.13	0/626	0.30	0/857
23	Z	0.11	0/695	0.30	0/939
24	a	0.14	0/1199	0.39	0/1623
25	b	0.13	0/905	0.33	0/1231
26	c	0.13	0/1368	0.34	0/1871
27	d	0.15	0/1491	0.34	0/2011
28	e	0.13	0/912	0.35	0/1241
29	f	0.10	0/350	0.28	0/473
30	g	0.11	0/1031	0.27	0/1394
31	h	0.11	0/889	0.26	0/1190

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	i	0.15	0/2773	0.39	1/3768 (0.0%)
33	j	0.18	0/819	0.41	0/1117
34	k	0.15	0/759	0.34	0/1029
35	l	0.14	0/4845	0.36	0/6595
36	m	0.15	0/938	0.34	0/1271
37	n	0.12	0/491	0.33	0/663
38	o	0.13	0/1092	0.37	1/1481 (0.1%)
39	p	0.13	0/1590	0.33	0/2155
40	r	0.14	0/3723	0.36	0/5078
41	s	0.18	0/2464	0.41	0/3369
42	u	0.12	0/1436	0.31	0/1938
43	v	0.13	0/1022	0.37	0/1377
44	w	0.12	0/2639	0.34	0/3576
All	All	0.14	0/66887	0.35	5/90711 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	124	MET	CA-C-N	6.39	126.31	119.85
3	C	124	MET	C-N-CA	6.39	126.31	119.85
32	i	92	PRO	CA-N-CD	-5.71	104.01	112.00
1	A	209	GLU	N-CA-C	5.16	116.90	111.28
38	o	59	VAL	N-CA-C	5.08	115.63	108.36

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	3318	0	3280	71	0
2	B	1412	0	1363	33	0
3	C	1248	0	1254	21	0
4	E	971	0	975	14	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	691	0	704	15	0
6	G	673	0	652	25	0
6	X	695	0	669	21	0
7	H	910	0	950	26	0
8	I	780	0	808	19	0
9	J	2613	0	2629	37	0
10	K	355	0	329	7	0
11	L	1016	0	1016	18	0
12	M	5296	0	5326	82	0
13	N	1204	0	1162	22	0
14	O	1671	0	1673	29	0
15	P	1738	0	1693	34	0
16	Q	3377	0	3319	65	0
17	S	567	0	565	7	0
18	T	741	0	702	12	0
19	U	643	0	642	10	0
20	V	1014	0	1014	19	0
21	W	1167	0	1155	22	0
22	Y	600	0	539	19	0
23	Z	674	0	643	7	0
24	a	1165	0	1174	24	0
25	b	878	0	896	24	0
26	c	1312	0	1206	31	0
27	d	1458	0	1425	23	0
28	e	886	0	833	23	0
29	f	342	0	341	3	0
30	g	1000	0	994	12	0
31	h	867	0	871	18	0
32	i	2710	0	2874	54	0
33	j	800	0	855	19	0
34	k	748	0	799	18	0
35	l	4720	0	4797	96	0
36	m	919	0	920	26	0
37	n	479	0	486	7	0
38	o	1062	0	1072	14	0
39	p	1534	0	1470	22	0
40	r	3631	0	3839	81	0
41	s	2394	0	2508	60	0
42	u	1398	0	1378	22	0
43	v	998	0	919	28	0
44	w	2579	0	2529	45	0
45	A	8	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	B	16	0	0	0	0
45	C	8	0	0	1	0
45	M	16	0	0	0	0
46	A	31	0	19	2	0
47	A	44	0	27	4	0
48	C	52	0	88	5	0
48	e	52	0	88	1	0
48	g	52	0	88	5	0
48	m	52	0	88	4	0
48	r	52	0	88	7	0
49	G	35	0	0	2	0
49	X	35	0	0	3	0
50	J	48	0	25	2	0
51	M	4	0	0	0	0
51	O	4	0	0	1	0
52	M	1	0	0	0	0
53	N	51	0	46	0	0
53	a	91	0	132	8	0
53	i	66	0	76	4	0
53	l	100	0	156	5	0
53	r	199	0	307	17	0
54	Q	51	0	82	1	0
54	i	47	0	71	5	0
54	l	92	0	138	6	0
54	m	41	0	59	2	0
54	r	51	0	82	6	0
54	s	51	0	82	4	0
55	T	1	0	0	0	0
56	s	28	0	31	4	0
57	w	27	0	11	1	0
All	All	66660	0	67032	1089	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 8.

All (1089) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:112:SER:CB	49:X:201:8Q1:O1	1.67	1.39
20:V:107:SER:HB3	20:V:110:ILE:CG2	1.57	1.32
50:J:401:NDP:O4D	50:J:401:NDP:C4D	1.68	1.19

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:A:503:NAI:C1B	47:A:503:NAI:O4B	1.63	1.12
20:V:107:SER:HB3	20:V:110:ILE:HG22	1.14	1.10
45:C:301:SF4:S4	16:Q:223:HIS:CD2	2.51	1.03
6:G:126:PHE:CB	6:G:128:PHE:HE1	1.76	0.99
20:V:107:SER:CB	20:V:110:ILE:HG22	1.93	0.97
20:V:69:ILE:HG21	20:V:100:THR:HG21	1.48	0.93
41:s:24:GLU:HG2	41:s:271:LEU:HD22	1.55	0.89
20:V:65:ALA:O	20:V:69:ILE:HG12	1.73	0.88
32:i:72:MET:HE1	34:k:43:MET:HE1	1.57	0.86
41:s:281:ARG:HB2	41:s:284:GLN:HG3	1.56	0.85
6:G:126:PHE:CB	6:G:128:PHE:CE1	2.61	0.84
24:a:169:TYR:HH	30:g:2:THR:N	1.74	0.84
15:P:64:TYR:HH	15:P:103:HIS:HE2	1.27	0.82
1:A:121:GLU:HB2	47:A:503:NAI:H42N	1.61	0.82
20:V:107:SER:HB3	20:V:110:ILE:HG21	1.62	0.81
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.64	0.80
42:u:80:GLU:HG3	42:u:81:PRO:HD3	1.65	0.78
1:A:210:THR:HB	1:A:224:ARG:H	1.48	0.78
33:j:18:VAL:HG22	41:s:222:MET:HG3	1.65	0.77
33:j:13:LEU:HD13	41:s:10:ILE:HD13	1.68	0.76
17:S:5:ILE:HG12	41:s:26:LYS:HG2	1.67	0.76
24:a:137:MET:HE1	37:n:42:SER:HB3	1.68	0.75
35:l:100:ILE:HD13	35:l:341:MET:HE3	1.67	0.75
39:p:176:GLU:HG2	39:p:177:ARG:HG2	1.69	0.75
1:A:50:ASP:O	1:A:59:ARG:NH2	2.20	0.75
22:Y:54:GLN:OE1	35:l:446:ASN:ND2	2.21	0.74
22:Y:65:MET:HE3	35:l:375:ILE:HG12	1.69	0.74
35:l:401:MET:HE3	35:l:482:MET:HG2	1.68	0.74
1:A:398:ARG:NH1	12:M:155:GLU:OE2	2.21	0.74
18:T:46:ASP:O	18:T:52:ARG:NH1	2.20	0.73
1:A:398:ARG:NH2	1:A:408:GLU:OE1	2.21	0.72
1:A:89:GLY:HA2	1:A:244:ASN:HD22	1.54	0.72
34:k:8:ILE:HG21	34:k:43:MET:HB2	1.72	0.72
1:A:102:MET:HG2	1:A:149:MET:HB3	1.70	0.72
6:X:123:GLU:HG2	6:X:129:GLU:HA	1.72	0.72
4:E:37:ARG:HA	6:G:120:MET:HE1	1.72	0.71
5:F:39:LYS:HE3	5:F:39:LYS:HA	1.72	0.71
9:J:162:GLU:HG2	9:J:163:LYS:HG3	1.72	0.71
15:P:83:GLU:OE1	15:P:142:ARG:NH2	2.23	0.71
32:i:108:LEU:HD11	32:i:191:THR:HG21	1.72	0.70
2:B:165:ASP:OD1	16:Q:368:ARG:NH2	2.25	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:302:LEU:HB2	16:Q:401:GLU:HB2	1.73	0.69
37:n:47:ARG:NH1	37:n:53:GLU:OE1	2.22	0.69
34:k:80:MET:HE2	36:m:172:THR:HA	1.74	0.69
1:A:385:CYS:HB2	45:A:501:SF4:S4	2.33	0.69
25:b:100:ARG:HB2	35:l:60:GLU:HB2	1.73	0.69
26:c:100:ASN:HB2	26:c:103:GLU:HG3	1.76	0.68
32:i:155:LEU:HD22	32:i:278:MET:HE1	1.76	0.68
14:O:88:ARG:NH2	14:O:190:ASP:OD2	2.26	0.68
30:g:56:VAL:HG21	40:r:17:MET:HE1	1.76	0.68
40:r:210:TYR:O	40:r:213:HIS:ND1	2.27	0.68
34:k:98:CYS:HB2	35:l:580:GLN:HB2	1.75	0.68
53:r:503:CDL:H312	53:r:503:CDL:H742	1.74	0.68
42:u:139:GLU:N	42:u:139:GLU:OE2	2.27	0.67
32:i:92:PRO:O	32:i:94:ALA:N	2.26	0.67
14:O:177:LEU:HB2	14:O:185:MET:HE1	1.77	0.67
37:n:54:GLU:N	37:n:54:GLU:OE1	2.28	0.67
32:i:177:LYS:NZ	34:k:97:GLN:O	2.23	0.67
2:B:111:GLU:O	2:B:141:ARG:NH1	2.27	0.67
3:C:59:ARG:NH1	48:C:302:PLX:O3	2.27	0.67
16:Q:52:MET:O	32:i:171:ASN:ND2	2.27	0.67
15:P:44:ARG:HB3	15:P:45:PRO:HD3	1.77	0.66
2:B:68:ARG:NH2	16:Q:260:GLU:OE2	2.29	0.66
40:r:307:TRP:HA	40:r:310:MET:HE2	1.76	0.66
21:W:51:MET:HE2	41:s:311:THR:HB	1.76	0.66
2:B:177:THR:HG21	2:B:182:GLU:HB2	1.77	0.66
15:P:154:GLU:OE2	15:P:180:ASN:ND2	2.28	0.66
3:C:113:MET:HE1	16:Q:86:PRO:HB2	1.76	0.65
39:p:29:SER:HB3	39:p:76:HIS:CD2	2.32	0.65
41:s:25:ARG:HD2	56:s:402:UQ:HM21	1.79	0.65
7:H:50:GLN:O	7:H:54:GLU:HG3	1.95	0.65
25:b:110:ILE:HG12	27:d:16:ARG:HB3	1.77	0.65
32:i:179:MET:HE1	32:i:251:MET:HE1	1.78	0.65
38:o:50:GLN:O	38:o:56:ARG:HD3	1.96	0.65
12:M:213:MET:HE1	12:M:713:ALA:HB1	1.77	0.65
40:r:122:PHE:HE1	40:r:238:LEU:HB3	1.61	0.65
1:A:132:ARG:HB3	1:A:165:GLU:HG3	1.78	0.65
33:j:95:LEU:HD13	41:s:302:MET:HG2	1.78	0.65
34:k:23:ARG:HD3	36:m:23:LYS:HB2	1.78	0.65
2:B:184:LEU:HB3	11:L:112:MET:HE2	1.79	0.65
12:M:556:THR:HA	12:M:579:MET:HE1	1.78	0.65
33:j:64:LEU:HD13	36:m:165:VAL:HG22	1.78	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:81:ARG:NH1	20:V:89:ASN:OD1	2.29	0.65
16:Q:104:GLU:OE1	41:s:134:ARG:NH2	2.30	0.65
25:b:99:GLU:OE2	35:l:2:ASN:ND2	2.30	0.65
39:p:29:SER:HB3	39:p:76:HIS:HD2	1.62	0.65
44:w:246:LEU:HD12	44:w:255:VAL:HG11	1.77	0.65
9:J:192:ARG:NH1	9:J:198:ALA:O	2.30	0.64
1:A:40:ARG:NH1	1:A:289:GLU:O	2.30	0.64
1:A:210:THR:HG22	1:A:224:ARG:HG2	1.79	0.64
25:b:104:ILE:HB	43:v:48:ASP:HB3	1.78	0.64
35:l:161:ARG:NH1	35:l:238:GLU:OE1	2.30	0.64
20:V:69:ILE:HG21	20:V:100:THR:CG2	2.24	0.64
1:A:244:ASN:OD1	1:A:245:VAL:N	2.30	0.64
5:F:40:ARG:HH12	5:F:84:ALA:HB1	1.61	0.64
53:r:504:CDL:H271	53:r:504:CDL:H742	1.80	0.64
5:F:89:ARG:O	5:F:93:ASN:ND2	2.26	0.64
10:K:76:LEU:HD23	10:K:76:LEU:H	1.62	0.64
6:X:69:SER:OG	6:X:70:ASP:N	2.31	0.64
27:d:110:LEU:HD11	35:l:203:MET:HG2	1.79	0.64
1:A:311:TRP:NE1	1:A:333:GLU:OE2	2.29	0.63
1:A:409:ILE:HG23	1:A:439:ILE:HD12	1.80	0.63
32:i:72:MET:HE2	32:i:76:ILE:HG13	1.78	0.63
44:w:242:LYS:HA	44:w:246:LEU:HD23	1.79	0.63
1:A:48:ARG:NH2	14:O:226:GLU:OE2	2.31	0.63
22:Y:94:ASP:HB3	22:Y:99:ILE:HB	1.79	0.63
28:e:119:ARG:O	28:e:123:GLU:HG3	1.98	0.63
26:c:46:GLU:OE1	26:c:46:GLU:N	2.23	0.63
27:d:163:MET:HG3	28:e:149:LEU:HD11	1.79	0.63
5:F:33:VAL:O	5:F:36:PHE:HB3	1.98	0.63
6:X:112:SER:CB	49:X:201:8Q1:P24	2.86	0.63
35:l:338:MET:HA	35:l:341:MET:HG3	1.80	0.63
41:s:69:SER:O	41:s:73:ILE:HD12	1.99	0.63
14:O:38:LEU:O	14:O:124:ARG:NH2	2.31	0.63
44:w:125:ASP:O	44:w:130:ARG:NH2	2.32	0.63
9:J:132:ARG:NH2	50:J:401:NDP:O2X	2.32	0.62
11:L:109:ASN:ND2	11:L:111:LEU:O	2.32	0.62
41:s:24:GLU:CG	41:s:271:LEU:HD22	2.27	0.62
11:L:88:GLN:NE2	12:M:141:ASP:OD2	2.31	0.62
26:c:70:MET:SD	26:c:70:MET:N	2.73	0.62
5:F:46:LYS:HE2	12:M:674:LEU:HD21	1.81	0.62
6:G:144:ILE:O	6:G:148:ILE:HD12	1.99	0.62
12:M:308:ARG:NH2	12:M:578:PRO:O	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:196:ALA:O	16:Q:197:MET:HG3	1.99	0.62
39:p:56:ASP:HB3	39:p:59:LYS:HB2	1.81	0.62
28:e:129:ARG:HG2	28:e:134:LEU:HB2	1.82	0.62
1:A:140:GLU:OE2	1:A:256:ARG:NH2	2.32	0.62
20:V:88:LEU:O	20:V:92:ILE:HG13	1.99	0.62
25:b:78:PRO:O	25:b:82:ILE:HD12	1.99	0.62
32:i:211:MET:HG3	32:i:333:SER:HB2	1.82	0.62
12:M:150:ARG:NH2	16:Q:359:ASP:OD1	2.32	0.62
20:V:12:ILE:HB	20:V:21:LYS:HD3	1.82	0.62
49:X:201:8Q1:N36	49:X:201:8Q1:O40	2.32	0.62
26:c:155:PRO:HG3	43:v:4:HIS:CD2	2.34	0.62
9:J:157:LYS:NZ	9:J:197:GLU:OE1	2.30	0.62
9:J:163:LYS:NZ	9:J:253:ILE:O	2.32	0.62
32:i:54:GLU:HG3	34:k:93:LEU:HD22	1.80	0.61
53:i:401:CDL:H141	53:i:401:CDL:H371	1.82	0.61
13:N:42:ASP:HB2	13:N:48:TYR:HE1	1.64	0.61
53:r:503:CDL:H421	53:r:503:CDL:H602	1.83	0.61
1:A:185:ASN:OD1	1:A:190:GLY:N	2.30	0.61
33:j:65:PHE:O	33:j:69:ILE:HG13	2.00	0.61
37:n:28:ASP:OD2	40:r:3:LYS:NZ	2.33	0.61
40:r:225:ILE:HG13	40:r:229:MET:HE2	1.82	0.61
41:s:102:VAL:HG11	41:s:154:LEU:HD11	1.82	0.61
32:i:255:PRO:HG2	40:r:123:GLU:HB2	1.83	0.61
43:v:18:ASP:OD2	43:v:21:ARG:NH2	2.34	0.61
1:A:277:ASN:HD21	14:O:181:VAL:HB	1.64	0.60
6:G:88:LYS:HD3	6:G:98:LEU:HD21	1.82	0.60
25:b:86:LEU:HD11	35:l:9:LEU:HD12	1.82	0.60
8:I:42:PRO:HB3	21:W:6:VAL:HG11	1.84	0.60
1:A:64:LYS:HD2	14:O:249:LEU:HD23	1.83	0.60
24:a:134:GLU:HA	24:a:137:MET:HE3	1.83	0.60
33:j:25:PRO:HB2	41:s:60:PRO:HD3	1.82	0.60
2:B:93:LEU:O	8:I:34:ARG:NH2	2.34	0.60
31:h:18:MET:HE3	34:k:56:ALA:HA	1.83	0.60
3:C:158:PRO:HB2	9:J:92:MET:HE3	1.82	0.60
9:J:212:ARG:O	9:J:216:TYR:CB	2.50	0.60
21:W:38:VAL:O	21:W:42:THR:HG23	2.02	0.60
41:s:51:ASP:HB3	56:s:402:UQ:H8	1.84	0.60
2:B:89:GLU:OE2	13:N:34:ARG:NH2	2.35	0.60
35:l:286:LEU:HD22	35:l:411:MET:SD	2.42	0.60
41:s:62:ARG:HH21	41:s:68:ILE:HB	1.66	0.60
42:u:49:GLU:OE1	42:u:135:ARG:NH2	2.34	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:O	1:A:88:ARG:NH1	2.35	0.60
3:C:53:LEU:HD22	48:C:302:PLX:H342	1.84	0.60
12:M:137:CYS:HB3	12:M:140:GLN:HB2	1.84	0.60
25:b:123:PHE:HD2	43:v:40:VAL:HG11	1.67	0.60
53:a:201:CDL:H531	54:l:703:PEE:H56	1.83	0.60
26:c:170:ARG:HG2	43:v:53:LEU:HD13	1.83	0.60
32:i:289:ASN:HA	32:i:292:PHE:CE2	2.36	0.60
9:J:140:ASP:OD1	9:J:140:ASP:N	2.35	0.59
38:o:59:VAL:HG13	40:r:422:HIS:CE1	2.36	0.59
22:Y:94:ASP:OD1	43:v:107:ARG:NH1	2.35	0.59
35:l:55:MET:HE2	35:l:471:ASN:HB3	1.82	0.59
35:l:227:PHE:O	35:l:230:HIS:ND1	2.34	0.59
6:G:84:LEU:O	6:G:88:LYS:HG2	2.03	0.59
11:L:84:ARG:NH1	11:L:88:GLN:O	2.35	0.59
6:X:90:TYR:HE1	23:Z:44:PRO:HB2	1.67	0.59
48:g:201:PLX:H301	32:i:347:ASN:HB3	1.83	0.59
32:i:139:LEU:HD11	32:i:187:MET:HE1	1.85	0.59
40:r:312:ALA:O	40:r:316:MET:HG3	2.01	0.59
22:Y:61:PHE:HE1	35:l:459:ILE:HD11	1.67	0.59
35:l:526:LEU:HD12	35:l:530:PRO:HG2	1.84	0.59
36:m:25:SER:O	36:m:28:TYR:N	2.34	0.59
26:c:116:ARG:HG2	54:l:702:PEE:H49	1.83	0.59
35:l:250:SER:HB2	35:l:333:ALA:HA	1.84	0.59
11:L:78:ARG:HH12	12:M:249:GLU:HG3	1.66	0.59
9:J:369:VAL:HG12	9:J:370:LYS:HG2	1.85	0.59
28:e:89:VAL:HG21	40:r:25:ILE:HG23	1.84	0.59
26:c:154:GLN:HE22	35:l:486:MET:HE1	1.68	0.59
33:j:60:ILE:HG21	36:m:168:ILE:HG21	1.85	0.59
12:M:650:SER:OG	12:M:652:ASN:OD1	2.20	0.59
13:N:32:ASP:OD2	13:N:58:ARG:NH2	2.36	0.59
24:a:137:MET:HG2	27:d:83:LEU:HD12	1.83	0.59
20:V:62:THR:HG23	20:V:104:ARG:HG2	1.85	0.59
35:l:512:LYS:O	39:p:36:LYS:NZ	2.36	0.59
6:G:75:THR:OG1	6:G:156:GLU:OE1	2.20	0.58
35:l:491:LEU:O	35:l:495:ILE:HD12	2.03	0.58
38:o:58:GLY:HA2	40:r:425:ASN:CG	2.28	0.58
44:w:54:THR:O	44:w:55:GLU:HG3	2.03	0.58
6:X:120:MET:HE1	39:p:21:LYS:HA	1.85	0.58
36:m:175:ASN:OD1	44:w:289:ARG:NH2	2.36	0.58
13:N:106:ARG:HB2	13:N:109:ILE:HG13	1.85	0.58
41:s:101:GLY:O	41:s:105:MET:HG3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:90:GLY:HA3	15:P:238:PRO:HB2	1.84	0.58
35:l:419:THR:HA	35:l:422:TYR:CE2	2.39	0.58
9:J:212:ARG:O	9:J:216:TYR:HB2	2.03	0.58
39:p:95:GLU:HG3	40:r:418:LYS:HD3	1.85	0.58
41:s:85:MET:SD	41:s:108:MET:HB2	2.44	0.58
32:i:154:MET:HE3	32:i:154:MET:HA	1.86	0.58
12:M:509:ASP:OD1	12:M:509:ASP:N	2.36	0.58
32:i:233:THR:HG23	32:i:237:MET:HE3	1.86	0.58
16:Q:192:LEU:HD12	16:Q:197:MET:HA	1.86	0.57
40:r:403:THR:HA	40:r:406:TYR:CE2	2.39	0.57
1:A:210:THR:CG2	1:A:224:ARG:HG2	2.33	0.57
9:J:192:ARG:NH2	9:J:262:THR:OG1	2.38	0.57
24:a:95:GLU:OE2	53:a:201:CDL:O1	2.22	0.57
1:A:270:ASN:HD22	1:A:338:ASP:HB2	1.69	0.57
16:Q:99:MET:HE1	16:Q:447:VAL:HG21	1.86	0.57
35:l:119:LYS:NZ	53:r:503:CDL:OA3	2.37	0.57
44:w:128:SER:HB3	44:w:173:MET:HE3	1.86	0.57
7:H:38:ILE:HG21	7:H:45:ARG:HB2	1.86	0.57
25:b:10:LEU:O	25:b:14:GLN:HG3	2.05	0.57
35:l:391:SER:O	35:l:395:ILE:HG12	2.04	0.57
44:w:118:TYR:OH	57:w:401:ADP:O2'	2.21	0.57
1:A:98:LYS:NZ	47:A:503:NAI:O3B	2.37	0.57
11:L:80:PHE:HE1	11:L:100:GLU:HG2	1.69	0.57
26:c:123:PRO:HD2	35:l:525:MET:HE1	1.86	0.57
35:l:559:GLU:O	35:l:563:PRO:HD2	2.05	0.57
9:J:306:GLU:HG2	9:J:315:THR:HG22	1.87	0.57
28:e:113:ARG:HH12	40:r:452:LYS:HD2	1.70	0.57
33:j:88:LEU:HD13	41:s:309:ILE:HD12	1.87	0.57
43:v:33:GLU:OE1	43:v:33:GLU:N	2.31	0.57
43:v:83:GLU:H	43:v:83:GLU:CD	2.13	0.57
35:l:375:ILE:HD12	35:l:458:LEU:HD11	1.87	0.57
31:h:69:ARG:O	31:h:73:MET:HG2	2.04	0.57
3:C:83:ARG:NH1	16:Q:212:GLU:OE2	2.22	0.57
12:M:624:ARG:NH1	12:M:628:GLU:OE1	2.31	0.57
35:l:562:LEU:HB3	35:l:563:PRO:HD3	1.85	0.56
3:C:124:MET:HE3	3:C:128:ARG:HD3	1.88	0.56
7:H:72:LEU:HD23	7:H:80:VAL:HG11	1.87	0.56
15:P:43:THR:HA	15:P:47:ILE:HD12	1.87	0.56
53:a:201:CDL:H322	54:l:703:PEE:H62	1.86	0.56
11:L:163:ASN:O	11:L:171:ARG:HA	2.06	0.56
21:W:144:THR:HB	41:s:96:ILE:HG23	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:l:83:ASP:OD2	35:l:262:ARG:NH1	2.33	0.56
6:G:83:VAL:HG21	6:G:145:VAL:HG12	1.87	0.56
12:M:389:THR:O	12:M:390:THR:OG1	2.22	0.56
12:M:676:ASN:O	12:M:678:GLN:NE2	2.37	0.56
15:P:187:ILE:HG23	15:P:188:LEU:HG	1.87	0.56
19:U:26:GLY:HA3	54:s:401:PEE:H37	1.87	0.56
33:j:68:GLU:HG3	36:m:161:LEU:HD13	1.87	0.56
12:M:419:ARG:NH1	12:M:439:THR:O	2.38	0.56
27:d:43:ARG:HH21	27:d:47:LEU:HD21	1.70	0.56
40:r:14:MET:SD	40:r:30:HIS:ND1	2.76	0.56
1:A:113:LEU:HD13	1:A:149:MET:HE1	1.88	0.56
20:V:73:THR:HB	20:V:93:GLY:HA2	1.88	0.56
16:Q:140:ASP:OD2	16:Q:143:SER:OG	2.23	0.56
1:A:89:GLY:O	47:A:503:NAI:H2N	2.06	0.56
40:r:191:SER:HB3	54:r:501:PEE:H3	1.87	0.56
1:A:222:LYS:HB2	11:L:175:LYS:HZ3	1.70	0.55
9:J:238:GLN:HG2	9:J:266:VAL:HB	1.87	0.55
20:V:96:ALA:O	20:V:100:THR:HG23	2.07	0.55
33:j:5:LEU:HD23	41:s:2:PHE:HD2	1.71	0.55
40:r:61:LEU:HB2	40:r:457:PRO:HD3	1.88	0.55
16:Q:302:LEU:HD11	16:Q:406:GLU:HG3	1.87	0.55
15:P:44:ARG:HB3	15:P:45:PRO:CD	2.36	0.55
32:i:106:LEU:HD22	32:i:187:MET:HE2	1.89	0.55
40:r:433:GLU:O	40:r:437:MET:HG2	2.06	0.55
1:A:41:ILE:O	1:A:137:LYS:NZ	2.38	0.55
12:M:382:ARG:HG2	12:M:386:LEU:HD11	1.88	0.55
12:M:690:THR:HG22	12:M:691:ILE:H	1.71	0.55
1:A:169:LEU:O	1:A:173:ILE:HG13	2.06	0.55
2:B:63:TRP:HB3	2:B:66:LEU:HD12	1.89	0.55
2:B:171:PRO:HB3	13:N:93:MET:HE1	1.88	0.55
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.88	0.55
42:u:59:GLU:O	42:u:63:VAL:HG13	2.07	0.55
44:w:214:ILE:HG22	44:w:217:ARG:HD3	1.88	0.55
1:A:372:GLU:OE1	14:O:33:GLY:N	2.40	0.55
40:r:122:PHE:CE1	40:r:238:LEU:HB3	2.41	0.55
41:s:170:GLU:OE1	42:u:98:ARG:NH1	2.40	0.55
1:A:282:VAL:HG13	1:A:356:VAL:HG21	1.88	0.55
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.89	0.55
21:W:73:PRO:HA	42:u:44:MET:HE2	1.89	0.55
30:g:4:MET:O	30:g:10:ARG:NH1	2.40	0.55
43:v:45:GLU:N	43:v:45:GLU:OE1	2.34	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:27:ARG:NH1	16:Q:212:GLU:OE1	2.36	0.55
54:Q:501:PEE:H38	19:U:25:ILE:HG12	1.89	0.55
22:Y:65:MET:HE1	35:l:378:LEU:HD12	1.87	0.55
24:a:139:ILE:HG23	40:r:54:LEU:HD23	1.89	0.55
1:A:319:PRO:HG2	1:A:347:THR:HG21	1.88	0.55
53:a:201:CDL:H191	53:a:201:CDL:H732	1.89	0.55
27:d:71:VAL:HG11	27:d:87:GLU:HB3	1.88	0.54
43:v:51:LEU:HD21	43:v:64:ILE:HD13	1.88	0.54
4:E:89:GLU:OE1	4:E:98:LYS:NZ	2.33	0.54
40:r:101:LEU:HD13	53:r:504:CDL:H441	1.90	0.54
35:l:465:GLY:O	35:l:469:SER:OG	2.22	0.54
40:r:226:ALA:HA	40:r:229:MET:HE3	1.89	0.54
5:F:48:ASN:HB3	5:F:51:LEU:HB3	1.90	0.54
36:m:168:ILE:O	36:m:172:THR:OG1	2.25	0.54
16:Q:149:GLN:NE2	16:Q:309:ASP:OD2	2.34	0.54
41:s:62:ARG:HD3	41:s:64:ALA:H	1.73	0.54
40:r:201:MET:HE2	54:r:501:PEE:H42	1.89	0.54
40:r:269:MET:HE1	40:r:396:MET:SD	2.48	0.54
21:W:62:ILE:O	21:W:66:GLU:HG2	2.07	0.54
12:M:388:ASN:HB3	12:M:511:LYS:HE2	1.90	0.53
23:Z:24:ILE:HD11	23:Z:46:GLY:HA3	1.90	0.53
1:A:48:ARG:O	10:K:74:ARG:NH1	2.36	0.53
24:a:141:GLN:O	24:a:145:GLU:HG3	2.08	0.53
38:o:59:VAL:HG22	40:r:423:ILE:HG23	1.90	0.53
35:l:396:ILE:HG21	35:l:490:ALA:HB2	1.90	0.53
1:A:125:CYS:SG	14:O:180:CYS:N	2.82	0.53
37:n:43:LEU:HA	37:n:46:LYS:HZ2	1.73	0.53
44:w:146:ALA:HB1	44:w:157:VAL:HG21	1.91	0.53
9:J:236:VAL:HG12	9:J:272:LEU:HD22	1.89	0.53
44:w:165:SER:HB3	44:w:245:PHE:CE1	2.43	0.53
54:i:402:PEE:H34	40:r:155:ALA:HB2	1.90	0.53
35:l:83:ASP:CG	35:l:262:ARG:HH12	2.17	0.53
35:l:298:ILE:O	35:l:302:VAL:HG23	2.09	0.53
41:s:221:ALA:O	41:s:225:MET:HG3	2.09	0.53
12:M:299:ARG:HH11	12:M:705:GLN:HG3	1.72	0.53
24:a:152:LYS:HD3	30:g:96:VAL:HG21	1.91	0.53
32:i:42:PRO:HG2	36:m:167:VAL:HG22	1.90	0.53
2:B:77:LEU:HD13	41:s:31:MET:HE3	1.90	0.53
12:M:136:GLU:HG2	12:M:242:PRO:HG3	1.90	0.53
12:M:217:GLU:HG3	12:M:412:PRO:HB3	1.90	0.53
6:X:138:LEU:HD13	6:X:144:ILE:HG12	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:412:VAL:HB	16:Q:421:ARG:HB3	1.91	0.53
34:k:25:HIS:O	34:k:28:SER:N	2.34	0.53
12:M:34:VAL:HG23	12:M:41:VAL:HG13	1.91	0.52
12:M:210:ILE:HD11	12:M:212:LYS:HE2	1.91	0.52
44:w:215:GLN:O	44:w:219:GLN:HG2	2.09	0.52
4:E:71:ALA:HA	49:G:201:8Q1:O40	2.09	0.52
9:J:135:GLU:OE2	9:J:179:ARG:NH1	2.42	0.52
14:O:146:ASP:OD1	14:O:146:ASP:N	2.36	0.52
35:l:97:THR:O	35:l:101:MET:HG3	2.08	0.52
35:l:414:ILE:HG12	53:l:701:CDL:H631	1.91	0.52
42:u:83:THR:HA	42:u:86:TRP:CD1	2.44	0.52
44:w:180:ARG:NH1	44:w:316:GLU:OE2	2.41	0.52
26:c:153:TYR:HB3	35:l:403:TYR:HD1	1.74	0.52
27:d:33:LEU:HD12	27:d:36:ILE:HD11	1.91	0.52
41:s:10:ILE:HD11	41:s:83:LEU:HD13	1.91	0.52
3:C:66:THR:HG21	3:C:76:MET:HE2	1.90	0.52
6:G:94:ASP:OD1	6:G:94:ASP:N	2.40	0.52
31:h:89:GLU:OE1	31:h:91:LYS:NZ	2.43	0.52
2:B:78:PHE:O	8:I:12:ARG:NH2	2.42	0.52
8:I:95:VAL:O	15:P:105:ASN:ND2	2.42	0.52
12:M:390:THR:HA	12:M:600:GLU:HG2	1.91	0.52
54:i:402:PEE:H27	35:l:563:PRO:HA	1.91	0.52
40:r:237:LYS:HD2	40:r:316:MET:HB3	1.90	0.52
24:a:144:ALA:O	24:a:148:GLU:HG2	2.10	0.52
9:J:172:ALA:HA	9:J:181:LEU:HB3	1.91	0.52
15:P:45:PRO:O	16:Q:162:GLN:NE2	2.41	0.52
23:Z:57:PHE:O	35:l:434:LYS:NZ	2.33	0.52
31:h:7:GLN:NE2	31:h:15:ASP:OD1	2.40	0.52
33:j:15:SER:HA	41:s:76:ILE:HD12	1.91	0.52
35:l:511:LEU:HD12	39:p:39:TYR:HD2	1.74	0.51
36:m:31:LEU:HA	36:m:34:ILE:HD12	1.92	0.51
53:r:503:CDL:H572	53:r:503:CDL:H871	1.93	0.51
7:H:37:GLN:HB2	7:H:95:LEU:HD11	1.91	0.51
9:J:315:THR:O	9:J:319:VAL:HG13	2.10	0.51
16:Q:259:GLU:OE1	16:Q:338:ARG:NH2	2.35	0.51
1:A:290:GLU:HG3	1:A:291:GLU:N	2.24	0.51
12:M:275:PRO:HB3	12:M:286:ILE:HG23	1.91	0.51
13:N:2:GLU:HG3	13:N:4:VAL:HG22	1.90	0.51
22:Y:72:ARG:NH2	22:Y:76:ASP:OD2	2.37	0.51
53:a:201:CDL:H432	27:d:44:PRO:HB3	1.93	0.51
26:c:78:LEU:HD23	26:c:106:HIS:HA	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:265:MET:HE2	32:i:343:LEU:HD21	1.92	0.51
32:i:334:THR:HG21	53:r:504:CDL:H391	1.92	0.51
48:g:201:PLX:H1C2	31:h:2:PRO:HD2	1.92	0.51
35:l:393:ASP:O	35:l:397:GLU:HG3	2.10	0.51
53:r:503:CDL:H511	53:r:503:CDL:HA62	1.92	0.51
53:r:503:CDL:H652	53:r:503:CDL:H862	1.93	0.51
8:I:46:SER:O	8:I:52:ASN:ND2	2.44	0.51
22:Y:97:LEU:HG	43:v:104:ARG:HB2	1.90	0.51
24:a:96:ALA:HB2	27:d:61:TYR:CE2	2.45	0.51
16:Q:274:ASP:OD1	16:Q:323:ARG:NH1	2.40	0.51
44:w:86:PHE:HB2	44:w:159:LEU:HD23	1.93	0.51
16:Q:184:ILE:HD11	16:Q:251:PHE:CZ	2.45	0.51
21:W:34:SER:O	21:W:38:VAL:HG23	2.11	0.51
35:l:10:THR:O	35:l:14:ILE:HG23	2.11	0.51
54:r:501:PEE:H69	48:r:502:PLX:H381	1.93	0.51
9:J:38:HIS:NE2	13:N:132:LYS:HD2	2.26	0.51
24:a:140:LEU:HD21	40:r:177:LEU:HB3	1.92	0.51
32:i:280:THR:O	32:i:284:MET:HG2	2.10	0.51
40:r:216:LEU:HD23	40:r:287:ALA:HB1	1.93	0.51
1:A:33:GLY:O	1:A:302:LYS:NZ	2.40	0.51
28:e:125:LEU:HD21	28:e:129:ARG:CZ	2.41	0.51
29:f:47:THR:HG23	30:g:65:LEU:HD22	1.93	0.51
54:r:501:PEE:H36	54:r:501:PEE:H79	1.93	0.51
25:b:7:ASP:OD1	25:b:7:ASP:N	2.42	0.50
4:E:123:TYR:CZ	12:M:320:GLU:HG3	2.46	0.50
13:N:73:THR:HG22	13:N:77:VAL:HG12	1.93	0.50
25:b:32:GLU:HG3	39:p:115:TYR:HA	1.93	0.50
43:v:60:ALA:O	43:v:64:ILE:HG12	2.11	0.50
49:G:201:8Q1:O40	49:G:201:8Q1:N36	2.45	0.50
9:J:57:THR:HG21	9:J:120:VAL:HG12	1.93	0.50
22:Y:51:THR:HG22	22:Y:53:SER:H	1.76	0.50
27:d:29:PRO:O	27:d:33:LEU:HB2	2.11	0.50
35:l:220:ALA:HB1	35:l:314:MET:HE1	1.93	0.50
35:l:536:LEU:HB3	35:l:537:PRO:HD3	1.93	0.50
1:A:296:LEU:HD13	1:A:332:CYS:HB2	1.94	0.50
30:g:19:GLU:O	30:g:22:SER:OG	2.28	0.50
5:F:37:ILE:HA	5:F:41:TYR:HB2	1.93	0.50
6:G:148:ILE:HD12	6:G:148:ILE:H	1.77	0.50
12:M:36:VAL:HG22	12:M:102:ILE:HD12	1.94	0.50
27:d:144:SER:OG	27:d:158:LYS:NZ	2.38	0.50
32:i:57:THR:HA	34:k:77:LEU:HD13	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:26:HIS:CD2	39:p:79:PRO:HB3	2.46	0.50
41:s:62:ARG:NH2	41:s:66:SER:O	2.45	0.50
3:C:125:PRO:HB2	41:s:58:LYS:HE3	1.94	0.50
7:H:38:ILE:CG2	7:H:45:ARG:HB2	2.41	0.50
7:H:69:GLU:HG3	7:H:77:ILE:HG12	1.94	0.50
15:P:87:PHE:CE2	15:P:144:LYS:HD2	2.47	0.50
22:Y:45:ARG:HG2	35:l:439:PRO:HB3	1.92	0.50
24:a:136:THR:HG21	40:r:48:ASN:HD22	1.75	0.50
48:e:201:PLX:H382	40:r:67:VAL:HG12	1.94	0.50
1:A:159:ARG:NH2	14:O:176:CYS:O	2.34	0.50
1:A:214:GLU:HG2	11:L:175:LYS:HZ2	1.77	0.50
2:B:86:TYR:CD1	2:B:87:PRO:HA	2.47	0.50
12:M:266:ARG:HG2	12:M:267:THR:HG23	1.94	0.50
22:Y:43:ARG:HG3	22:Y:48:PRO:HA	1.93	0.50
32:i:95:MET:HE2	32:i:149:ILE:HA	1.94	0.50
7:H:44:TYR:HB2	15:P:68:ILE:HG23	1.94	0.50
7:H:76:GLN:O	7:H:79:GLU:HG2	2.12	0.50
41:s:46:LEU:HD23	41:s:49:ILE:HD12	1.94	0.50
25:b:14:GLN:HE22	39:p:157:ALA:HB3	1.77	0.49
32:i:276:ILE:HG21	54:r:501:PEE:H7	1.94	0.49
34:k:45:THR:HG23	36:m:52:LEU:HD13	1.94	0.49
35:l:293:ILE:HD13	35:l:418:LEU:HD22	1.94	0.49
5:F:57:GLU:O	12:M:655:ARG:NH2	2.45	0.49
18:T:39:THR:HG22	18:T:62:VAL:HG22	1.93	0.49
25:b:87:LYS:HE3	25:b:88:TYR:CZ	2.47	0.49
35:l:360:GLY:HA3	35:l:435:PRO:HA	1.94	0.49
44:w:343:TYR:HA	44:w:352:ILE:HD12	1.93	0.49
4:E:34:GLU:CD	4:E:37:ARG:HH21	2.20	0.49
10:K:89:LEU:O	10:K:93:LEU:HG	2.12	0.49
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.94	0.49
15:P:213:ASP:HB3	15:P:216:VAL:HG22	1.94	0.49
18:T:122:HIS:O	18:T:122:HIS:ND1	2.39	0.49
26:c:185:GLU:HG2	43:v:37:ARG:HG2	1.94	0.49
15:P:113:ASP:HB2	16:Q:425:LYS:HG3	1.94	0.49
26:c:140:MET:HE1	35:l:411:MET:SD	2.52	0.49
35:l:473:PRO:HG2	35:l:475:MET:HE2	1.95	0.49
42:u:137:LEU:HD12	42:u:138:PRO:HD2	1.94	0.49
44:w:110:GLY:HA2	44:w:134:TRP:CD2	2.47	0.49
1:A:263:ALA:HA	1:A:271:SER:HB2	1.94	0.49
5:F:68:ARG:NH2	12:M:364:ASP:OD1	2.46	0.49
36:m:57:PHE:HD1	41:s:107:ALA:HB1	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:53:TYR:CE2	42:u:44:MET:HG3	2.47	0.49
24:a:120:TRP:O	24:a:124:THR:HG22	2.13	0.49
4:E:116:THR:O	4:E:121:LYS:NZ	2.45	0.49
16:Q:446:ASP:OD1	16:Q:446:ASP:N	2.45	0.49
26:c:81:ARG:NH2	38:o:14:LEU:O	2.43	0.49
40:r:373:ILE:HD11	40:r:444:LEU:HD23	1.93	0.49
40:r:392:THR:O	40:r:396:MET:HG2	2.12	0.49
7:H:66:LYS:HB3	7:H:66:LYS:HE3	1.53	0.49
21:W:120:MET:HE1	31:h:73:MET:SD	2.53	0.49
24:a:136:THR:HG21	40:r:48:ASN:ND2	2.28	0.49
28:e:143:ASP:OD1	28:e:146:LYS:NZ	2.41	0.49
35:l:233:LEU:HB3	35:l:234:PRO:HD3	1.94	0.49
36:m:25:SER:O	36:m:27:ILE:N	2.45	0.49
6:G:141:PRO:O	6:G:145:VAL:HG13	2.12	0.49
16:Q:461:VAL:O	16:Q:463:ARG:NH1	2.46	0.49
3:C:193:TRP:HA	3:C:196:ARG:HG2	1.94	0.48
11:L:86:ASN:ND2	12:M:275:PRO:HG2	2.29	0.48
13:N:120:THR:HG22	13:N:122:GLN:H	1.77	0.48
44:w:95:ASP:OD1	44:w:95:ASP:N	2.45	0.48
6:X:113:LEU:O	6:X:116:VAL:HG12	2.13	0.48
53:a:201:CDL:H541	54:l:703:PEE:H16	1.95	0.48
35:l:172:ILE:HG21	40:r:408:LEU:HD12	1.94	0.48
33:j:73:LEU:O	41:s:160:TYR:OH	2.31	0.48
53:l:701:CDL:H622	53:l:701:CDL:H591	1.53	0.48
1:A:116:ASN:ND2	1:A:207:GLY:O	2.40	0.48
9:J:279:TYR:O	9:J:283:VAL:HG22	2.14	0.48
16:Q:424:ILE:HB	16:Q:463:ARG:HD2	1.95	0.48
32:i:298:TYR:O	32:i:303:THR:OG1	2.31	0.48
35:l:331:MET:HE1	35:l:468:ILE:HD12	1.94	0.48
1:A:185:ASN:O	1:A:187:CYS:N	2.47	0.48
48:m:201:PLX:H351	48:m:201:PLX:H322	1.61	0.48
26:c:156:VAL:HG12	43:v:99:MET:HG3	1.95	0.48
27:d:43:ARG:O	27:d:47:LEU:HG	2.14	0.48
40:r:337:VAL:HG21	40:r:345:ALA:HB2	1.95	0.48
41:s:72:ILE:O	41:s:76:ILE:HG12	2.14	0.48
44:w:258:TYR:OH	44:w:272:ASP:OD2	2.30	0.48
12:M:194:ASP:OD2	12:M:212:LYS:HD3	2.14	0.48
22:Y:105:ASP:N	22:Y:105:ASP:OD1	2.46	0.48
26:c:153:TYR:OH	43:v:8:ARG:NH1	2.33	0.48
35:l:264:TYR:CD2	35:l:265:PRO:HD3	2.47	0.48
44:w:208:ASP:N	44:w:258:TYR:O	2.36	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:GLU:HB2	2:B:144:ARG:HB3	1.96	0.48
6:G:99:SER:O	6:G:102:SER:OG	2.29	0.48
7:H:38:ILE:O	7:H:45:ARG:NH1	2.44	0.48
17:S:69:ILE:HD13	42:u:20:VAL:HG13	1.95	0.48
32:i:265:MET:HE1	42:u:167:LEU:HD11	1.95	0.48
36:m:152:TRP:HZ3	48:m:201:PLX:H132	1.78	0.48
39:p:100:PRO:HG3	40:r:419:TYR:CE1	2.47	0.48
40:r:282:LEU:HG	40:r:342:MET:HG3	1.95	0.48
1:A:119:GLU:CG	1:A:127:ASP:HB2	2.44	0.48
7:H:99:PRO:HD2	7:H:100:TRP:CZ3	2.49	0.48
12:M:638:THR:O	12:M:642:VAL:HG23	2.14	0.48
17:S:50:ARG:O	17:S:54:ILE:HG23	2.13	0.48
26:c:87:ASP:OD2	26:c:90:TYR:N	2.47	0.48
40:r:196:TRP:CD1	40:r:250:LEU:HB3	2.48	0.48
16:Q:274:ASP:CG	16:Q:323:ARG:HH12	2.22	0.47
32:i:128:LEU:O	32:i:132:THR:OG1	2.23	0.47
5:F:23:LEU:HD12	5:F:34:ARG:HG2	1.96	0.47
35:l:452:ASN:HA	35:l:455:LYS:HG2	1.94	0.47
39:p:57:MET:HE2	39:p:57:MET:HA	1.95	0.47
43:v:28:ASP:N	43:v:28:ASP:OD1	2.47	0.47
1:A:456:GLN:OE1	1:A:457:HIS:ND1	2.47	0.47
15:P:69:LEU:HD22	15:P:96:VAL:HG22	1.97	0.47
19:U:38:TYR:HB2	41:s:310:MET:O	2.14	0.47
22:Y:68:TRP:CZ2	22:Y:72:ARG:HD2	2.49	0.47
26:c:58:ARG:HD2	38:o:35:GLU:HG3	1.95	0.47
35:l:327:LEU:O	35:l:331:MET:HG2	2.14	0.47
40:r:12:LEU:HB2	40:r:13:PRO:HD3	1.97	0.47
41:s:66:SER:HB2	41:s:122:ALA:O	2.13	0.47
9:J:174:ILE:HG23	9:J:175:LYS:HG2	1.96	0.47
13:N:10:GLY:O	13:N:14:VAL:HG23	2.15	0.47
22:Y:81:LEU:HD23	35:l:488:MET:HE1	1.96	0.47
31:h:97:HIS:HA	31:h:102:GLU:HB3	1.96	0.47
32:i:20:VAL:HG11	32:i:137:ALA:HB1	1.97	0.47
35:l:292:ALA:HB2	35:l:304:PHE:HB3	1.96	0.47
41:s:24:GLU:HA	41:s:271:LEU:HD13	1.96	0.47
1:A:48:ARG:HD3	10:K:70:ASN:O	2.13	0.47
2:B:122:VAL:HG21	16:Q:385:TYR:HD1	1.78	0.47
2:B:151:LYS:HA	3:C:141:GLY:HA2	1.96	0.47
6:G:105:MET:HG2	6:G:139:MET:HE1	1.94	0.47
6:G:116:VAL:O	6:G:120:MET:HG2	2.15	0.47
26:c:168:LEU:HA	26:c:168:LEU:HD12	1.80	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:81:ILE:O	7:H:85:GLU:HG3	2.14	0.47
12:M:29:SER:OG	12:M:30:ASN:OD1	2.30	0.47
12:M:250:SER:OG	12:M:251:ILE:N	2.48	0.47
12:M:636:TYR:CD1	12:M:642:VAL:HG22	2.50	0.47
14:O:164:THR:CG2	14:O:169:PHE:H	2.28	0.47
35:l:62:ILE:HD13	35:l:81:LYS:HA	1.95	0.47
53:l:701:CDL:H711	53:l:701:CDL:H742	1.67	0.47
42:u:83:THR:HA	42:u:86:TRP:NE1	2.30	0.47
1:A:248:VAL:O	1:A:251:SER:OG	2.29	0.47
2:B:76:TYR:HE2	41:s:33:LEU:HB2	1.77	0.47
3:C:71:CYS:HB3	16:Q:141:TYR:HB2	1.97	0.47
4:E:15:THR:OG1	11:L:55:VAL:O	2.29	0.47
8:I:12:ARG:HD3	8:I:20:LEU:HD22	1.97	0.47
9:J:168:SER:O	9:J:202:LYS:HA	2.15	0.47
18:T:29:VAL:HG22	18:T:66:PHE:CE1	2.50	0.47
21:W:129:THR:HG22	21:W:132:GLU:HG2	1.96	0.47
53:a:201:CDL:H212	53:a:201:CDL:H761	1.97	0.47
9:J:319:VAL:HA	9:J:322:VAL:HG12	1.97	0.47
16:Q:127:LYS:HB3	16:Q:131:GLN:HB3	1.96	0.47
2:B:188:GLU:HG2	18:T:62:VAL:HA	1.97	0.47
13:N:60:ARG:HH22	13:N:95:ASP:HA	1.80	0.47
24:a:78:THR:HG21	28:e:96:SER:O	2.15	0.47
32:i:311:MET:HE2	32:i:311:MET:HB2	1.77	0.47
40:r:306:PRO:HA	40:r:458:LEU:HD22	1.97	0.47
42:u:9:THR:OG1	42:u:12:ASP:OD2	2.32	0.47
1:A:70:LEU:HD21	1:A:189:SER:HA	1.97	0.46
48:C:302:PLX:H31	13:N:75:TRP:CD2	2.50	0.46
9:J:328:THR:HG22	9:J:330:PRO:HD3	1.97	0.46
11:L:89:SER:O	12:M:59:GLN:NE2	2.46	0.46
16:Q:196:ALA:C	16:Q:197:MET:HG3	2.40	0.46
20:V:88:LEU:HD22	20:V:92:ILE:HD11	1.97	0.46
20:V:140:LYS:HE3	20:V:140:LYS:HB3	1.56	0.46
35:l:488:MET:O	35:l:492:ILE:HG23	2.14	0.46
41:s:14:LEU:HD22	41:s:225:MET:HE3	1.96	0.46
1:A:109:ARG:NH1	1:A:237:GLY:O	2.48	0.46
2:B:77:LEU:HB2	41:s:31:MET:HG3	1.97	0.46
7:H:98:LYS:HA	7:H:100:TRP:CH2	2.50	0.46
19:U:51:TYR:HB3	36:m:136:PHE:HE2	1.80	0.46
21:W:68:ARG:NH2	36:m:134:GLY:HA2	2.29	0.46
12:M:373:PRO:HB3	12:M:487:THR:HG22	1.97	0.46
28:e:70:ASN:O	28:e:73:SER:HB2	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:f:72:ARG:HH12	30:g:19:GLU:HA	1.79	0.46
35:l:481:THR:HB	43:v:92:HIS:ND1	2.30	0.46
38:o:59:VAL:HG22	40:r:423:ILE:HG12	1.97	0.46
1:A:445:GLU:OE2	1:A:449:ARG:NH2	2.46	0.46
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.98	0.46
22:Y:87:PRO:HG3	43:v:96:VAL:HG22	1.96	0.46
28:e:113:ARG:NH1	40:r:452:LYS:HD2	2.30	0.46
41:s:267:THR:O	41:s:271:LEU:HG	2.15	0.46
3:C:121:TYR:CE1	3:C:128:ARG:HD2	2.51	0.46
7:H:30:LYS:O	7:H:34:VAL:HG23	2.15	0.46
15:P:125:ARG:HH22	15:P:201:ASP:CG	2.23	0.46
35:l:420:ALA:O	35:l:424:THR:HG22	2.15	0.46
40:r:48:ASN:N	40:r:48:ASN:OD1	2.48	0.46
3:C:79:MET:HE3	3:C:86:MET:HE2	1.97	0.46
7:H:35:LEU:HD13	7:H:49:GLU:HG3	1.98	0.46
12:M:347:ASP:CB	12:M:594:ALA:HB1	2.46	0.46
12:M:387:LEU:HD12	12:M:514:ASN:HB3	1.96	0.46
14:O:151:ALA:HB1	14:O:202:GLU:OE1	2.16	0.46
19:U:47:ARG:HH11	19:U:47:ARG:HG2	1.81	0.46
2:B:140:ARG:HG3	12:M:238:PHE:CG	2.51	0.46
3:C:88:ARG:HA	41:s:37:PRO:HA	1.97	0.46
35:l:173:LEU:HD12	40:r:405:LEU:HD21	1.98	0.46
1:A:126:LYS:O	1:A:130:ILE:HG12	2.15	0.46
12:M:222:ILE:HA	12:M:225:ILE:HG12	1.98	0.46
24:a:169:TYR:OH	30:g:2:THR:N	2.42	0.46
40:r:398:MET:O	40:r:402:ILE:HG13	2.15	0.46
43:v:17:PRO:HB3	43:v:105:GLU:OE1	2.15	0.46
7:H:27:LEU:HD13	7:H:84:ALA:HB3	1.98	0.46
6:X:129:GLU:HB2	39:p:82:PHE:CD2	2.50	0.46
26:c:131:LYS:HB2	26:c:131:LYS:HE2	1.77	0.46
35:l:49:VAL:HB	35:l:50:PRO:HD3	1.97	0.46
35:l:410:LEU:O	35:l:414:ILE:HG13	2.15	0.46
37:n:50:ARG:HB2	37:n:53:GLU:HB2	1.98	0.46
43:v:69:CYS:HB3	43:v:80:CYS:HB2	1.86	0.46
44:w:166:ASP:OD1	44:w:187:TYR:OH	2.34	0.46
1:A:455:LEU:O	1:A:458:GLN:NE2	2.49	0.46
12:M:254:MET:HE1	12:M:700:ILE:HB	1.98	0.46
21:W:43:LEU:HG	41:s:179:TRP:HE1	1.81	0.46
6:X:82:ARG:O	6:X:86:VAL:HG23	2.16	0.46
27:d:99:ASP:OD2	27:d:142:ARG:NH1	2.49	0.46
34:k:57:ASN:HB3	36:m:143:ILE:HG13	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:s:179:TRP:O	41:s:183:MET:HG3	2.15	0.46
12:M:89:VAL:HB	12:M:94:MET:HE3	1.97	0.45
22:Y:43:ARG:NH1	22:Y:47:PHE:O	2.47	0.45
35:l:505:ASN:O	35:l:508:THR:OG1	2.32	0.45
40:r:87:GLU:O	40:r:92:LYS:NZ	2.49	0.45
54:s:401:PEE:H64	54:s:401:PEE:H59	1.60	0.45
1:A:256:ARG:HG2	14:O:245:VAL:HG22	1.98	0.45
8:I:74:LYS:HD2	8:I:74:LYS:HA	1.78	0.45
32:i:68:MET:HE2	32:i:68:MET:HA	1.96	0.45
54:r:501:PEE:H24	54:r:501:PEE:H30	1.81	0.45
6:G:104:PHE:HB2	6:G:139:MET:HE3	1.99	0.45
16:Q:181:LEU:HD21	16:Q:210:MET:HB2	1.97	0.45
31:h:86:LEU:HD22	31:h:91:LYS:HD2	1.99	0.45
1:A:185:ASN:C	1:A:187:CYS:H	2.23	0.45
9:J:132:ARG:HA	9:J:132:ARG:HD3	1.69	0.45
14:O:137:THR:HG22	14:O:138:THR:H	1.81	0.45
16:Q:414:ASP:OD1	16:Q:416:SER:OG	2.30	0.45
32:i:12:THR:HG21	36:m:163:ILE:HG21	1.98	0.45
34:k:33:LEU:HD23	34:k:36:MET:HE2	1.98	0.45
48:m:201:PLX:H312	48:m:201:PLX:H282	1.85	0.45
1:A:62:TRP:CD2	1:A:181:LEU:HD13	2.51	0.45
12:M:624:ARG:NH2	12:M:637:ASP:OD1	2.45	0.45
36:m:55:MET:HA	36:m:55:MET:HE2	1.98	0.45
40:r:204:MET:HE3	40:r:261:PHE:CD1	2.52	0.45
40:r:260:PRO:HG3	48:r:502:PLX:H132	1.98	0.45
42:u:47:ARG:NH2	42:u:53:PRO:HG3	2.32	0.45
1:A:290:GLU:HG3	1:A:291:GLU:H	1.82	0.45
12:M:405:THR:OG1	12:M:410:GLU:OE1	2.34	0.45
12:M:457:SER:OG	12:M:459:ASN:OD1	2.22	0.45
14:O:110:MET:O	14:O:114:GLU:HG3	2.15	0.45
15:P:125:ARG:NH2	15:P:201:ASP:OD1	2.49	0.45
6:X:80:LYS:HE3	6:X:80:LYS:HB3	1.58	0.45
6:X:126:PHE:CD2	6:X:148:ILE:HD13	2.52	0.45
25:b:81:ILE:HG23	54:l:703:PEE:H58	1.99	0.45
30:g:73:PHE:HE2	48:g:201:PLX:H392	1.81	0.45
36:m:45:LEU:HD23	36:m:50:SER:HA	1.98	0.45
48:m:201:PLX:H342	48:m:201:PLX:H372	1.65	0.45
6:G:105:MET:HE2	6:G:105:MET:HA	1.98	0.45
7:H:99:PRO:HD2	7:H:100:TRP:CE3	2.51	0.45
16:Q:259:GLU:O	16:Q:263:THR:HG22	2.17	0.45
25:b:109:THR:HG22	25:b:116:VAL:HG12	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:320:THR:OG1	44:w:300:ASN:HB2	2.16	0.45
36:m:17:PHE:HA	36:m:20:PHE:CE1	2.51	0.45
2:B:135:ARG:HD3	2:B:141:ARG:HG3	1.98	0.45
13:N:4:VAL:O	13:N:8:ARG:HG2	2.17	0.45
15:P:119:VAL:HG12	15:P:121:THR:HG22	1.98	0.45
23:Z:75:PHE:O	23:Z:79:VAL:HG13	2.16	0.45
27:d:89:GLU:O	27:d:93:ARG:HG3	2.17	0.45
35:l:503:GLU:OE1	35:l:503:GLU:HA	2.17	0.45
38:o:58:GLY:HA2	40:r:425:ASN:ND2	2.31	0.45
41:s:21:THR:HB	56:s:402:UQ:HM23	1.98	0.45
41:s:79:LEU:HD23	41:s:79:LEU:HA	1.85	0.45
2:B:74:LEU:HB2	41:s:272:TRP:CZ2	2.52	0.45
12:M:133:GLN:O	12:M:137:CYS:HB2	2.17	0.45
25:b:110:ILE:HG22	25:b:113:THR:H	1.82	0.45
26:c:148:GLU:OE2	35:l:405:ASN:ND2	2.35	0.45
27:d:37:PHE:CE2	35:l:3:PRO:HB3	2.52	0.45
27:d:102:ILE:HD11	28:e:125:LEU:HD22	1.98	0.45
35:l:53:MET:HE2	35:l:53:MET:HB3	1.83	0.45
40:r:340:ARG:O	40:r:340:ARG:HG3	2.17	0.45
40:r:371:PRO:O	40:r:448:THR:OG1	2.34	0.45
6:G:128:PHE:CZ	6:G:148:ILE:HG23	2.52	0.45
12:M:395:GLU:OE2	12:M:417:ARG:NH1	2.46	0.45
12:M:467:LYS:HB2	12:M:467:LYS:HE3	1.66	0.45
5:F:45:LYS:HB3	12:M:671:LEU:HD21	1.99	0.44
6:G:119:ILE:O	6:G:123:GLU:HG3	2.17	0.44
7:H:56:LEU:HA	7:H:59:VAL:HG12	1.98	0.44
12:M:198:THR:HG21	12:M:209:TYR:HB2	1.99	0.44
14:O:182:ASN:HB3	14:O:194:GLU:HB3	2.00	0.44
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.53	0.44
21:W:128:ARG:NH1	31:h:102:GLU:OE2	2.40	0.44
25:b:108:ASP:OD1	43:v:68:LYS:NZ	2.43	0.44
26:c:117:VAL:HG21	35:l:539:TYR:HB2	2.00	0.44
35:l:356:ILE:HA	35:l:359:MET:HG2	1.99	0.44
40:r:105:PHE:O	40:r:109:THR:OG1	2.26	0.44
41:s:173:TRP:HB3	41:s:175:ILE:HG22	2.00	0.44
2:B:192:ASN:ND2	18:T:61:GLU:OE2	2.34	0.44
12:M:399:VAL:HG22	12:M:428:LYS:HB3	1.99	0.44
13:N:53:LYS:HD2	13:N:53:LYS:HA	1.81	0.44
21:W:100:ASP:OD1	31:h:82:GLN:NE2	2.50	0.44
24:a:147:ALA:HB2	40:r:173:SER:HB2	1.98	0.44
34:k:32:CYS:O	34:k:36:MET:HG3	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:357:THR:O	40:r:361:VAL:HG23	2.18	0.44
44:w:295:ARG:HA	44:w:298:VAL:HG22	1.98	0.44
1:A:288:VAL:HG21	1:A:303:HIS:CD2	2.52	0.44
5:F:68:ARG:HG3	5:F:74:GLU:HG2	2.00	0.44
11:L:139:GLU:HG3	11:L:145:PHE:HE2	1.83	0.44
12:M:389:THR:OG1	12:M:514:ASN:ND2	2.33	0.44
6:X:120:MET:HE1	39:p:21:LYS:HG3	1.98	0.44
22:Y:51:THR:O	22:Y:54:GLN:HG2	2.16	0.44
24:a:60:SER:HB3	39:p:107:TRP:HA	1.99	0.44
24:a:94:GLY:HA2	24:a:116:PRO:HG3	1.99	0.44
48:g:201:PLX:H72	48:g:201:PLX:H101	1.78	0.44
35:l:366:MET:HB2	35:l:445:GLU:OE2	2.18	0.44
44:w:351:TRP:O	44:w:355:LYS:HG3	2.17	0.44
2:B:177:THR:HG22	2:B:179:THR:H	1.82	0.44
17:S:12:MET:SD	41:s:20:LEU:HA	2.58	0.44
23:Z:13:LYS:HD2	23:Z:13:LYS:HA	1.78	0.44
41:s:1:MET:HE3	41:s:1:MET:HB3	1.82	0.44
1:A:392:MET:HE1	1:A:432:ALA:HA	1.99	0.44
46:A:502:FMN:H9	46:A:502:FMN:H1'1	1.78	0.44
6:G:114:ASP:N	6:G:114:ASP:OD1	2.51	0.44
26:c:81:ARG:NE	26:c:85:GLU:OE2	2.50	0.44
27:d:80:LYS:HA	27:d:80:LYS:HD3	1.73	0.44
31:h:7:GLN:O	31:h:11:GLY:N	2.49	0.44
32:i:213:LEU:HD13	53:i:401:CDL:H131	2.00	0.44
40:r:233:ALA:HA	40:r:320:GLY:HA2	1.99	0.44
41:s:141:SER:HB3	41:s:289:LEU:HD22	1.99	0.44
1:A:385:CYS:O	1:A:389:VAL:HB	2.18	0.44
48:C:302:PLX:H251	48:C:302:PLX:H52	1.80	0.44
8:I:97:PRO:HD3	15:P:61:PHE:CE1	2.51	0.44
27:d:42:ASP:O	27:d:46:THR:OG1	2.30	0.44
30:g:87:LEU:HD23	30:g:87:LEU:HA	1.88	0.44
36:m:57:PHE:CZ	41:s:111:LEU:HD11	2.52	0.44
53:r:503:CDL:H581	53:r:503:CDL:H851	2.00	0.44
43:v:103:GLU:OE2	43:v:103:GLU:HA	2.17	0.44
1:A:102:MET:O	1:A:102:MET:HG3	2.17	0.44
2:B:192:ASN:OD1	18:T:63:ASN:ND2	2.44	0.44
9:J:298:TYR:HA	9:J:301:VAL:HG12	1.99	0.44
21:W:128:ARG:HH12	31:h:102:GLU:CD	2.25	0.44
38:o:59:VAL:HG13	40:r:422:HIS:HE1	1.81	0.44
39:p:132:SER:OG	39:p:163:LEU:HB2	2.17	0.44
44:w:125:ASP:OD1	44:w:125:ASP:N	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:94:LEU:HD23	9:J:97:MET:HE3	2.00	0.44
10:K:78:HIS:CE1	10:K:79:HIS:CE1	3.05	0.44
12:M:153:PHE:CZ	12:M:155:GLU:HB2	2.53	0.44
12:M:456:ALA:O	12:M:499:ASN:ND2	2.51	0.44
32:i:236:LYS:HG2	32:i:237:MET:HG3	1.99	0.44
38:o:56:ARG:NH2	40:r:422:HIS:O	2.50	0.44
53:r:504:CDL:H662	53:r:504:CDL:H612	1.98	0.44
3:C:71:CYS:HB3	16:Q:141:TYR:CB	2.47	0.44
5:F:23:LEU:O	5:F:57:GLU:HA	2.17	0.44
7:H:94:MET:HE1	15:P:99:PHE:HD1	1.82	0.44
12:M:543:LYS:HB2	12:M:543:LYS:HE2	1.75	0.44
25:b:73:THR:HG23	25:b:74:HIS:ND1	2.33	0.44
12:M:454:ASP:OD1	12:M:454:ASP:N	2.51	0.43
6:X:111:ASP:OD1	6:X:112:SER:N	2.51	0.43
44:w:350:LYS:HE3	44:w:351:TRP:H	1.83	0.43
7:H:6:LYS:NZ	7:H:78:GLU:OE2	2.51	0.43
9:J:212:ARG:O	9:J:216:TYR:HB3	2.18	0.43
12:M:49:VAL:HG13	12:M:102:ILE:HD13	2.00	0.43
20:V:102:GLY:HA3	20:V:111:GLY:CA	2.48	0.43
27:d:81:ASP:O	27:d:85:MET:HG3	2.18	0.43
40:r:176:PHE:CE1	40:r:245:ARG:HB3	2.53	0.43
43:v:22:MET:HE1	43:v:102:PHE:CD2	2.53	0.43
1:A:367:ILE:O	1:A:371:ILE:HG12	2.19	0.43
2:B:211:TYR:CZ	8:I:39:PRO:HG3	2.52	0.43
16:Q:204:PHE:HA	16:Q:207:ARG:HB2	2.00	0.43
28:e:57:GLU:OE1	44:w:320:GLY:HA3	2.18	0.43
31:h:17:TRP:CD1	31:h:17:TRP:H	2.36	0.43
32:i:1:MET:HE2	32:i:1:MET:HB3	1.81	0.43
44:w:213:GLU:O	44:w:217:ARG:HG3	2.18	0.43
5:F:42:VAL:HG23	12:M:671:LEU:HG	2.00	0.43
41:s:11:ILE:HB	41:s:12:PRO:HD3	2.00	0.43
44:w:135:LEU:O	44:w:139:ARG:HG3	2.17	0.43
2:B:98:ARG:HB3	2:B:169:GLU:CD	2.43	0.43
4:E:101:THR:OG1	15:P:219:VAL:O	2.26	0.43
12:M:377:ALA:O	12:M:380:ASP:HB2	2.18	0.43
14:O:203:GLU:O	14:O:207:GLU:HG3	2.18	0.43
6:X:137:LYS:HB3	6:X:137:LYS:HE2	1.80	0.43
32:i:291:TYR:CE2	54:i:402:PEE:H49	2.54	0.43
35:l:529:TYR:HB3	35:l:530:PRO:HD3	2.00	0.43
44:w:129:TYR:CD1	44:w:183:CYS:HB3	2.54	0.43
8:I:27:ARG:HE	8:I:27:ARG:HB2	1.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O:75:LYS:HB2	14:O:75:LYS:HE3	1.80	0.43
23:Z:53:TYR:CE2	35:l:434:LYS:HG3	2.53	0.43
27:d:33:LEU:HD23	35:l:49:VAL:HG13	2.01	0.43
31:h:39:GLU:OE2	42:u:144:SER:OG	2.29	0.43
35:l:464:ALA:HA	35:l:467:ILE:HG22	2.01	0.43
40:r:127:VAL:HB	40:r:128:PRO:HD3	1.99	0.43
40:r:410:MET:HE2	40:r:410:MET:HB3	1.91	0.43
8:I:70:MET:HG3	15:P:66:ALA:HB1	2.00	0.43
18:T:60:LYS:HG2	18:T:62:VAL:HG23	2.01	0.43
6:X:85:TYR:O	6:X:89:LEU:HD12	2.19	0.43
26:c:84:GLN:O	26:c:98:ARG:NH1	2.52	0.43
28:e:87:MET:HE3	28:e:87:MET:HB3	1.96	0.43
33:j:73:LEU:HD13	36:m:55:MET:HE1	2.00	0.43
35:l:183:VAL:HG21	40:r:400:MET:HE1	2.00	0.43
35:l:557:TRP:O	35:l:561:ILE:HG12	2.18	0.43
40:r:371:PRO:HD2	53:r:503:CDL:H391	1.99	0.43
48:r:502:PLX:H92	48:r:502:PLX:H121	1.82	0.43
41:s:184:MET:HE1	41:s:296:LEU:HB3	1.99	0.43
42:u:158:LEU:HD23	42:u:158:LEU:HA	1.86	0.43
8:I:40:LYS:HB3	8:I:40:LYS:HE2	1.81	0.43
9:J:115:SER:HA	9:J:118:LYS:HG2	2.01	0.43
9:J:303:ARG:HB2	9:J:316:ARG:HD3	2.01	0.43
12:M:472:PRO:O	12:M:510:TRP:NE1	2.43	0.43
16:Q:65:PRO:HB2	16:Q:67:ASN:O	2.19	0.43
32:i:115:VAL:HG12	32:i:180:ALA:HB1	2.01	0.43
36:m:23:LYS:N	36:m:24:PRO:HD3	2.33	0.43
38:o:8:PRO:HG3	38:o:14:LEU:HD13	2.01	0.43
44:w:102:LYS:H	44:w:102:LYS:HG2	1.53	0.43
12:M:306:MET:HB2	12:M:583:ILE:HB	2.01	0.43
13:N:85:GLU:HG2	13:N:86:TRP:H	1.84	0.43
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.84	0.43
16:Q:251:PHE:HB3	16:Q:341:LEU:HD11	2.00	0.43
21:W:10:MET:SD	21:W:11:PRO:HD2	2.59	0.43
21:W:51:MET:HA	41:s:313:SER:HB2	2.01	0.43
6:X:77:GLU:OE2	6:X:80:LYS:NZ	2.52	0.43
25:b:82:ILE:HD11	35:l:13:THR:HG21	2.01	0.43
54:m:202:PEE:H27	54:m:202:PEE:H21	1.88	0.43
39:p:63:LEU:O	39:p:64:LEU:HB3	2.18	0.43
40:r:37:ILE:HD13	40:r:37:ILE:HA	1.89	0.43
44:w:72:ARG:CZ	44:w:72:ARG:HB3	2.48	0.43
44:w:235:GLN:NE2	44:w:239:ASN:OD1	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:64:PRO:HB3	3:C:102:VAL:HG13	2.00	0.43
8:I:27:ARG:HD3	16:Q:209:LYS:HD3	2.01	0.43
12:M:489:ILE:O	12:M:493:VAL:HG23	2.19	0.43
14:O:133:GLN:HG2	14:O:174:VAL:HG11	2.01	0.43
24:a:113:PHE:HB2	24:a:119:ARG:HG2	2.01	0.43
35:l:213:LEU:HB3	35:l:273:VAL:HG11	2.01	0.43
37:n:17:VAL:HG13	40:r:7:PRO:HB3	2.01	0.43
40:r:340:ARG:O	40:r:340:ARG:CG	2.67	0.43
56:s:402:UQ:H121	56:s:402:UQ:H101	1.62	0.43
43:v:12:ASP:OD1	43:v:15:LYS:HB2	2.19	0.43
44:w:170:LEU:HD22	44:w:187:TYR:CD1	2.54	0.43
2:B:110:GLU:HB2	18:T:71:ILE:HB	2.01	0.42
12:M:61:PRO:HB2	12:M:77:MET:HG3	2.01	0.42
15:P:94:ILE:O	15:P:98:THR:OG1	2.23	0.42
15:P:103:HIS:CD2	15:P:105:ASN:HB2	2.54	0.42
16:Q:184:ILE:HD11	16:Q:251:PHE:HZ	1.83	0.42
30:g:15:PHE:O	30:g:80:ARG:NH1	2.50	0.42
32:i:234:TRP:CE3	32:i:304:MET:HG2	2.54	0.42
32:i:291:TYR:HA	40:r:151:PHE:HZ	1.84	0.42
32:i:323:MET:HE3	32:i:323:MET:HB2	1.91	0.42
44:w:58:LYS:HZ3	44:w:278:CYS:HB2	1.84	0.42
1:A:66:LYS:HE3	1:A:188:GLY:O	2.19	0.42
2:B:205:ILE:O	2:B:209:TYR:HB3	2.18	0.42
4:E:16:SER:HA	11:L:54:ALA:HA	2.00	0.42
9:J:298:TYR:CD2	9:J:319:VAL:HB	2.55	0.42
12:M:451:ILE:O	12:M:455:ILE:HG12	2.19	0.42
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	2.01	0.42
27:d:164:LEU:HD23	28:e:149:LEU:HD13	2.01	0.42
36:m:72:THR:HG22	41:s:121:TRP:HH2	1.83	0.42
41:s:74:ALA:HB3	41:s:75:PRO:HD3	2.00	0.42
7:H:59:VAL:HG23	7:H:68:LEU:HD21	2.01	0.42
9:J:311:GLU:O	9:J:311:GLU:HG3	2.19	0.42
12:M:689:LEU:HD12	12:M:689:LEU:HA	1.82	0.42
13:N:43:LYS:HE3	13:N:44:TYR:CZ	2.54	0.42
16:Q:144:MET:HE2	16:Q:144:MET:HB2	1.92	0.42
16:Q:150:ALA:HB2	16:Q:400:ILE:HG12	2.02	0.42
16:Q:263:THR:O	16:Q:327:TYR:OH	2.36	0.42
6:X:92:LYS:HE2	6:X:92:LYS:HB2	1.85	0.42
25:b:28:LEU:HD22	25:b:32:GLU:HG2	2.00	0.42
35:l:467:ILE:O	35:l:471:ASN:HB2	2.19	0.42
40:r:201:MET:HE1	40:r:212:LEU:HD11	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:325:MET:HE2	40:r:362:ALA:HB2	2.01	0.42
48:r:502:PLX:H301	48:r:502:PLX:H331	1.55	0.42
41:s:235:ASN:ND2	41:s:267:THR:HA	2.33	0.42
43:v:83:GLU:CD	43:v:83:GLU:N	2.77	0.42
1:A:35:LEU:HD23	1:A:40:ARG:NH1	2.34	0.42
8:I:107:SER:C	8:I:109:ASP:H	2.27	0.42
12:M:252:ASP:OD2	12:M:290:THR:OG1	2.36	0.42
28:e:76:TYR:HB2	28:e:83:ASP:OD1	2.19	0.42
28:e:125:LEU:HD21	28:e:129:ARG:NH1	2.35	0.42
29:f:68:GLU:HG2	30:g:21:ARG:CZ	2.49	0.42
32:i:106:LEU:HG	32:i:138:PRO:HB2	2.02	0.42
48:r:502:PLX:H22	48:r:502:PLX:H1C3	1.76	0.42
10:K:98:MET:HB3	10:K:98:MET:HE3	1.74	0.42
15:P:115:THR:OG1	15:P:116:ALA:N	2.51	0.42
16:Q:188:THR:HB	16:Q:200:PHE:HA	1.99	0.42
22:Y:42:PRO:HB3	35:l:442:LEU:HD23	2.00	0.42
24:a:53:ARG:HB3	25:b:28:LEU:HD12	2.01	0.42
25:b:88:TYR:CZ	27:d:49:ARG:HG2	2.54	0.42
26:c:118:ASP:O	35:l:535:ARG:HD3	2.20	0.42
26:c:156:VAL:HG11	43:v:95:TYR:CZ	2.55	0.42
35:l:264:TYR:CG	35:l:265:PRO:HD3	2.54	0.42
14:O:152:ILE:HD11	14:O:201:ILE:HG12	2.02	0.42
15:P:173:MET:HE1	15:P:189:THR:HG23	2.01	0.42
19:U:23:PHE:CD2	54:s:401:PEE:H58	2.55	0.42
20:V:141:VAL:O	20:V:141:VAL:HG23	2.20	0.42
6:X:113:LEU:O	6:X:117:GLU:HG3	2.19	0.42
26:c:153:TYR:HB3	35:l:403:TYR:CD1	2.52	0.42
35:l:266:LEU:O	35:l:269:THR:HG22	2.19	0.42
1:A:110:PRO:O	1:A:238:CYS:HB3	2.20	0.42
9:J:83:PRO:HG3	9:J:119:VAL:HG11	2.02	0.42
16:Q:47:PHE:CD2	16:Q:52:MET:HE1	2.54	0.42
18:T:69:ASP:O	18:T:73:GLU:HG3	2.20	0.42
19:U:14:ALA:O	19:U:15:LYS:HG2	2.20	0.42
53:a:201:CDL:H341	53:a:201:CDL:H372	1.65	0.42
44:w:267:GLU:CD	44:w:267:GLU:H	2.28	0.42
6:G:104:PHE:HD1	6:G:108:LEU:HD12	1.84	0.42
12:M:634:LEU:HD13	12:M:636:TYR:OH	2.20	0.42
14:O:111:ARG:NH1	14:O:114:GLU:OE2	2.52	0.42
14:O:131:HIS:O	14:O:188:ILE:HA	2.20	0.42
16:Q:397:TYR:OH	16:Q:406:GLU:OE1	2.38	0.42
54:i:402:PEE:H42	54:i:402:PEE:H35	1.70	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:r:147:LEU:HD22	40:r:151:PHE:HE2	1.83	0.42
43:v:52:MET:HB2	43:v:55:GLN:HB2	2.02	0.42
1:A:380:GLY:O	1:A:386:ARG:NH1	2.51	0.42
4:E:28:ALA:HB1	4:E:79:VAL:HG11	2.02	0.42
6:G:105:MET:HG2	6:G:139:MET:CE	2.50	0.42
6:G:119:ILE:HD13	6:G:135:ALA:HB1	2.01	0.42
15:P:125:ARG:HD3	15:P:126:PHE:CZ	2.55	0.42
19:U:78:LEU:HD23	19:U:78:LEU:HA	1.88	0.42
6:X:86:VAL:HB	6:X:122:MET:HE1	2.02	0.42
33:j:17:LEU:HA	33:j:20:ILE:HG12	2.01	0.42
33:j:90:MET:SD	36:m:151:THR:HG23	2.60	0.42
53:r:503:CDL:H591	53:r:503:CDL:H332	2.01	0.42
1:A:278:ILE:HG21	1:A:304:ALA:HB2	2.02	0.42
46:A:502:FMN:O4'	46:A:502:FMN:O2'	2.35	0.42
3:C:161:ILE:HG13	3:C:180:LEU:HB2	2.01	0.42
12:M:94:MET:HE2	12:M:94:MET:HB2	1.75	0.42
12:M:306:MET:HE3	12:M:316:TYR:CE1	2.55	0.42
13:N:97:PRO:HG2	13:N:100:THR:HG23	2.01	0.42
28:e:152:ASP:OD1	28:e:152:ASP:N	2.53	0.42
33:j:81:THR:C	33:j:83:ASN:H	2.28	0.42
38:o:80:PHE:HE1	38:o:86:THR:HG21	1.83	0.42
44:w:148:GLU:O	44:w:152:SER:OG	2.25	0.42
1:A:209:GLU:OE2	1:A:226:LYS:NZ	2.35	0.41
1:A:256:ARG:O	14:O:245:VAL:HA	2.20	0.41
2:B:88:PHE:CZ	13:N:30:ALA:HA	2.55	0.41
2:B:100:GLU:O	2:B:170:GLY:N	2.36	0.41
12:M:48:THR:HA	12:M:95:PRO:HA	2.02	0.41
33:j:86:THR:O	33:j:90:MET:HG2	2.20	0.41
35:l:362:LEU:HB2	35:l:431:PHE:HD1	1.84	0.41
44:w:213:GLU:OE1	44:w:217:ARG:HD2	2.19	0.41
7:H:9:THR:HG23	7:H:16:VAL:HG22	2.02	0.41
9:J:316:ARG:O	9:J:319:VAL:HG22	2.20	0.41
10:K:87:LEU:HD12	14:O:85:LEU:HD13	2.02	0.41
14:O:133:GLN:HG3	14:O:172:ILE:HG12	2.02	0.41
16:Q:152:SER:HB3	16:Q:229:PRO:HA	2.02	0.41
16:Q:203:MET:HE2	16:Q:258:LEU:HD22	2.02	0.41
24:a:78:THR:HG22	28:e:100:VAL:HG11	2.03	0.41
32:i:79:LEU:HB2	34:k:47:ILE:HD13	2.02	0.41
53:i:401:CDL:H122	53:i:401:CDL:H151	1.88	0.41
35:l:102:GLU:OE1	35:l:456:ARG:NH2	2.35	0.41
40:r:186:LEU:HD23	40:r:186:LEU:HA	1.90	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:s:401:PEE:H67	54:s:401:PEE:H73	1.79	0.41
4:E:81:LEU:HD23	4:E:81:LEU:HA	1.95	0.41
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	2.02	0.41
35:l:534:HIS:CE1	54:l:702:PEE:H16	2.55	0.41
39:p:152:GLU:H	39:p:152:GLU:HG2	1.68	0.41
40:r:133:ILE:HG12	40:r:223:ALA:HB2	2.00	0.41
40:r:225:ILE:HD13	40:r:331:ASN:HB2	2.02	0.41
44:w:88:GLU:OE1	44:w:161:ARG:NH1	2.53	0.41
1:A:279:SER:OG	1:A:280:GLY:N	2.51	0.41
5:F:30:SER:OG	5:F:63:PRO:HG3	2.21	0.41
9:J:83:PRO:HA	9:J:106:MET:O	2.20	0.41
16:Q:181:LEU:HD23	16:Q:207:ARG:HG2	2.02	0.41
48:g:201:PLX:H22	48:g:201:PLX:H1C3	1.80	0.41
31:h:54:LYS:HE2	31:h:54:LYS:HB2	1.92	0.41
32:i:128:LEU:HD12	32:i:216:PHE:HB3	2.02	0.41
35:l:161:ARG:NH2	39:p:88:GLY:O	2.54	0.41
35:l:400:ASN:HB3	35:l:486:MET:SD	2.60	0.41
39:p:46:ALA:O	39:p:50:GLU:HG2	2.20	0.41
40:r:87:GLU:OE2	40:r:91:ARG:HD2	2.19	0.41
53:r:504:CDL:H722	53:r:504:CDL:H322	2.02	0.41
42:u:111:VAL:CG1	42:u:117:TRP:HB2	2.49	0.41
44:w:59:VAL:HG13	44:w:201:PRO:HA	2.03	0.41
9:J:231:LEU:O	9:J:274:PHE:HB2	2.20	0.41
12:M:637:ASP:N	12:M:641:GLN:OE1	2.37	0.41
6:X:89:LEU:HD22	23:Z:48:ASN:HA	2.02	0.41
25:b:69:ILE:HD12	25:b:69:ILE:HA	1.91	0.41
33:j:90:MET:HE3	33:j:90:MET:HA	2.03	0.41
41:s:174:MET:O	41:s:174:MET:HG3	2.20	0.41
42:u:80:GLU:O	42:u:84:GLU:HG3	2.20	0.41
1:A:268:GLU:HG2	1:A:269:ARG:HG2	2.03	0.41
12:M:319:TRP:HZ3	12:M:584:LEU:HD22	1.85	0.41
15:P:161:LYS:HA	15:P:161:LYS:HD3	1.91	0.41
17:S:39:ALA:O	54:m:202:PEE:N	2.54	0.41
21:W:93:GLU:OE1	31:h:92:TYR:OH	2.29	0.41
24:a:137:MET:HE3	24:a:137:MET:HB2	1.95	0.41
26:c:113:ILE:C	26:c:115:ASN:H	2.28	0.41
26:c:125:SER:O	26:c:129:MET:HG3	2.20	0.41
28:e:143:ASP:HA	28:e:144:PRO:HD3	1.97	0.41
35:l:144:TRP:CE2	35:l:223:LYS:HD2	2.56	0.41
40:r:445:LEU:O	40:r:448:THR:HG22	2.20	0.41
42:u:60:GLY:O	42:u:63:VAL:HG22	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:54:THR:O	44:w:56:THR:HG22	2.20	0.41
44:w:165:SER:HB3	44:w:245:PHE:CZ	2.55	0.41
2:B:198:GLU:HG2	13:N:108:TYR:HE1	1.85	0.41
4:E:80:ASP:OD1	4:E:80:ASP:N	2.50	0.41
7:H:64:ASP:OD1	7:H:65:VAL:N	2.53	0.41
12:M:354:LEU:HD22	12:M:548:LEU:HD22	2.01	0.41
15:P:196:HIS:HA	15:P:197:PRO:HD3	1.91	0.41
25:b:16:ARG:O	25:b:20:ARG:HG3	2.21	0.41
32:i:221:HIS:HB2	32:i:323:MET:HE1	2.02	0.41
35:l:78:LEU:HD11	53:r:503:CDL:H251	2.02	0.41
35:l:495:ILE:O	35:l:499:MET:HG3	2.21	0.41
38:o:59:VAL:CG1	40:r:422:HIS:HE1	2.34	0.41
40:r:119:TYR:O	40:r:123:GLU:HG2	2.20	0.41
40:r:190:TRP:CE2	48:r:502:PLX:H1A3	2.55	0.41
48:C:302:PLX:H21	48:C:302:PLX:H1C3	1.69	0.41
16:Q:184:ILE:HG12	16:Q:203:MET:HE3	2.02	0.41
16:Q:303:ARG:HG3	16:Q:401:GLU:HB3	2.03	0.41
16:Q:345:SER:HB2	21:W:19:ILE:HD12	2.03	0.41
34:k:55:LEU:O	34:k:58:MET:HE3	2.21	0.41
35:l:289:ALA:O	35:l:293:ILE:HG23	2.21	0.41
40:r:22:MET:HE3	40:r:22:MET:HB3	1.80	0.41
53:r:503:CDL:H652	53:r:503:CDL:H622	1.67	0.41
41:s:7:LEU:HA	41:s:10:ILE:HG22	2.03	0.41
3:C:61:SER:OG	41:s:54:LYS:HD3	2.20	0.41
4:E:93:THR:HG23	4:E:103:ILE:HD11	2.02	0.41
6:G:115:GLN:O	6:G:119:ILE:HG13	2.21	0.41
12:M:304:GLN:HB2	12:M:316:TYR:CD1	2.56	0.41
14:O:132:ILE:HD11	14:O:169:PHE:HD2	1.86	0.41
17:S:1:MET:HB2	17:S:3:PHE:CZ	2.55	0.41
21:W:70:ALA:HB2	42:u:125:LEU:HD13	2.03	0.41
32:i:38:LEU:HD12	32:i:38:LEU:HA	1.95	0.41
32:i:317:PHE:HZ	44:w:141:LEU:HD21	1.86	0.41
42:u:38:LYS:HB3	42:u:39:PRO:HD3	2.03	0.41
44:w:314:LEU:O	44:w:318:THR:HG22	2.21	0.41
1:A:149:MET:HE2	1:A:149:MET:HB2	1.77	0.41
7:H:51:ILE:HD11	8:I:94:ALA:HB3	2.03	0.41
7:H:76:GLN:O	7:H:78:GLU:N	2.54	0.41
8:I:40:LYS:HB2	21:W:7:LYS:H	1.86	0.41
13:N:122:GLN:HA	18:T:59:GLN:HG2	2.03	0.41
20:V:102:GLY:HA3	20:V:111:GLY:HA2	2.02	0.41
22:Y:100:LEU:O	22:Y:102:ASP:N	2.49	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:90:VAL:HG22	40:r:28:THR:HG21	2.02	0.41
31:h:19:THR:HA	32:i:84:TRP:HB2	2.03	0.41
32:i:13:VAL:HG13	32:i:36:ASN:ND2	2.35	0.41
33:j:84:LEU:HD23	33:j:84:LEU:HA	1.87	0.41
44:w:58:LYS:NZ	44:w:278:CYS:HB2	2.36	0.41
12:M:372:PHE:CD1	12:M:373:PRO:HD2	2.56	0.40
16:Q:53:TYR:HE1	54:i:402:PEE:H2	1.85	0.40
16:Q:68:ASP:O	32:i:49:ASN:ND2	2.54	0.40
16:Q:357:LYS:HD3	16:Q:364:SER:HB3	2.02	0.40
16:Q:404:LYS:HE2	16:Q:457:VAL:HB	2.03	0.40
17:S:43:TYR:CZ	21:W:68:ARG:HG3	2.56	0.40
20:V:120:LEU:HD11	48:r:502:PLX:H382	2.02	0.40
35:l:144:TRP:HH2	35:l:256:GLY:HA2	1.86	0.40
40:r:97:THR:HG21	53:r:504:CDL:H242	2.03	0.40
1:A:251:SER:OG	1:A:252:PRO:HD3	2.21	0.40
2:B:79:ARG:NH2	8:I:20:LEU:HD21	2.37	0.40
3:C:69:LEU:HD23	16:Q:94:VAL:HG11	2.03	0.40
6:G:112:SER:O	6:G:116:VAL:HG23	2.21	0.40
9:J:316:ARG:O	9:J:320:GLU:HG2	2.21	0.40
12:M:347:ASP:HB3	12:M:594:ALA:HB1	2.02	0.40
13:N:2:GLU:O	13:N:6:VAL:HG23	2.21	0.40
14:O:185:MET:HB3	14:O:194:GLU:HA	2.03	0.40
15:P:201:ASP:OD1	15:P:201:ASP:N	2.38	0.40
25:b:36:PRO:HA	25:b:37:PRO:HD3	1.91	0.40
28:e:84:LEU:HG	28:e:88:ARG:HD2	2.04	0.40
28:e:136:LEU:HD13	28:e:136:LEU:HA	1.98	0.40
32:i:40:MET:HE1	32:i:129:LEU:HD23	2.02	0.40
1:A:338:ASP:N	1:A:338:ASP:OD1	2.54	0.40
3:C:124:MET:HA	3:C:125:PRO:HD3	1.73	0.40
3:C:154:ASP:HA	3:C:157:VAL:O	2.21	0.40
4:E:88:MET:HE2	15:P:184:LEU:O	2.21	0.40
6:G:103:HIS:CE1	6:G:139:MET:HE2	2.56	0.40
11:L:58:LYS:HE2	11:L:58:LYS:HB2	1.94	0.40
15:P:109:LYS:HE3	15:P:109:LYS:HB3	1.91	0.40
16:Q:249:LYS:HA	21:W:19:ILE:HG23	2.04	0.40
24:a:154:LEU:HD23	24:a:154:LEU:HA	1.95	0.40
26:c:113:ILE:HD11	26:c:116:ARG:HD2	2.03	0.40
26:c:185:GLU:HB2	43:v:35:LYS:O	2.21	0.40
32:i:38:LEU:HD12	34:k:73:LEU:HD22	2.03	0.40
32:i:325:LEU:HD12	53:i:401:CDL:H121	2.03	0.40
35:l:500:LEU:HD21	53:l:701:CDL:H342	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:w:353:TRP:H	44:w:353:TRP:CD1	2.39	0.40
12:M:47:THR:HG23	12:M:51:GLN:HB2	2.03	0.40
12:M:58:MET:HG2	12:M:59:GLN:N	2.36	0.40
14:O:185:MET:HE2	51:O:301:FES:S1	2.62	0.40
16:Q:156:GLU:OE2	16:Q:171:ARG:NH2	2.51	0.40
19:U:53:TYR:CZ	42:u:44:MET:HG3	2.56	0.40
26:c:38:PRO:HG2	38:o:71:ALA:HB2	2.02	0.40
27:d:15:ARG:O	27:d:15:ARG:CG	2.70	0.40
28:e:74:HIS:HB2	28:e:83:ASP:OD2	2.21	0.40
32:i:9:LEU:HD13	32:i:42:PRO:HB2	2.03	0.40
32:i:347:ASN:OD1	32:i:347:ASN:N	2.54	0.40
39:p:76:HIS:O	39:p:78:GLN:N	2.55	0.40
41:s:105:MET:SD	41:s:162:LEU:HD11	2.62	0.40
44:w:350:LYS:HA	44:w:350:LYS:HD2	1.93	0.40
2:B:210:LEU:HD12	8:I:38:PRO:HB3	2.03	0.40
7:H:94:MET:HE1	15:P:99:PHE:CD1	2.55	0.40
16:Q:432:LEU:HD12	16:Q:432:LEU:HA	1.93	0.40
18:T:29:VAL:HG21	18:T:64:GLU:OE2	2.21	0.40
31:h:17:TRP:HE3	34:k:55:LEU:HD13	1.86	0.40
53:l:701:CDL:H421	53:l:701:CDL:H391	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	429/433 (99%)	415 (97%)	14 (3%)	0	100	100
2	B	174/176 (99%)	173 (99%)	1 (1%)	0	100	100
3	C	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
4	E	113/115 (98%)	111 (98%)	2 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	84/86 (98%)	79 (94%)	5 (6%)	0	100	100
6	G	86/88 (98%)	86 (100%)	0	0	100	100
6	X	86/88 (98%)	83 (96%)	3 (4%)	0	100	100
7	H	110/112 (98%)	101 (92%)	9 (8%)	0	100	100
8	I	93/112 (83%)	80 (86%)	13 (14%)	0	100	100
9	J	327/342 (96%)	316 (97%)	10 (3%)	1 (0%)	36	65
10	K	40/43 (93%)	40 (100%)	0	0	100	100
11	L	123/125 (98%)	121 (98%)	2 (2%)	0	100	100
12	M	688/690 (100%)	670 (97%)	17 (2%)	1 (0%)	48	77
13	N	142/144 (99%)	139 (98%)	3 (2%)	0	100	100
14	O	215/217 (99%)	205 (95%)	10 (5%)	0	100	100
15	P	206/208 (99%)	197 (96%)	9 (4%)	0	100	100
16	Q	412/430 (96%)	398 (97%)	14 (3%)	0	100	100
17	S	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
18	T	94/96 (98%)	92 (98%)	2 (2%)	0	100	100
19	U	81/83 (98%)	79 (98%)	2 (2%)	0	100	100
20	V	138/140 (99%)	132 (96%)	5 (4%)	1 (1%)	18	48
21	W	140/142 (99%)	136 (97%)	4 (3%)	0	100	100
22	Y	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
23	Z	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
24	a	138/140 (99%)	135 (98%)	3 (2%)	0	100	100
25	b	99/126 (79%)	94 (95%)	5 (5%)	0	100	100
26	c	154/156 (99%)	145 (94%)	9 (6%)	0	100	100
27	d	173/175 (99%)	171 (99%)	2 (1%)	0	100	100
28	e	105/107 (98%)	101 (96%)	4 (4%)	0	100	100
29	f	40/49 (82%)	39 (98%)	1 (2%)	0	100	100
30	g	119/121 (98%)	116 (98%)	3 (2%)	0	100	100
31	h	103/105 (98%)	99 (96%)	4 (4%)	0	100	100
32	i	345/347 (99%)	332 (96%)	11 (3%)	2 (1%)	21	51
33	j	95/115 (83%)	88 (93%)	7 (7%)	0	100	100
34	k	96/98 (98%)	87 (91%)	9 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	l	601/606 (99%)	577 (96%)	24 (4%)	0	100	100
36	m	125/175 (71%)	115 (92%)	10 (8%)	0	100	100
37	n	54/56 (96%)	54 (100%)	0	0	100	100
38	o	126/128 (98%)	119 (94%)	7 (6%)	0	100	100
39	p	176/178 (99%)	166 (94%)	10 (6%)	0	100	100
40	r	457/459 (100%)	448 (98%)	9 (2%)	0	100	100
41	s	299/318 (94%)	287 (96%)	12 (4%)	0	100	100
42	u	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
43	v	122/125 (98%)	115 (94%)	7 (6%)	0	100	100
44	w	318/320 (99%)	305 (96%)	13 (4%)	0	100	100
All	All	8067/8325 (97%)	7770 (96%)	292 (4%)	5 (0%)	49	77

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
32	i	93	VAL
32	i	92	PRO
12	M	283	GLU
9	J	38	HIS
20	V	46	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/346 (100%)	339 (98%)	6 (2%)	53	82
2	B	151/151 (100%)	149 (99%)	2 (1%)	61	86
3	C	132/132 (100%)	130 (98%)	2 (2%)	57	84
4	E	107/107 (100%)	106 (99%)	1 (1%)	70	90
5	F	76/76 (100%)	74 (97%)	2 (3%)	40	73

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	G	71/81 (88%)	70 (99%)	1 (1%)	59	85
6	X	75/81 (93%)	74 (99%)	1 (1%)	61	86
7	H	99/99 (100%)	98 (99%)	1 (1%)	68	89
8	I	87/97 (90%)	85 (98%)	2 (2%)	44	76
9	J	276/296 (93%)	272 (99%)	4 (1%)	59	85
10	K	41/42 (98%)	39 (95%)	2 (5%)	22	54
11	L	113/113 (100%)	113 (100%)	0	100	100
12	M	580/580 (100%)	572 (99%)	8 (1%)	59	85
13	N	130/130 (100%)	128 (98%)	2 (2%)	57	84
14	O	183/183 (100%)	181 (99%)	2 (1%)	65	88
15	P	190/190 (100%)	188 (99%)	2 (1%)	65	88
16	Q	361/370 (98%)	357 (99%)	4 (1%)	65	88
17	S	58/58 (100%)	58 (100%)	0	100	100
18	T	79/79 (100%)	78 (99%)	1 (1%)	61	86
19	U	69/69 (100%)	68 (99%)	1 (1%)	59	85
20	V	99/101 (98%)	94 (95%)	5 (5%)	21	53
21	W	122/123 (99%)	121 (99%)	1 (1%)	73	90
22	Y	63/63 (100%)	63 (100%)	0	100	100
23	Z	65/65 (100%)	65 (100%)	0	100	100
24	a	122/122 (100%)	118 (97%)	4 (3%)	33	67
25	b	97/119 (82%)	96 (99%)	1 (1%)	68	89
26	c	140/141 (99%)	137 (98%)	3 (2%)	47	77
27	d	154/155 (99%)	151 (98%)	3 (2%)	50	79
28	e	98/99 (99%)	95 (97%)	3 (3%)	35	69
29	f	35/45 (78%)	35 (100%)	0	100	100
30	g	108/108 (100%)	106 (98%)	2 (2%)	50	79
31	h	93/93 (100%)	92 (99%)	1 (1%)	65	88
32	i	311/311 (100%)	307 (99%)	4 (1%)	61	86
33	j	88/100 (88%)	88 (100%)	0	100	100
34	k	85/85 (100%)	84 (99%)	1 (1%)	63	86
35	l	518/540 (96%)	512 (99%)	6 (1%)	63	86

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
36	m	91/141 (64%)	89 (98%)	2 (2%)	45 77
37	n	53/53 (100%)	53 (100%)	0	100 100
38	o	113/113 (100%)	111 (98%)	2 (2%)	51 80
39	p	159/159 (100%)	158 (99%)	1 (1%)	78 93
40	r	410/410 (100%)	403 (98%)	7 (2%)	53 82
41	s	263/275 (96%)	258 (98%)	5 (2%)	50 79
42	u	153/153 (100%)	151 (99%)	2 (1%)	61 86
43	v	98/111 (88%)	95 (97%)	3 (3%)	35 69
44	w	280/283 (99%)	277 (99%)	3 (1%)	65 88
All	All	7041/7248 (97%)	6938 (98%)	103 (2%)	55 84

All (103) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	LEU
1	A	95	THR
1	A	134	ASP
1	A	210	THR
1	A	307	VAL
1	A	334	THR
2	B	47	SER
2	B	76	TYR
3	C	71	CYS
3	C	188	LYS
4	E	96	VAL
5	F	26	ARG
5	F	64	LYS
6	G	117	GLU
7	H	67	LYS
8	I	16	SER
8	I	92	LYS
9	J	140	ASP
9	J	214	LEU
9	J	293	LEU
9	J	298	TYR
10	K	97	ARG
10	K	107	SER
12	M	361	VAL
12	M	364	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	M	515	ILE
12	M	544	VAL
12	M	640	ASP
12	M	657	ASP
12	M	671	LEU
12	M	682	ASP
13	N	68	MET
13	N	80	SER
14	O	137	THR
14	O	232	THR
15	P	127	GLU
15	P	226	LEU
16	Q	80	LEU
16	Q	147	ASN
16	Q	217	VAL
16	Q	446	ASP
18	T	43	GLN
19	U	74	GLN
20	V	89	ASN
20	V	110	ILE
20	V	120	LEU
20	V	140	LYS
20	V	141	VAL
21	W	64	ASP
6	X	77	GLU
24	a	77	LEU
24	a	127	ASP
24	a	173	THR
24	a	186	THR
25	b	91	THR
26	c	78	LEU
26	c	169	GLU
26	c	182	VAL
27	d	34	THR
27	d	134	GLN
27	d	136	SER
28	e	55	LEU
28	e	136	LEU
28	e	137	MET
30	g	13	LEU
30	g	18	ASN
31	h	88	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	i	67	SER
32	i	132	THR
32	i	344	SER
32	i	347	ASN
34	k	39	SER
35	l	23	ASN
35	l	70	THR
35	l	71	LEU
35	l	190	LEU
35	l	387	THR
35	l	455	LYS
36	m	27	ILE
36	m	46	ASN
38	o	85	LYS
38	o	114	LYS
39	p	24	LEU
40	r	35	SER
40	r	45	LEU
40	r	139	GLN
40	r	179	ILE
40	r	248	THR
40	r	303	ILE
40	r	367	LEU
41	s	24	GLU
41	s	72	ILE
41	s	81	LEU
41	s	151	LEU
41	s	251	THR
42	u	109	GLU
42	u	111	VAL
43	v	68	LYS
43	v	78	LEU
43	v	80	CYS
44	w	95	ASP
44	w	175	ARG
44	w	250	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	393	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	436	GLN
1	A	441	HIS
1	A	458	GLN
3	C	111	ASN
4	E	72	HIS
5	F	25	GLN
5	F	62	GLN
5	F	80	ASN
6	G	103	HIS
6	G	142	GLN
8	I	29	GLN
9	J	122	HIS
9	J	128	ASN
9	J	376	ASN
10	K	79	HIS
11	L	85	ASN
11	L	86	ASN
12	M	123	ASN
12	M	278	HIS
12	M	336	ASN
12	M	388	ASN
12	M	677	GLN
13	N	12	GLN
13	N	13	GLN
14	O	41	HIS
14	O	133	GLN
14	O	182	ASN
15	P	196	HIS
16	Q	234	GLN
17	S	40	HIS
17	S	61	HIS
18	T	120	GLN
23	Z	48	ASN
24	a	90	ASN
24	a	132	ASN
26	c	154	GLN
30	g	119	HIS
32	i	63	GLN
32	i	91	ASN
32	i	310	ASN
35	l	67	HIS
35	l	165	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
35	l	170	GLN
35	l	192	HIS
35	l	471	ASN
38	o	52	ASN
39	p	12	HIS
39	p	51	HIS
39	p	75	GLN
40	r	175	ASN
40	r	399	ASN
40	r	421	HIS
40	r	422	HIS
40	r	424	ASN
41	s	47	GLN
41	s	235	ASN
41	s	250	HIS
41	s	287	HIS
42	u	30	HIS
42	u	163	HIS
43	v	4	HIS
43	v	65	GLN
44	w	92	HIS
44	w	223	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
16	2MR	Q	118	16	10,12,13	2.01	1 (10%)	5,13,15	6.04	3 (60%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	Q	118	2MR	CZ-NE	5.74	1.46	1.34

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	Q	118	2MR	NE-CZ-NH2	12.34	130.79	119.48
16	Q	118	2MR	CD-NE-CZ	4.21	131.28	123.36
16	Q	118	2MR	CQ2-NH2-CZ	3.36	130.86	123.65

There are no chirality outliers.

All (2) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 35 ligands modelled in this entry, 2 are monoatomic - leaving 33 for Mogul analysis.

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
54	PEE	l	702	-	45,45,50	1.25	6 (13%)	48,50,55	1.03	2 (4%)
54	PEE	l	703	-	45,45,50	1.24	6 (13%)	48,50,55	0.99	2 (4%)
48	PLX	g	201	-	51,51,51	1.21	3 (5%)	53,59,59	0.61	1 (1%)
49	8Q1	X	201	-	32,34,34	1.63	6 (18%)	39,43,43	1.55	6 (15%)
54	PEE	Q	501	-	50,50,50	1.18	6 (12%)	53,55,55	0.97	2 (3%)
50	NDP	J	401	-	51,52,52	4.31	25 (49%)	71,80,80	2.18	15 (21%)
45	SF4	C	301	16,3	0,12,12	-	-	-		
45	SF4	B	301	2	0,12,12	-	-	-		
54	PEE	r	501	-	50,50,50	1.18	6 (12%)	53,55,55	1.01	2 (3%)
45	SF4	A	501	1	0,12,12	-	-	-		
51	FES	M	803	12	0,4,4	-	-	-		
45	SF4	M	802	12	0,12,12	-	-	-		
54	PEE	i	402	-	46,46,50	1.23	6 (13%)	49,51,55	1.00	2 (4%)
53	CDL	a	201	-	90,90,99	1.16	8 (8%)	96,102,111	0.91	4 (4%)
54	PEE	s	401	-	50,50,50	1.17	6 (12%)	53,55,55	0.96	2 (3%)
47	NAI	A	503	-	47,48,48	4.02	22 (46%)	64,73,73	1.68	11 (17%)
45	SF4	M	801	12	0,12,12	-	-	-		
53	CDL	l	701	-	99,99,99	1.12	9 (9%)	105,111,111	0.85	4 (3%)
45	SF4	B	302	2	0,12,12	-	-	-		
51	FES	O	301	14	0,4,4	-	-	-		
56	UQ	s	402	-	28,28,63	3.32	7 (25%)	36,37,79	2.78	12 (33%)
48	PLX	m	201	-	51,51,51	1.22	4 (7%)	53,59,59	0.61	1 (1%)
57	ADP	w	401	-	28,29,29	3.19	9 (32%)	43,45,45	1.93	9 (20%)
54	PEE	m	202	-	40,40,50	1.17	5 (12%)	43,45,55	1.01	2 (4%)
49	8Q1	G	201	-	32,34,34	1.61	6 (18%)	39,43,43	1.49	6 (15%)
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.23	8 (16%)
53	CDL	N	201	-	50,50,99	1.42	9 (18%)	56,62,111	1.18	4 (7%)
53	CDL	r	504	-	99,99,99	1.11	9 (9%)	105,111,111	0.85	4 (3%)
48	PLX	C	302	-	51,51,51	1.22	4 (7%)	53,59,59	0.61	1 (1%)
53	CDL	i	401	-	65,65,99	1.30	8 (12%)	71,77,111	1.03	4 (5%)
53	CDL	r	503	-	98,98,99	1.12	8 (8%)	104,110,111	0.90	4 (3%)
48	PLX	r	502	-	51,51,51	1.20	4 (7%)	53,59,59	0.63	1 (1%)
48	PLX	e	201	-	51,51,51	1.21	5 (9%)	53,59,59	0.60	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	PEE	l	702	-	-	21/49/49/54	-
54	PEE	l	703	-	-	20/49/49/54	-
48	PLX	g	201	-	-	24/55/55/55	-
49	8Q1	X	201	-	-	19/41/41/41	-
54	PEE	Q	501	-	-	24/54/54/54	-
50	NDP	J	401	-	-	6/34/77/77	0/5/5/5
45	SF4	C	301	16,3	-	-	0/6/5/5
45	SF4	B	301	2	-	-	0/6/5/5
54	PEE	r	501	-	-	30/54/54/54	-
45	SF4	A	501	1	-	-	0/6/5/5
51	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	802	12	-	-	0/6/5/5
54	PEE	i	402	-	-	24/50/50/54	-
53	CDL	a	201	-	-	51/101/101/110	-
54	PEE	s	401	-	-	28/54/54/54	-
53	CDL	l	701	-	-	55/110/110/110	-
47	NAI	A	503	-	-	7/29/72/72	0/5/5/5
45	SF4	M	801	12	-	-	0/6/5/5
45	SF4	B	302	2	-	-	0/6/5/5
51	FES	O	301	14	-	-	0/1/1/1
56	UQ	s	402	-	-	9/21/45/87	0/1/1/1
48	PLX	m	201	-	-	30/55/55/55	-
57	ADP	w	401	-	-	4/16/32/32	0/3/3/3
54	PEE	m	202	-	-	17/44/44/54	-
49	8Q1	G	201	-	-	17/41/41/41	-
46	FMN	A	502	-	-	3/18/18/18	0/3/3/3
53	CDL	N	201	-	-	33/61/61/110	-
53	CDL	r	504	-	-	60/110/110/110	-
48	PLX	C	302	-	-	28/55/55/55	-
53	CDL	i	401	-	-	37/76/76/110	-
53	CDL	r	503	-	-	56/109/109/110	-
48	PLX	r	502	-	-	30/55/55/55	-
48	PLX	e	201	-	-	30/55/55/55	-

All (189) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C3B-C2B	-13.14	1.24	1.53
50	J	401	NDP	O4D-C4D	10.76	1.68	1.45
47	A	503	NAI	C3D-C4D	-10.35	1.26	1.53
50	J	401	NDP	C3D-C4D	-9.93	1.27	1.53
56	s	402	UQ	C13-C14	9.64	1.55	1.33
47	A	503	NAI	O4B-C1B	9.41	1.63	1.42
56	s	402	UQ	C8-C9	9.23	1.54	1.33
57	w	401	ADP	C3'-C4'	-8.96	1.30	1.53
47	A	503	NAI	O4B-C4B	-8.26	1.26	1.45
56	s	402	UQ	C18-C19	7.92	1.56	1.32
50	J	401	NDP	O4B-C4B	-7.88	1.27	1.45
57	w	401	ADP	O4'-C4'	7.81	1.62	1.45
47	A	503	NAI	C2D-C1D	-7.67	1.29	1.53
50	J	401	NDP	C2N-C3N	7.53	1.55	1.35
50	J	401	NDP	C6N-C5N	7.31	1.55	1.33
47	A	503	NAI	C2B-C1B	-7.31	1.30	1.53
47	A	503	NAI	O4D-C4D	6.94	1.60	1.45
50	J	401	NDP	PN-O3	6.75	1.66	1.59
57	w	401	ADP	PA-O3A	6.63	1.66	1.59
47	A	503	NAI	PA-O3	6.47	1.66	1.59
50	J	401	NDP	P2B-O2B	6.13	1.70	1.59
47	A	503	NAI	C2D-C3D	6.06	1.69	1.53
50	J	401	NDP	PA-O3	5.83	1.65	1.59
50	J	401	NDP	C6A-N6A	5.78	1.49	1.34
47	A	503	NAI	PN-O3	5.67	1.65	1.59
47	A	503	NAI	O4D-C1D	5.65	1.55	1.42
50	J	401	NDP	C3B-C4B	5.53	1.67	1.53
57	w	401	ADP	C6-N6	5.46	1.48	1.34
47	A	503	NAI	C7N-N7N	5.29	1.48	1.33
47	A	503	NAI	C4N-C3N	-5.28	1.40	1.50
49	X	201	8Q1	C39-N41	5.14	1.45	1.33
49	X	201	8Q1	C34-N36	5.11	1.45	1.33
49	G	201	8Q1	C34-N36	5.11	1.45	1.33
50	J	401	NDP	C6N-N1N	5.10	1.49	1.37
47	A	503	NAI	C6A-N6A	5.09	1.47	1.34
49	G	201	8Q1	C39-N41	5.05	1.45	1.33
50	J	401	NDP	O4D-C1D	-4.97	1.30	1.42
50	J	401	NDP	O4B-C1B	4.77	1.53	1.42
50	J	401	NDP	C1B-N9A	-4.53	1.33	1.46
57	w	401	ADP	O4'-C1'	-4.50	1.31	1.42
47	A	503	NAI	O2B-C2B	4.35	1.53	1.43
50	J	401	NDP	O2D-C2D	-3.93	1.33	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	J	401	NDP	C7N-N7N	3.87	1.44	1.33
54	m	202	PEE	C18-C19	3.83	1.53	1.31
54	l	702	PEE	C18-C19	3.82	1.53	1.31
54	l	703	PEE	C18-C19	3.81	1.53	1.31
54	r	501	PEE	C18-C19	3.81	1.53	1.31
54	i	402	PEE	C18-C19	3.81	1.53	1.31
54	Q	501	PEE	C18-C19	3.81	1.53	1.31
54	s	401	PEE	C18-C19	3.79	1.53	1.31
54	i	402	PEE	C39-C38	3.75	1.53	1.31
54	r	501	PEE	C39-C38	3.73	1.52	1.31
54	l	702	PEE	C39-C38	3.73	1.52	1.31
54	l	703	PEE	C39-C38	3.73	1.52	1.31
54	Q	501	PEE	C39-C38	3.72	1.52	1.31
54	s	401	PEE	C39-C38	3.72	1.52	1.31
47	A	503	NAI	C7N-C3N	3.61	1.56	1.48
46	A	502	FMN	C4A-N5	3.52	1.38	1.30
53	i	401	CDL	OA8-CA7	3.47	1.43	1.33
53	l	701	CDL	OA8-CA7	3.46	1.43	1.33
53	r	504	CDL	OA8-CA7	3.45	1.43	1.33
53	N	201	CDL	OA8-CA7	3.42	1.43	1.33
53	a	201	CDL	OA8-CA7	3.41	1.43	1.33
47	A	503	NAI	C4N-C5N	-3.40	1.40	1.49
53	r	503	CDL	OA8-CA7	3.37	1.43	1.33
57	w	401	ADP	C8-N9	-3.33	1.31	1.37
50	J	401	NDP	C8A-N9A	-3.18	1.32	1.37
57	w	401	ADP	O2'-C2'	-3.15	1.35	1.43
53	N	201	CDL	OA6-CA5	3.11	1.43	1.34
53	a	201	CDL	OB6-CB5	3.08	1.43	1.34
50	J	401	NDP	C7N-C3N	3.07	1.55	1.48
53	i	401	CDL	OB6-CB5	3.06	1.42	1.34
53	r	503	CDL	OB6-CB5	3.05	1.42	1.34
53	r	504	CDL	OB6-CB5	3.04	1.42	1.34
53	N	201	CDL	OB8-CB7	3.04	1.42	1.33
53	l	701	CDL	OB6-CB5	3.03	1.42	1.34
53	l	701	CDL	OA6-CA5	3.03	1.42	1.34
53	l	701	CDL	OB8-CB7	3.02	1.42	1.33
53	i	401	CDL	OB8-CB7	3.02	1.42	1.33
53	r	503	CDL	OB8-CB7	3.02	1.42	1.33
53	r	504	CDL	OA6-CA5	3.00	1.42	1.34
53	N	201	CDL	OB6-CB5	3.00	1.42	1.34
53	r	504	CDL	OB8-CB7	2.98	1.42	1.33
53	a	201	CDL	OB8-CB7	2.98	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	w	401	ADP	O3'-C3'	2.97	1.50	1.43
50	J	401	NDP	O3D-C3D	2.97	1.50	1.43
50	J	401	NDP	C5A-N7A	-2.97	1.33	1.39
53	r	503	CDL	OA6-CA5	2.95	1.42	1.34
53	a	201	CDL	OA6-CA5	2.95	1.42	1.34
53	i	401	CDL	OA6-CA5	2.92	1.42	1.34
48	e	201	PLX	O6-C4	-2.90	1.40	1.44
48	C	302	PLX	O6-C4	-2.83	1.41	1.44
48	g	201	PLX	O6-C4	-2.82	1.41	1.44
48	m	201	PLX	O6-C4	-2.76	1.41	1.44
47	A	503	NAI	C8A-N9A	-2.71	1.32	1.37
56	s	402	UQ	C6-C1	2.71	1.54	1.46
50	J	401	NDP	O2B-C2B	2.65	1.53	1.44
53	r	503	CDL	OA6-CA4	-2.61	1.40	1.46
53	a	201	CDL	OA6-CA4	-2.58	1.40	1.46
54	r	501	PEE	O2-C2	-2.57	1.40	1.46
46	A	502	FMN	C10-N1	2.57	1.38	1.33
53	r	504	CDL	OA6-CA4	-2.57	1.40	1.46
54	s	401	PEE	O2-C2	-2.57	1.40	1.46
53	i	401	CDL	OA6-CA4	-2.55	1.40	1.46
54	l	703	PEE	O2-C2	-2.53	1.40	1.46
54	i	402	PEE	O2-C2	-2.52	1.40	1.46
47	A	503	NAI	PN-O5D	2.52	1.69	1.59
54	Q	501	PEE	O3-C30	2.51	1.40	1.33
54	l	703	PEE	O3-C30	2.51	1.40	1.33
54	Q	501	PEE	O2-C2	-2.49	1.40	1.46
49	X	201	8Q1	C1-S44	2.49	1.82	1.76
53	l	701	CDL	OA6-CA4	-2.48	1.40	1.46
48	m	201	PLX	C7-C6	2.48	1.55	1.50
54	l	702	PEE	O2-C2	-2.47	1.40	1.46
54	s	401	PEE	O3-C30	2.47	1.40	1.33
57	w	401	ADP	C5-N7	-2.47	1.34	1.39
54	i	402	PEE	O3-C30	2.46	1.40	1.33
47	A	503	NAI	C6N-C5N	2.46	1.40	1.33
54	m	202	PEE	O2-C2	-2.46	1.40	1.46
54	l	702	PEE	O3-C30	2.45	1.40	1.33
54	r	501	PEE	O3-C30	2.45	1.40	1.33
48	r	502	PLX	C7-C6	2.43	1.55	1.50
50	J	401	NDP	C2D-C3D	2.43	1.59	1.53
48	C	302	PLX	C7-C6	2.39	1.55	1.50
54	m	202	PEE	O3-C30	2.38	1.40	1.33
49	G	201	8Q1	C1-S44	2.38	1.81	1.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	l	702	PEE	O2-C10	2.38	1.41	1.34
47	A	503	NAI	C5B-C4B	2.37	1.58	1.51
48	e	201	PLX	C7-C6	2.36	1.55	1.50
54	m	202	PEE	O2-C10	2.35	1.40	1.34
54	Q	501	PEE	O2-C10	2.35	1.40	1.34
49	X	201	8Q1	C6-C1	2.33	1.53	1.50
53	l	701	CDL	OB6-CB4	-2.31	1.41	1.46
47	A	503	NAI	O3B-C3B	-2.31	1.37	1.43
48	g	201	PLX	C7-C6	2.31	1.55	1.50
53	l	701	CDL	PB2-OB2	2.30	1.68	1.59
54	i	402	PEE	O2-C10	2.30	1.40	1.34
53	N	201	CDL	OB6-CB4	-2.29	1.41	1.46
49	G	201	8Q1	C6-C1	2.29	1.53	1.50
49	X	201	8Q1	O35-C34	-2.29	1.19	1.23
53	r	503	CDL	PB2-OB2	2.28	1.68	1.59
49	G	201	8Q1	O35-C34	-2.28	1.19	1.23
54	l	703	PEE	O2-C10	2.28	1.40	1.34
53	r	503	CDL	OB6-CB4	-2.28	1.41	1.46
53	N	201	CDL	PB2-OB2	2.27	1.68	1.59
53	i	401	CDL	PB2-OB5	2.27	1.68	1.59
49	G	201	8Q1	O40-C39	-2.27	1.18	1.23
53	i	401	CDL	OB6-CB4	-2.26	1.41	1.46
53	r	504	CDL	PB2-OB5	2.25	1.68	1.59
53	i	401	CDL	PB2-OB2	2.25	1.68	1.59
53	a	201	CDL	OB6-CB4	-2.25	1.41	1.46
54	r	501	PEE	O2-C10	2.25	1.40	1.34
53	r	504	CDL	PB2-OB2	2.24	1.68	1.59
48	r	502	PLX	O6-C4	-2.24	1.41	1.44
54	s	401	PEE	O2-C10	2.24	1.40	1.34
53	r	504	CDL	OB6-CB4	-2.23	1.41	1.46
53	r	503	CDL	PB2-OB5	2.23	1.68	1.59
53	N	201	CDL	PB2-OB5	2.23	1.68	1.59
50	J	401	NDP	PA-O5B	2.22	1.68	1.59
53	l	701	CDL	PB2-OB5	2.22	1.68	1.59
49	X	201	8Q1	O40-C39	-2.21	1.18	1.23
53	a	201	CDL	PB2-OB2	2.21	1.68	1.59
53	a	201	CDL	PB2-OB5	2.21	1.68	1.59
48	C	302	PLX	P1-O4	2.21	1.68	1.59
48	r	502	PLX	P1-O4	2.20	1.68	1.59
48	g	201	PLX	P1-O4	2.20	1.68	1.59
54	m	202	PEE	O3-C3	-2.18	1.40	1.45
48	m	201	PLX	P1-O4	2.18	1.67	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	N	201	CDL	OA6-CA4	-2.18	1.41	1.46
54	l	702	PEE	O3-C3	-2.16	1.40	1.45
48	e	201	PLX	P1-O4	2.16	1.67	1.59
54	Q	501	PEE	O3-C3	-2.14	1.40	1.45
54	r	501	PEE	O3-C3	-2.14	1.40	1.45
56	s	402	UQ	O4-C4	-2.13	1.18	1.23
56	s	402	UQ	O3-CM3	-2.12	1.40	1.45
54	s	401	PEE	O3-C3	-2.12	1.40	1.45
50	J	401	NDP	O7N-C7N	-2.11	1.19	1.24
54	i	402	PEE	O3-C3	-2.11	1.40	1.45
48	m	201	PLX	P1-O1	2.10	1.67	1.59
48	r	502	PLX	P1-O1	2.09	1.67	1.59
54	l	703	PEE	O3-C3	-2.09	1.40	1.45
48	C	302	PLX	P1-O1	2.08	1.67	1.59
47	A	503	NAI	C5A-N7A	-2.06	1.35	1.39
48	e	201	PLX	P1-O1	2.06	1.67	1.59
53	N	201	CDL	C11-CA5	2.05	1.56	1.50
56	s	402	UQ	C7-C8	2.03	1.53	1.50
48	e	201	PLX	C1-C2	2.02	1.57	1.51
53	r	504	CDL	C11-CA5	2.01	1.56	1.50
53	l	701	CDL	C11-CA5	2.01	1.56	1.50

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
56	s	402	UQ	C7-C8-C9	-9.60	110.29	126.83
50	J	401	NDP	C3N-C2N-N1N	-7.33	112.45	123.20
50	J	401	NDP	C1D-N1N-C2N	-7.23	109.23	121.14
50	J	401	NDP	C6N-N1N-C2N	-6.08	112.81	119.32
56	s	402	UQ	C12-C13-C14	-6.05	113.77	127.62
49	X	201	8Q1	C6-C1-S44	5.64	120.12	113.40
57	w	401	ADP	C5-C4-N3	-5.57	119.05	126.72
50	J	401	NDP	C5A-C4A-N3A	-5.50	119.14	126.72
47	A	503	NAI	C5A-C4A-N3A	-5.41	119.27	126.72
49	G	201	8Q1	C6-C1-S44	5.34	119.77	113.40
50	J	401	NDP	C1D-N1N-C6N	-5.23	109.71	120.77
56	s	402	UQ	C10-C9-C8	-4.63	111.74	123.63
56	s	402	UQ	C11-C9-C8	-4.50	111.06	121.17
57	w	401	ADP	N3-C2-N1	-4.47	121.82	128.58
47	A	503	NAI	N3A-C2A-N1A	-4.44	121.86	128.58
57	w	401	ADP	N3-C4-N9	4.42	134.68	127.17
56	s	402	UQ	C15-C14-C13	-4.23	112.77	123.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
53	N	201	CDL	OA6-CA5-C11	4.21	120.58	111.48
50	J	401	NDP	N3A-C2A-N1A	-4.14	122.32	128.58
53	r	503	CDL	OA6-CA5-C11	4.10	120.36	111.48
53	r	503	CDL	OB6-CB5-C51	4.06	120.27	111.48
54	r	501	PEE	O2-C10-C11	4.05	120.25	111.48
54	l	702	PEE	O2-C10-C11	4.05	120.25	111.48
53	a	201	CDL	OB6-CB5-C51	4.02	120.18	111.48
53	r	504	CDL	OB6-CB5-C51	4.02	120.17	111.48
54	m	202	PEE	O2-C10-C11	4.02	120.17	111.48
54	i	402	PEE	O2-C10-C11	4.01	120.16	111.48
53	a	201	CDL	OA6-CA5-C11	4.01	120.15	111.48
56	s	402	UQ	C16-C14-C13	-3.99	112.21	121.17
56	s	402	UQ	C17-C18-C19	-3.98	114.39	127.64
53	N	201	CDL	OB6-CB5-C51	3.97	120.06	111.48
53	l	701	CDL	OA6-CA5-C11	3.96	120.05	111.48
53	i	401	CDL	OB6-CB5-C51	3.95	120.03	111.48
53	i	401	CDL	OA6-CA5-C11	3.92	119.97	111.48
50	J	401	NDP	N3A-C4A-N9A	3.86	133.74	127.17
54	Q	501	PEE	O2-C10-C11	3.86	119.83	111.48
54	l	703	PEE	O2-C10-C11	3.86	119.83	111.48
54	s	401	PEE	O2-C10-C11	3.81	119.73	111.48
47	A	503	NAI	N3A-C4A-N9A	3.78	133.60	127.17
53	l	701	CDL	OB6-CB5-C51	3.76	119.62	111.48
53	r	504	CDL	OA6-CA5-C11	3.73	119.56	111.48
47	A	503	NAI	C2A-N3A-C4A	3.69	120.84	111.83
57	w	401	ADP	N9-C8-N7	-3.61	108.81	113.94
50	J	401	NDP	C2A-N3A-C4A	3.59	120.59	111.83
57	w	401	ADP	C2-N3-C4	3.56	120.52	111.83
47	A	503	NAI	C4A-C5A-N7A	-3.50	106.58	110.58
49	X	201	8Q1	O4-C1-C6	-3.46	119.99	123.98
47	A	503	NAI	C5A-N7A-C8A	3.39	108.78	103.45
49	G	201	8Q1	O4-C1-C6	-3.35	120.11	123.98
56	s	402	UQ	C7-C6-C5	-3.34	119.17	124.89
57	w	401	ADP	C5-N7-C8	3.33	108.69	103.45
47	A	503	NAI	N9A-C8A-N7A	-3.28	109.28	113.94
56	s	402	UQ	C21-C19-C18	-3.27	112.83	122.66
50	J	401	NDP	C4A-C5A-N7A	-3.27	106.85	110.58
47	A	503	NAI	C3D-C2D-C1D	3.23	107.57	101.46
57	w	401	ADP	C4-N9-C8	3.21	109.11	105.74
46	A	502	FMN	C4-N3-C2	-3.16	120.02	125.64
50	J	401	NDP	N9A-C8A-N7A	-3.09	109.55	113.94
50	J	401	NDP	C5A-N7A-C8A	3.03	108.21	103.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	w	401	ADP	C4-C5-N7	-3.03	107.12	110.58
56	s	402	UQ	CM5-C5-C6	-2.88	119.72	124.45
54	r	501	PEE	O3-C30-C31	2.86	120.56	111.83
54	Q	501	PEE	O3-C30-C31	2.86	120.55	111.83
56	s	402	UQ	C20-C19-C18	-2.83	114.16	122.66
53	i	401	CDL	OA8-CA7-C31	2.79	120.34	111.83
47	A	503	NAI	C4D-O4D-C1D	-2.77	103.36	109.47
54	l	702	PEE	O3-C30-C31	2.76	120.26	111.83
53	N	201	CDL	OB8-CB7-C71	2.76	120.26	111.83
53	N	201	CDL	OA8-CA7-C31	2.76	120.25	111.83
53	a	201	CDL	OB8-CB7-C71	2.75	120.21	111.83
53	i	401	CDL	OB8-CB7-C71	2.74	120.20	111.83
53	r	503	CDL	OB8-CB7-C71	2.73	120.15	111.83
53	l	701	CDL	OB8-CB7-C71	2.70	120.06	111.83
54	s	401	PEE	O3-C30-C31	2.69	120.04	111.83
54	l	703	PEE	O3-C30-C31	2.68	120.00	111.83
47	A	503	NAI	C2D-C3D-C4D	2.67	107.77	102.61
54	i	402	PEE	O3-C30-C31	2.65	119.91	111.83
46	A	502	FMN	C4A-C4-N3	2.65	119.99	113.25
53	r	504	CDL	OA8-CA7-C31	2.64	119.89	111.83
53	r	504	CDL	OB8-CB7-C71	2.62	119.83	111.83
53	l	701	CDL	OA8-CA7-C31	2.62	119.81	111.83
53	r	503	CDL	OA8-CA7-C31	2.61	119.78	111.83
48	g	201	PLX	C1A-N1-C1	2.59	120.20	109.91
54	m	202	PEE	O3-C30-C31	2.59	119.72	111.83
49	X	201	8Q1	C43-S44-C1	2.57	109.45	101.84
48	e	201	PLX	C1A-N1-C1	2.56	120.07	109.91
49	G	201	8Q1	C37-C38-C39	2.49	116.54	112.39
48	r	502	PLX	C1A-N1-C1	2.47	119.74	109.91
46	A	502	FMN	O4-C4-C4A	-2.45	120.05	126.53
53	a	201	CDL	OA8-CA7-C31	2.45	119.31	111.83
46	A	502	FMN	C4A-C10-N10	2.42	119.95	116.48
50	J	401	NDP	C4A-N9A-C8A	2.41	108.27	105.74
48	m	201	PLX	C1A-N1-C1	2.40	119.44	109.91
49	X	201	8Q1	C37-C38-C39	2.37	116.35	112.39
47	A	503	NAI	C4A-N9A-C8A	2.37	108.23	105.74
46	A	502	FMN	C5A-C9A-N10	2.36	120.10	117.97
48	C	302	PLX	C1A-N1-C1	2.35	119.24	109.91
49	X	201	8Q1	C38-C39-N41	2.32	120.57	116.34
46	A	502	FMN	C10-C4A-N5	-2.31	120.09	124.81
46	A	502	FMN	C9A-C5A-N5	-2.29	120.03	122.45
49	G	201	8Q1	C38-C39-N41	2.27	120.48	116.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	G	201	8Q1	C43-S44-C1	2.22	108.41	101.84
49	X	201	8Q1	O4-C1-S44	-2.20	119.89	122.68
50	J	401	NDP	C2B-C1B-N9A	-2.19	110.15	113.75
50	J	401	NDP	C2B-C3B-C4B	2.16	106.64	101.99
56	s	402	UQ	C7-C6-C1	2.09	120.95	118.52
50	J	401	NDP	C2D-C3D-C4D	2.05	106.56	102.61
49	G	201	8Q1	O4-C1-S44	-2.01	120.12	122.68
46	A	502	FMN	C4A-C10-N1	-2.01	119.65	124.59
57	w	401	ADP	C2'-C3'-C4'	2.01	106.50	102.61

There are no chirality outliers.

All (663) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-O2'
46	A	502	FMN	N10-C1'-C2'-C3'
48	C	302	PLX	C3-O4-P1-O1
48	C	302	PLX	C3-O4-P1-O2
48	C	302	PLX	C3-O4-P1-O3
48	C	302	PLX	N1-C1-C2-O1
48	e	201	PLX	O7-C6-O6-C4
48	e	201	PLX	C2-O1-P1-O4
48	e	201	PLX	C2-O1-P1-O2
48	e	201	PLX	C2-O1-P1-O3
48	e	201	PLX	O9-C24-O8-C5
48	e	201	PLX	O9-C24-C25-C26
48	g	201	PLX	O7-C6-O6-C4
48	m	201	PLX	O7-C6-C7-C8
48	m	201	PLX	O7-C6-O6-C4
48	r	502	PLX	O7-C6-O6-C4
48	r	502	PLX	C5-C4-O6-C6
48	r	502	PLX	C3-O4-P1-O1
48	r	502	PLX	C3-O4-P1-O2
48	r	502	PLX	C2-O1-P1-O4
48	r	502	PLX	C2-O1-P1-O2
48	r	502	PLX	O9-C24-O8-C5
48	r	502	PLX	O9-C24-C25-C26
49	G	201	8Q1	O4-C1-S44-C43
49	G	201	8Q1	C6-C1-S44-C43
49	G	201	8Q1	C28-C29-C32-C34
49	G	201	8Q1	C28-C29-C32-O33
49	G	201	8Q1	C30-C29-C32-C34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
49	G	201	8Q1	C30-C29-C32-O33
49	G	201	8Q1	C31-C29-C32-C34
49	G	201	8Q1	C31-C29-C32-O33
49	G	201	8Q1	N36-C37-C38-C39
49	G	201	8Q1	C42-C43-S44-C1
49	G	201	8Q1	C28-O27-P24-O3
49	G	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C1-C6-C7-C8
49	X	201	8Q1	C28-C29-C32-C34
49	X	201	8Q1	C28-C29-C32-O33
49	X	201	8Q1	C30-C29-C32-C34
49	X	201	8Q1	C30-C29-C32-O33
49	X	201	8Q1	C31-C29-C32-C34
49	X	201	8Q1	C31-C29-C32-O33
49	X	201	8Q1	N36-C37-C38-C39
49	X	201	8Q1	C28-O27-P24-O2
49	X	201	8Q1	C28-O27-P24-O1
53	N	201	CDL	CA2-C1-CB2-OB2
53	N	201	CDL	CA2-OA2-PA1-OA3
53	N	201	CDL	CA2-OA2-PA1-OA4
53	N	201	CDL	CA2-OA2-PA1-OA5
53	N	201	CDL	CA3-OA5-PA1-OA2
53	N	201	CDL	CA3-OA5-PA1-OA3
53	N	201	CDL	CA3-OA5-PA1-OA4
53	N	201	CDL	C11-CA5-OA6-CA4
53	N	201	CDL	CB2-OB2-PB2-OB3
53	N	201	CDL	CB2-OB2-PB2-OB4
53	N	201	CDL	CB2-OB2-PB2-OB5
53	N	201	CDL	CB3-OB5-PB2-OB2
53	N	201	CDL	CB3-OB5-PB2-OB3
53	N	201	CDL	CB3-OB5-PB2-OB4
53	a	201	CDL	CA2-OA2-PA1-OA3
53	a	201	CDL	CA2-OA2-PA1-OA4
53	a	201	CDL	CA2-OA2-PA1-OA5
53	a	201	CDL	CA3-OA5-PA1-OA2
53	a	201	CDL	CA3-OA5-PA1-OA4
53	a	201	CDL	CB2-OB2-PB2-OB3
53	a	201	CDL	CB2-OB2-PB2-OB5
53	a	201	CDL	CB3-OB5-PB2-OB2
53	a	201	CDL	CB3-OB5-PB2-OB4
53	i	401	CDL	CA2-OA2-PA1-OA3
53	i	401	CDL	CA2-OA2-PA1-OA4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	i	401	CDL	CA2-OA2-PA1-OA5
53	i	401	CDL	CA3-OA5-PA1-OA2
53	i	401	CDL	CA3-OA5-PA1-OA3
53	i	401	CDL	CA3-OA5-PA1-OA4
53	i	401	CDL	CB2-OB2-PB2-OB4
53	i	401	CDL	CB2-OB2-PB2-OB5
53	l	701	CDL	CA2-OA2-PA1-OA3
53	l	701	CDL	CA2-OA2-PA1-OA4
53	l	701	CDL	CA2-OA2-PA1-OA5
53	l	701	CDL	CA3-OA5-PA1-OA2
53	l	701	CDL	CB2-OB2-PB2-OB3
53	l	701	CDL	CB2-OB2-PB2-OB4
53	l	701	CDL	CB2-OB2-PB2-OB5
53	l	701	CDL	OB6-CB4-CB6-OB8
53	r	503	CDL	O1-C1-CA2-OA2
53	r	503	CDL	O1-C1-CB2-OB2
53	r	503	CDL	CA2-C1-CB2-OB2
53	r	503	CDL	CA2-OA2-PA1-OA3
53	r	503	CDL	CB3-OB5-PB2-OB2
53	r	503	CDL	CB3-OB5-PB2-OB3
53	r	503	CDL	CB3-OB5-PB2-OB4
53	r	504	CDL	CB2-C1-CA2-OA2
53	r	504	CDL	CA3-OA5-PA1-OA2
53	r	504	CDL	CA3-OA5-PA1-OA4
53	r	504	CDL	CB3-OB5-PB2-OB2
53	r	504	CDL	CB3-OB5-PB2-OB3
54	i	402	PEE	C11-C10-O2-C2
54	i	402	PEE	C4-O4P-P-O3P
54	i	402	PEE	C4-O4P-P-O1P
54	l	702	PEE	C11-C10-O2-C2
54	l	702	PEE	C4-O4P-P-O3P
54	l	702	PEE	C4-O4P-P-O2P
54	l	702	PEE	C4-O4P-P-O1P
54	m	202	PEE	C11-C10-O2-C2
54	m	202	PEE	O4P-C4-C5-N
54	r	501	PEE	C4-O4P-P-O3P
54	r	501	PEE	C4-O4P-P-O1P
54	s	401	PEE	C11-C10-O2-C2
54	s	401	PEE	O4-C10-O2-C2
54	s	401	PEE	C1-O3P-P-O1P
54	s	401	PEE	C1-O3P-P-O4P
54	s	401	PEE	C4-O4P-P-O3P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	s	401	PEE	C4-O4P-P-O2P
54	s	401	PEE	C4-O4P-P-O1P
56	s	402	UQ	C7-C8-C9-C10
56	s	402	UQ	C7-C8-C9-C11
56	s	402	UQ	C12-C11-C9-C8
56	s	402	UQ	C12-C11-C9-C10
57	w	401	ADP	C5'-O5'-PA-O1A
57	w	401	ADP	C5'-O5'-PA-O2A
53	r	503	CDL	OA9-CA7-OA8-CA6
53	i	401	CDL	OA9-CA7-OA8-CA6
53	N	201	CDL	OA7-CA5-OA6-CA4
53	r	504	CDL	OB7-CB5-OB6-CB4
54	i	402	PEE	O4-C10-O2-C2
54	l	702	PEE	O4-C10-O2-C2
54	m	202	PEE	O4-C10-O2-C2
53	r	503	CDL	C31-CA7-OA8-CA6
53	r	504	CDL	C51-CB5-OB6-CB4
53	i	401	CDL	C31-CA7-OA8-CA6
53	r	504	CDL	C71-CB7-OB8-CB6
54	s	401	PEE	C17-C18-C19-C20
54	l	703	PEE	O5-C30-O3-C3
53	N	201	CDL	O1-C1-CB2-OB2
53	a	201	CDL	O1-C1-CB2-OB2
53	l	701	CDL	O1-C1-CB2-OB2
54	l	702	PEE	C31-C30-O3-C3
53	r	504	CDL	OB9-CB7-OB8-CB6
54	l	702	PEE	O5-C30-O3-C3
54	m	202	PEE	C15-C16-C17-C18
54	l	703	PEE	C31-C30-O3-C3
56	s	402	UQ	C9-C11-C12-C13
53	l	701	CDL	C71-CB7-OB8-CB6
54	m	202	PEE	C31-C30-O3-C3
48	e	201	PLX	C12-C13-C14-C15
53	l	701	CDL	C11-C12-C13-C14
54	l	703	PEE	C37-C38-C39-C40
54	r	501	PEE	C17-C18-C19-C20
48	g	201	PLX	C7-C8-C9-C10
53	l	701	CDL	OB9-CB7-OB8-CB6
54	m	202	PEE	O5-C30-O3-C3
53	a	201	CDL	CA2-C1-CB2-OB2
53	r	503	CDL	CB2-C1-CA2-OA2
53	a	201	CDL	C71-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	r	503	CDL	C32-C33-C34-C35
53	r	503	CDL	C55-C56-C57-C58
48	r	502	PLX	C9-C10-C11-C12
48	r	502	PLX	C30-C31-C32-C33
53	i	401	CDL	C31-C32-C33-C34
53	r	503	CDL	C62-C63-C64-C65
48	m	201	PLX	C28-C29-C30-C31
53	l	701	CDL	C59-C60-C61-C62
53	r	503	CDL	C20-C21-C22-C23
53	l	701	CDL	CB7-C71-C72-C73
53	a	201	CDL	OA5-CA3-CA4-OA6
54	l	702	PEE	O3P-C1-C2-O2
53	l	701	CDL	OA6-CA4-CA6-OA8
53	r	504	CDL	OA6-CA4-CA6-OA8
54	Q	501	PEE	C37-C38-C39-C40
54	i	402	PEE	C17-C18-C19-C20
53	a	201	CDL	OB9-CB7-OB8-CB6
53	l	701	CDL	C35-C36-C37-C38
53	l	701	CDL	CB5-C51-C52-C53
48	m	201	PLX	C15-C16-C17-C18
48	g	201	PLX	C12-C13-C14-C15
53	l	701	CDL	C54-C55-C56-C57
53	i	401	CDL	CA7-C31-C32-C33
53	r	503	CDL	CA7-C31-C32-C33
53	r	503	CDL	CB5-C51-C52-C53
53	r	504	CDL	CA7-C31-C32-C33
53	r	504	CDL	CB7-C71-C72-C73
54	Q	501	PEE	C30-C31-C32-C33
53	r	503	CDL	CB7-C71-C72-C73
54	r	501	PEE	C10-C11-C12-C13
53	a	201	CDL	O1-C1-CA2-OA2
53	i	401	CDL	O1-C1-CA2-OA2
54	s	401	PEE	C31-C30-O3-C3
54	l	702	PEE	C37-C38-C39-C40
53	r	504	CDL	C74-C75-C76-C77
50	J	401	NDP	C2D-C1D-N1N-C6N
53	a	201	CDL	CB2-C1-CA2-OA2
53	i	401	CDL	CB2-C1-CA2-OA2
53	r	503	CDL	C71-CB7-OB8-CB6
48	m	201	PLX	C34-C35-C36-C37
56	s	402	UQ	C17-C18-C19-C20
48	m	201	PLX	O6-C6-C7-C8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	r	501	PEE	C11-C10-O2-C2
54	r	501	PEE	O4-C10-O2-C2
53	r	504	CDL	O1-C1-CA2-OA2
54	m	202	PEE	C31-C32-C33-C34
48	C	302	PLX	C28-C29-C30-C31
53	l	701	CDL	C71-C72-C73-C74
48	m	201	PLX	C32-C33-C34-C35
53	i	401	CDL	C37-C38-C39-C40
53	a	201	CDL	CB5-C51-C52-C53
48	g	201	PLX	C27-C28-C29-C30
53	l	701	CDL	C60-C61-C62-C63
48	g	201	PLX	C10-C11-C12-C13
48	g	201	PLX	C33-C34-C35-C36
48	m	201	PLX	C10-C11-C12-C13
48	r	502	PLX	C27-C28-C29-C30
49	X	201	8Q1	C9-C10-C11-C12
53	i	401	CDL	C52-C53-C54-C55
53	r	503	CDL	C73-C74-C75-C76
53	r	504	CDL	C14-C15-C16-C17
53	r	504	CDL	C56-C57-C58-C59
53	r	503	CDL	C75-C76-C77-C78
53	r	504	CDL	C12-C13-C14-C15
54	m	202	PEE	C12-C13-C14-C15
54	s	401	PEE	O5-C30-O3-C3
48	C	302	PLX	O7-C6-C7-C8
48	m	201	PLX	O9-C24-C25-C26
48	r	502	PLX	C12-C13-C14-C15
53	r	504	CDL	C71-C72-C73-C74
54	l	703	PEE	C33-C34-C35-C36
53	i	401	CDL	C11-C12-C13-C14
53	l	701	CDL	C73-C74-C75-C76
48	m	201	PLX	C27-C28-C29-C30
48	C	302	PLX	C17-C18-C19-C20
53	r	503	CDL	C71-C72-C73-C74
53	r	504	CDL	CB5-C51-C52-C53
48	g	201	PLX	C32-C33-C34-C35
53	l	701	CDL	C75-C76-C77-C78
53	r	503	CDL	C74-C75-C76-C77
53	r	503	CDL	C82-C83-C84-C85
54	i	402	PEE	C22-C23-C24-C25
54	l	703	PEE	C14-C15-C16-C17
53	r	503	CDL	OB9-CB7-OB8-CB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	701	CDL	C37-C38-C39-C40
48	m	201	PLX	C12-C13-C14-C15
53	l	701	CDL	C56-C57-C58-C59
53	i	401	CDL	C71-CB7-OB8-CB6
48	e	201	PLX	C14-C15-C16-C17
48	m	201	PLX	C7-C8-C9-C10
48	r	502	PLX	C15-C16-C17-C18
53	r	504	CDL	C73-C74-C75-C76
53	N	201	CDL	CA7-C31-C32-C33
53	a	201	CDL	C71-C72-C73-C74
53	l	701	CDL	C55-C56-C57-C58
54	l	703	PEE	C31-C32-C33-C34
48	C	302	PLX	C7-C8-C9-C10
54	l	702	PEE	C23-C24-C25-C26
48	e	201	PLX	C25-C26-C27-C28
53	r	504	CDL	C55-C56-C57-C58
54	i	402	PEE	C14-C15-C16-C17
54	l	703	PEE	C11-C10-O2-C2
54	Q	501	PEE	C15-C16-C17-C18
54	s	401	PEE	C37-C38-C39-C40
48	e	201	PLX	C30-C31-C32-C33
54	Q	501	PEE	C33-C34-C35-C36
53	a	201	CDL	C75-C76-C77-C78
53	i	401	CDL	CB5-C51-C52-C53
54	r	501	PEE	C30-C31-C32-C33
53	a	201	CDL	C37-C38-C39-C40
54	r	501	PEE	C41-C42-C43-C44
48	e	201	PLX	C11-C12-C13-C14
53	l	701	CDL	C40-C41-C42-C43
48	e	201	PLX	C28-C29-C30-C31
48	g	201	PLX	C25-C26-C27-C28
48	g	201	PLX	C30-C31-C32-C33
53	i	401	CDL	C35-C36-C37-C38
53	N	201	CDL	C71-CB7-OB8-CB6
48	e	201	PLX	C13-C14-C15-C16
48	g	201	PLX	C9-C10-C11-C12
53	i	401	CDL	C14-C15-C16-C17
53	r	504	CDL	C41-C42-C43-C44
54	Q	501	PEE	C34-C35-C36-C37
48	g	201	PLX	C11-C10-C9-C8
48	C	302	PLX	C13-C14-C15-C16
48	e	201	PLX	C27-C28-C29-C30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	m	201	PLX	C9-C10-C11-C12
53	r	504	CDL	C52-C53-C54-C55
53	a	201	CDL	C31-C32-C33-C34
53	N	201	CDL	C51-CB5-OB6-CB4
53	a	201	CDL	C51-CB5-OB6-CB4
53	r	503	CDL	C11-CA5-OA6-CA4
53	i	401	CDL	CB7-C71-C72-C73
54	s	401	PEE	C43-C44-C45-C46
54	i	402	PEE	C19-C20-C21-C22
56	s	402	UQ	C12-C13-C14-C15
48	e	201	PLX	C29-C30-C31-C32
53	N	201	CDL	C11-C12-C13-C14
53	i	401	CDL	C71-C72-C73-C74
48	e	201	PLX	C2-C1-N1-C1C
48	e	201	PLX	C2-C1-N1-C1A
48	r	502	PLX	C28-C29-C30-C31
54	r	501	PEE	C22-C23-C24-C25
53	r	503	CDL	C14-C15-C16-C17
53	r	504	CDL	C43-C44-C45-C46
56	s	402	UQ	C17-C18-C19-C21
48	m	201	PLX	C14-C15-C16-C17
53	i	401	CDL	OB9-CB7-OB8-CB6
53	N	201	CDL	OB7-CB5-OB6-CB4
53	a	201	CDL	OB7-CB5-OB6-CB4
48	C	302	PLX	O4-C3-C4-O6
53	r	503	CDL	C36-C37-C38-C39
48	r	502	PLX	C16-C17-C18-C19
53	a	201	CDL	C21-C22-C23-C24
53	r	503	CDL	C35-C36-C37-C38
54	Q	501	PEE	C21-C22-C23-C24
53	N	201	CDL	CB7-C71-C72-C73
54	i	402	PEE	C35-C36-C37-C38
48	m	201	PLX	C25-C26-C27-C28
53	r	503	CDL	C56-C57-C58-C59
48	C	302	PLX	C31-C32-C33-C34
54	s	401	PEE	C36-C37-C38-C39
48	C	302	PLX	C33-C34-C35-C36
48	g	201	PLX	C28-C29-C30-C31
53	r	504	CDL	C59-C60-C61-C62
53	r	503	CDL	OA7-CA5-OA6-CA4
54	l	703	PEE	O4-C10-O2-C2
53	l	701	CDL	C14-C15-C16-C17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	Q	501	PEE	C20-C21-C22-C23
48	C	302	PLX	C11-C12-C13-C14
53	r	504	CDL	C32-C33-C34-C35
53	r	504	CDL	C75-C76-C77-C78
53	r	503	CDL	C42-C43-C44-C45
48	e	201	PLX	C31-C32-C33-C34
53	l	701	CDL	C52-C53-C54-C55
54	i	402	PEE	C21-C22-C23-C24
54	r	501	PEE	C19-C20-C21-C22
53	N	201	CDL	OB9-CB7-OB8-CB6
48	e	201	PLX	C16-C17-C18-C19
48	r	502	PLX	C13-C14-C15-C16
48	C	302	PLX	O4-C3-C4-C5
53	a	201	CDL	OA5-CA3-CA4-CA6
53	a	201	CDL	OB5-CB3-CB4-CB6
54	l	702	PEE	O3P-C1-C2-C3
54	r	501	PEE	C11-C12-C13-C14
53	r	504	CDL	C78-C79-C80-C81
53	a	201	CDL	CA7-C31-C32-C33
54	l	702	PEE	C30-C31-C32-C33
48	r	502	PLX	C33-C34-C35-C36
48	r	502	PLX	C31-C32-C33-C34
53	l	701	CDL	C58-C59-C60-C61
53	l	701	CDL	CA3-CA4-CA6-OA8
53	l	701	CDL	CB3-CB4-CB6-OB8
53	r	504	CDL	CA3-CA4-CA6-OA8
54	r	501	PEE	C1-C2-C3-O3
53	r	504	CDL	C17-C18-C19-C20
48	e	201	PLX	C10-C11-C12-C13
53	N	201	CDL	C31-CA7-OA8-CA6
48	e	201	PLX	C2-C1-N1-C1B
54	s	401	PEE	C23-C24-C25-C26
48	e	201	PLX	C33-C34-C35-C36
54	Q	501	PEE	C13-C14-C15-C16
49	X	201	8Q1	C28-O27-P24-O3
48	r	502	PLX	C10-C11-C12-C13
53	l	701	CDL	C72-C73-C74-C75
54	Q	501	PEE	C14-C15-C16-C17
54	s	401	PEE	C21-C22-C23-C24
53	N	201	CDL	CA6-CA4-OA6-CA5
53	l	701	CDL	C39-C40-C41-C42
53	l	701	CDL	C62-C63-C64-C65

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
54	Q	501	PEE	C17-C18-C19-C20
54	m	202	PEE	C14-C15-C16-C17
53	r	504	CDL	C62-C63-C64-C65
53	N	201	CDL	C51-C52-C53-C54
53	r	503	CDL	C60-C61-C62-C63
54	l	703	PEE	C22-C23-C24-C25
53	i	401	CDL	OB6-CB4-CB6-OB8
54	l	702	PEE	O2-C2-C3-O3
53	l	701	CDL	C64-C65-C66-C67
54	r	501	PEE	C31-C30-O3-C3
53	r	503	CDL	C39-C40-C41-C42
48	r	502	PLX	C14-C15-C16-C17
48	r	502	PLX	C7-C8-C9-C10
53	N	201	CDL	C31-C32-C33-C34
53	a	201	CDL	C43-C44-C45-C46
53	i	401	CDL	C36-C37-C38-C39
54	l	702	PEE	C31-C32-C33-C34
53	r	504	CDL	C60-C61-C62-C63
53	i	401	CDL	C33-C34-C35-C36
54	Q	501	PEE	C10-C11-C12-C13
53	i	401	CDL	C73-C74-C75-C76
53	r	504	CDL	C13-C14-C15-C16
54	r	501	PEE	C36-C37-C38-C39
48	C	302	PLX	C27-C28-C29-C30
53	a	201	CDL	C14-C15-C16-C17
48	e	201	PLX	C7-C8-C9-C10
53	r	503	CDL	C37-C38-C39-C40
54	i	402	PEE	C24-C25-C26-C27
53	N	201	CDL	OB5-CB3-CB4-CB6
53	l	701	CDL	OA5-CA3-CA4-CA6
53	r	503	CDL	OA5-CA3-CA4-CA6
53	a	201	CDL	C34-C35-C36-C37
54	r	501	PEE	C23-C24-C25-C26
54	Q	501	PEE	C44-C45-C46-C47
48	C	302	PLX	C15-C16-C17-C18
54	l	703	PEE	C10-C11-C12-C13
48	g	201	PLX	C14-C15-C16-C17
54	r	501	PEE	C24-C25-C26-C27
53	r	504	CDL	C42-C43-C44-C45
54	l	703	PEE	C13-C14-C15-C16
53	N	201	CDL	OA9-CA7-OA8-CA6
53	r	504	CDL	C23-C24-C25-C26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	e	201	PLX	C36-C37-C38-C39
48	C	302	PLX	C9-C10-C11-C12
48	r	502	PLX	C3-C4-C5-O8
49	X	201	8Q1	O33-C32-C34-N36
53	r	504	CDL	CB3-CB4-CB6-OB8
54	i	402	PEE	C1-C2-C3-O3
54	l	703	PEE	C1-C2-C3-O3
53	a	201	CDL	C60-C61-C62-C63
53	a	201	CDL	C52-C53-C54-C55
48	e	201	PLX	C9-C10-C11-C12
53	r	504	CDL	C35-C36-C37-C38
53	a	201	CDL	OB5-CB3-CB4-OB6
53	l	701	CDL	OA5-CA3-CA4-OA6
53	r	503	CDL	OA5-CA3-CA4-OA6
53	r	504	CDL	C79-C80-C81-C82
48	m	201	PLX	C26-C27-C28-C29
53	r	503	CDL	C54-C55-C56-C57
53	r	503	CDL	C61-C62-C63-C64
54	r	501	PEE	C20-C21-C22-C23
49	X	201	8Q1	O4-C1-S44-C43
54	l	703	PEE	C32-C33-C34-C35
48	e	201	PLX	O6-C4-C5-O8
53	r	504	CDL	OB6-CB4-CB6-OB8
54	l	703	PEE	O2-C2-C3-O3
54	r	501	PEE	O2-C2-C3-O3
48	r	502	PLX	C11-C12-C13-C14
54	l	703	PEE	C30-C31-C32-C33
53	a	201	CDL	C33-C34-C35-C36
54	i	402	PEE	C13-C14-C15-C16
54	r	501	PEE	C16-C17-C18-C19
54	Q	501	PEE	C31-C30-O3-C3
48	m	201	PLX	C33-C34-C35-C36
53	r	503	CDL	C78-C79-C80-C81
53	r	504	CDL	C64-C65-C66-C67
53	l	701	CDL	C57-C58-C59-C60
53	i	401	CDL	C32-C33-C34-C35
48	g	201	PLX	C20-C21-C22-C23
54	s	401	PEE	C44-C45-C46-C47
54	l	702	PEE	C32-C33-C34-C35
49	X	201	8Q1	C6-C1-S44-C43
53	l	701	CDL	CA2-C1-CB2-OB2
48	C	302	PLX	C16-C17-C18-C19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
48	m	201	PLX	O4-C3-C4-C5
54	s	401	PEE	C38-C39-C40-C41
53	a	201	CDL	C74-C75-C76-C77
48	r	502	PLX	C20-C21-C22-C23
49	G	201	8Q1	C10-C11-C12-C13
53	r	504	CDL	C72-C73-C74-C75
54	r	501	PEE	O5-C30-O3-C3
53	l	701	CDL	C12-C13-C14-C15
49	X	201	8Q1	C7-C8-C9-C10
48	g	201	PLX	O4-C3-C4-O6
48	m	201	PLX	O4-C3-C4-O6
48	e	201	PLX	C3-C4-C5-O8
48	r	502	PLX	O6-C4-C5-O8
53	r	503	CDL	OB6-CB4-CB6-OB8
54	i	402	PEE	O2-C2-C3-O3
53	r	504	CDL	C82-C83-C84-C85
48	m	201	PLX	C7-C6-O6-C4
54	Q	501	PEE	O5-C30-O3-C3
49	G	201	8Q1	C7-C8-C9-C10
49	G	201	8Q1	C11-C10-C9-C8
54	Q	501	PEE	C42-C43-C44-C45
54	Q	501	PEE	C35-C36-C37-C38
54	r	501	PEE	C15-C16-C17-C18
54	l	703	PEE	C16-C17-C18-C19
53	a	201	CDL	C72-C73-C74-C75
53	l	701	CDL	C76-C77-C78-C79
48	g	201	PLX	C25-C24-O8-C5
48	m	201	PLX	C25-C24-O8-C5
48	m	201	PLX	C13-C14-C15-C16
53	a	201	CDL	C20-C21-C22-C23
54	i	402	PEE	C20-C21-C22-C23
54	i	402	PEE	C18-C19-C20-C21
53	a	201	CDL	C54-C55-C56-C57
50	J	401	NDP	O4D-C1D-N1N-C6N
48	g	201	PLX	O4-C3-C4-C5
53	r	503	CDL	C51-C52-C53-C54
48	m	201	PLX	C31-C32-C33-C34
48	C	302	PLX	C29-C30-C31-C32
54	i	402	PEE	C11-C12-C13-C14
53	r	504	CDL	C37-C38-C39-C40
48	e	201	PLX	O8-C24-C25-C26
53	N	201	CDL	OB5-CB3-CB4-OB6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	i	401	CDL	OA5-CA3-CA4-OA6
54	r	501	PEE	O3P-C1-C2-O2
48	m	201	PLX	C19-C20-C21-C22
54	Q	501	PEE	C23-C24-C25-C26
54	l	702	PEE	C21-C22-C23-C24
54	l	703	PEE	C18-C19-C20-C21
48	C	302	PLX	C30-C31-C32-C33
53	a	201	CDL	C73-C74-C75-C76
48	m	201	PLX	O6-C4-C5-O8
53	a	201	CDL	OA6-CA4-CA6-OA8
54	m	202	PEE	C22-C23-C24-C25
48	m	201	PLX	C3-C4-C5-O8
53	a	201	CDL	CA3-CA4-CA6-OA8
53	i	401	CDL	CB3-CB4-CB6-OB8
54	r	501	PEE	C31-C32-C33-C34
54	l	702	PEE	C14-C15-C16-C17
54	l	703	PEE	C34-C35-C36-C37
54	l	703	PEE	C38-C39-C40-C41
54	r	501	PEE	C33-C34-C35-C36
53	N	201	CDL	C71-C72-C73-C74
47	A	503	NAI	C5B-O5B-PA-O1A
47	A	503	NAI	C5B-O5B-PA-O2A
47	A	503	NAI	C5B-O5B-PA-O3
48	C	302	PLX	C2-O1-P1-O4
48	C	302	PLX	C2-O1-P1-O3
48	g	201	PLX	C3-O4-P1-O2
48	g	201	PLX	C2-O1-P1-O2
48	r	502	PLX	C2-O1-P1-O3
53	a	201	CDL	CB2-OB2-PB2-OB4
53	a	201	CDL	CB3-OB5-PB2-OB3
53	i	401	CDL	CB2-OB2-PB2-OB3
53	i	401	CDL	CB3-OB5-PB2-OB3
53	l	701	CDL	CB3-OB5-PB2-OB2
53	l	701	CDL	CB3-OB5-PB2-OB3
53	l	701	CDL	CB3-OB5-PB2-OB4
53	r	503	CDL	CA2-OA2-PA1-OA5
53	r	503	CDL	CB2-OB2-PB2-OB3
53	r	503	CDL	CB2-OB2-PB2-OB5
53	r	504	CDL	CA2-OA2-PA1-OA3
53	r	504	CDL	CA2-OA2-PA1-OA5
53	r	504	CDL	CA3-OA5-PA1-OA3
53	r	504	CDL	CB2-OB2-PB2-OB3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	r	504	CDL	CB2-OB2-PB2-OB4
53	r	504	CDL	CB2-OB2-PB2-OB5
54	m	202	PEE	C4-O4P-P-O3P
54	m	202	PEE	C4-O4P-P-O2P
54	m	202	PEE	C4-O4P-P-O1P
54	r	501	PEE	C1-O3P-P-O2P
54	r	501	PEE	C1-O3P-P-O1P
54	r	501	PEE	C1-O3P-P-O4P
54	s	401	PEE	C1-O3P-P-O2P
57	w	401	ADP	C5'-O5'-PA-O3A
53	l	701	CDL	C15-C16-C17-C18
54	i	402	PEE	C10-C11-C12-C13
53	r	504	CDL	CB4-CB3-OB5-PB2
53	l	701	CDL	C44-C45-C46-C47
54	s	401	PEE	C40-C41-C42-C43
53	r	504	CDL	C33-C34-C35-C36
53	r	504	CDL	C44-C45-C46-C47
54	Q	501	PEE	O3P-C1-C2-C3
54	r	501	PEE	O3P-C1-C2-C3
53	a	201	CDL	CA5-C11-C12-C13
54	Q	501	PEE	O3P-C1-C2-O2
48	e	201	PLX	C26-C27-C28-C29
53	l	701	CDL	C34-C35-C36-C37
49	X	201	8Q1	C13-C14-C15-C16
54	s	401	PEE	C32-C33-C34-C35
53	r	503	CDL	C33-C34-C35-C36
54	l	702	PEE	C1-C2-C3-O3
50	J	401	NDP	PN-O3-PA-O1A
53	a	201	CDL	C22-C23-C24-C25
48	r	502	PLX	C4-C5-O8-C24
48	g	201	PLX	C35-C36-C37-C38
48	g	201	PLX	O8-C24-C25-C26
54	s	401	PEE	C12-C13-C14-C15
53	r	504	CDL	C31-CA7-OA8-CA6
48	r	502	PLX	C29-C30-C31-C32
54	s	401	PEE	C24-C25-C26-C27
53	l	701	CDL	C41-C42-C43-C44
47	A	503	NAI	C2D-C1D-N1N-C2N
54	l	703	PEE	C23-C24-C25-C26
47	A	503	NAI	O4D-C1D-N1N-C2N
54	i	402	PEE	C31-C32-C33-C34
53	l	701	CDL	C53-C54-C55-C56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	r	504	CDL	CA5-C11-C12-C13
48	g	201	PLX	C13-C14-C15-C16
48	r	502	PLX	C18-C19-C20-C21
54	i	402	PEE	C34-C35-C36-C37
54	r	501	PEE	C12-C13-C14-C15
53	r	503	CDL	C52-C53-C54-C55
53	r	504	CDL	C51-C52-C53-C54
53	l	701	CDL	C24-C25-C26-C27
53	r	504	CDL	C20-C21-C22-C23
54	i	402	PEE	C32-C33-C34-C35
48	C	302	PLX	C12-C13-C14-C15
53	r	504	CDL	OA9-CA7-OA8-CA6
48	r	502	PLX	O8-C24-C25-C26
46	A	502	FMN	O2'-C2'-C3'-C4'
57	w	401	ADP	PB-O3A-PA-O2A
48	m	201	PLX	C18-C19-C20-C21
53	r	503	CDL	C19-C20-C21-C22
53	r	503	CDL	CB3-CB4-CB6-OB8
54	m	202	PEE	C11-C12-C13-C14
48	g	201	PLX	O9-C24-C25-C26
48	m	201	PLX	C30-C31-C32-C33
53	i	401	CDL	OA5-CA3-CA4-CA6
48	m	201	PLX	C35-C36-C37-C38
54	m	202	PEE	C16-C17-C18-C19
48	C	302	PLX	C26-C27-C28-C29
53	a	201	CDL	C56-C57-C58-C59
49	G	201	8Q1	C28-O27-P24-O1
54	Q	501	PEE	C18-C19-C20-C21
54	s	401	PEE	C10-C11-C12-C13
54	l	702	PEE	C16-C17-C18-C19
54	Q	501	PEE	C19-C20-C21-C22
54	Q	501	PEE	C16-C17-C18-C19
54	i	402	PEE	C38-C39-C40-C41
54	m	202	PEE	C18-C19-C20-C21
47	A	503	NAI	C2D-C1D-N1N-C6N
50	J	401	NDP	O4D-C4D-C5D-O5D
53	r	503	CDL	C58-C59-C60-C61
54	r	501	PEE	C44-C45-C46-C47
48	C	302	PLX	C25-C26-C27-C28
53	a	201	CDL	C36-C37-C38-C39
54	l	702	PEE	C15-C16-C17-C18
54	i	402	PEE	C36-C37-C38-C39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	i	401	CDL	C15-C16-C17-C18
53	r	504	CDL	C83-C84-C85-C86
54	l	702	PEE	C36-C37-C38-C39
53	a	201	CDL	OA7-CA5-OA6-CA4
53	l	701	CDL	C33-C34-C35-C36
54	s	401	PEE	O2-C10-C11-C12
54	s	401	PEE	O3-C30-C31-C32
48	e	201	PLX	C24-C25-C26-C27
49	G	201	8Q1	C9-C10-C11-C12
53	r	503	CDL	C72-C71-CB7-OB8
53	a	201	CDL	C11-CA5-OA6-CA4
49	X	201	8Q1	C29-C32-C34-O35
48	C	302	PLX	C32-C33-C34-C35
53	a	201	CDL	C76-C77-C78-C79
50	J	401	NDP	C2B-O2B-P2B-O3X
53	l	701	CDL	C31-C32-C33-C34
53	r	503	CDL	C83-C84-C85-C86
54	s	401	PEE	C34-C35-C36-C37
54	m	202	PEE	C1-C2-C3-O3
53	N	201	CDL	C72-C71-CB7-OB8
53	l	701	CDL	C32-C31-CA7-OA8
53	r	503	CDL	C12-C11-CA5-OA6
53	a	201	CDL	C18-C19-C20-C21
53	r	504	CDL	C39-C40-C41-C42
49	X	201	8Q1	C29-C32-C34-N36
48	C	302	PLX	C34-C35-C36-C37
56	s	402	UQ	C14-C16-C17-C18
50	J	401	NDP	C2B-O2B-P2B-O1X
54	s	401	PEE	O4-C10-C11-C12
53	l	701	CDL	C12-C11-CA5-OA6
54	Q	501	PEE	C22-C23-C24-C25
53	r	504	CDL	C52-C51-CB5-OB6
53	r	503	CDL	C72-C71-CB7-OB9
54	i	402	PEE	C30-C31-C32-C33
54	s	401	PEE	O5-C30-C31-C32
48	g	201	PLX	O9-C24-O8-C5
48	m	201	PLX	O9-C24-O8-C5
48	C	302	PLX	C18-C19-C20-C21
53	N	201	CDL	C72-C71-CB7-OB9
53	i	401	CDL	C12-C13-C14-C15
53	i	401	CDL	CA3-CA4-CA6-OA8
53	r	503	CDL	C44-C45-C46-C47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
53	l	701	CDL	C32-C31-CA7-OA9
53	r	503	CDL	C81-C82-C83-C84
53	r	503	CDL	C12-C11-CA5-OA7
47	A	503	NAI	O4D-C1D-N1N-C6N
54	Q	501	PEE	C38-C39-C40-C41

There are no ring outliers.

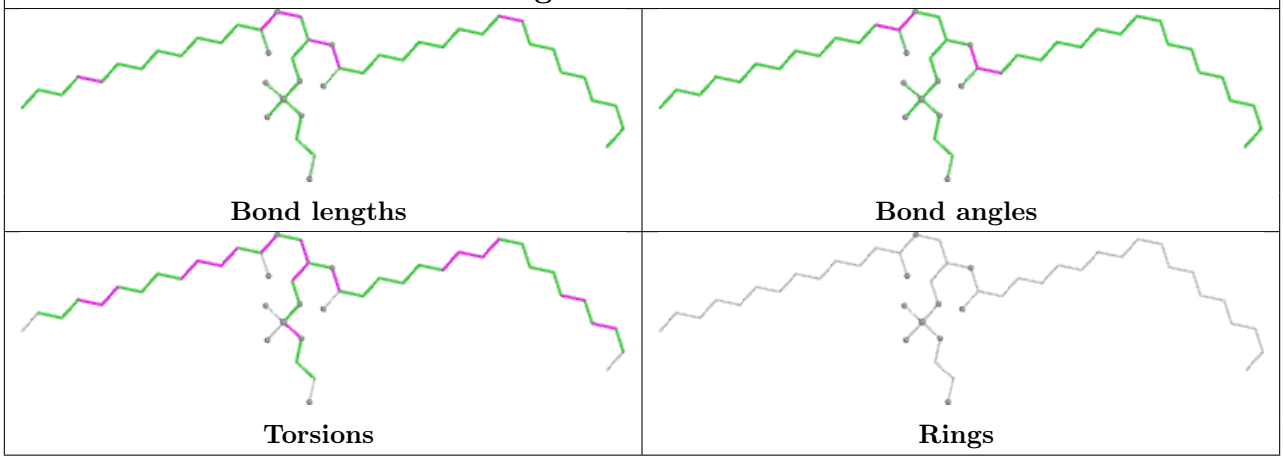
27 monomers are involved in 97 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	l	702	PEE	2	0
54	l	703	PEE	4	0
48	g	201	PLX	5	0
49	X	201	8Q1	3	0
54	Q	501	PEE	1	0
50	J	401	NDP	2	0
45	C	301	SF4	1	0
54	r	501	PEE	6	0
45	A	501	SF4	1	0
54	i	402	PEE	5	0
53	a	201	CDL	8	0
54	s	401	PEE	4	0
47	A	503	NAI	4	0
53	l	701	CDL	5	0
51	O	301	FES	1	0
56	s	402	UQ	4	0
48	m	201	PLX	4	0
57	w	401	ADP	1	0
54	m	202	PEE	2	0
49	G	201	8Q1	2	0
46	A	502	FMN	2	0
53	r	504	CDL	6	0
48	C	302	PLX	5	0
53	i	401	CDL	4	0
53	r	503	CDL	11	0
48	r	502	PLX	7	0
48	e	201	PLX	1	0

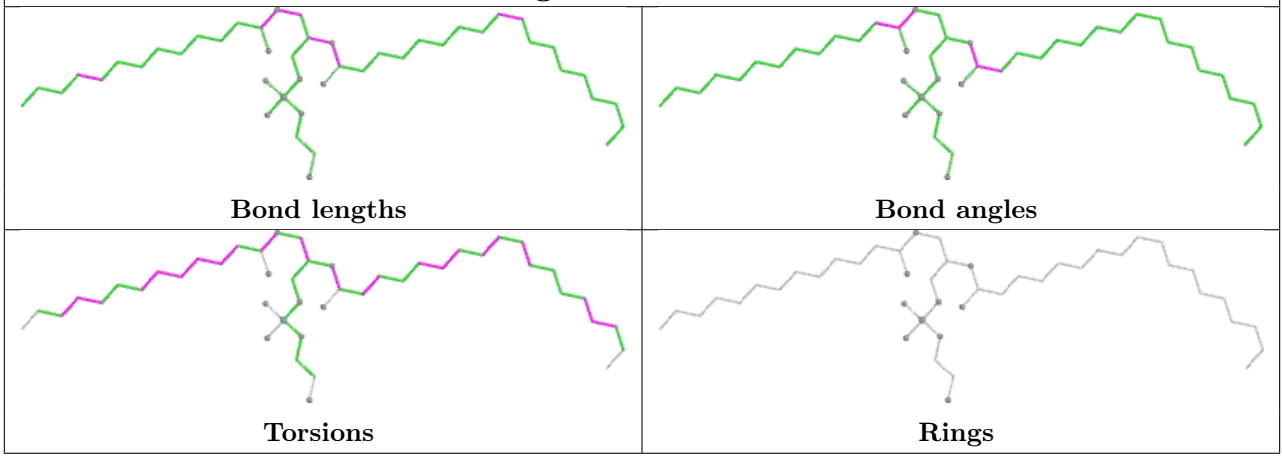
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is

within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

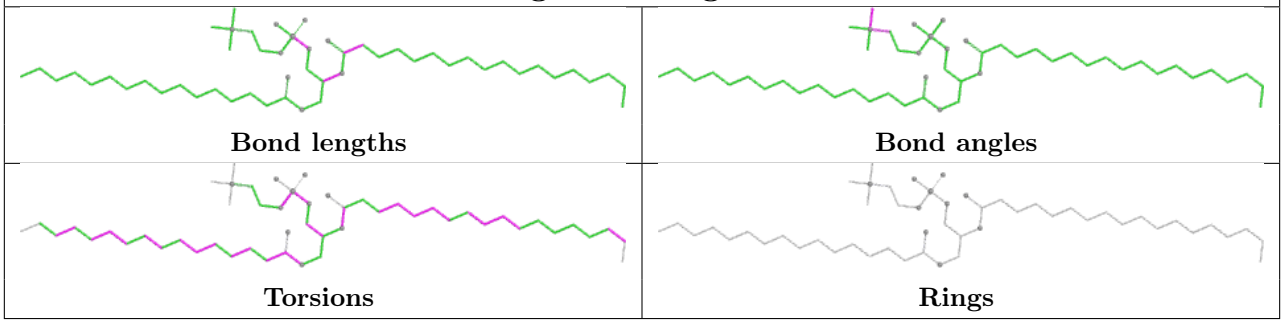
Ligand PEE l 702



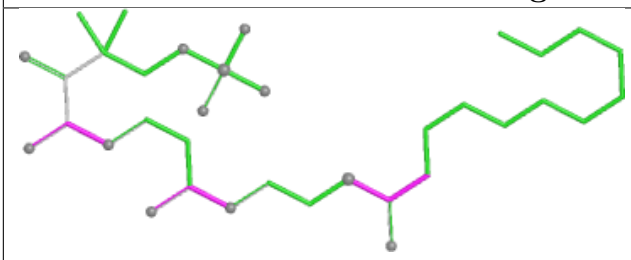
Ligand PEE l 703



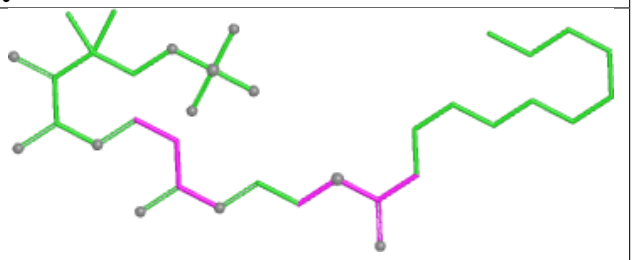
Ligand PLX g 201



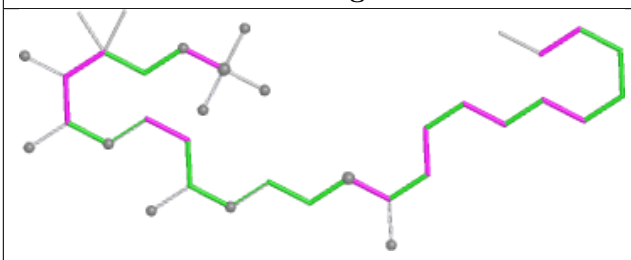
Ligand 8Q1 X 201



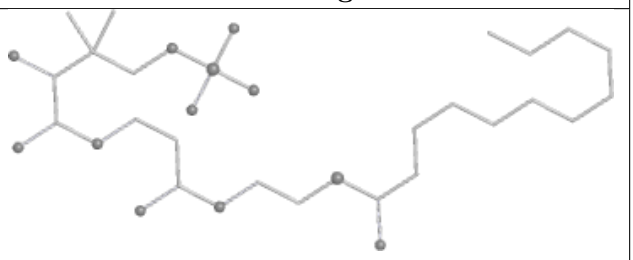
Bond lengths



Bond angles



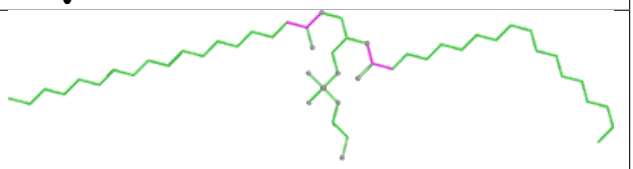
Torsions



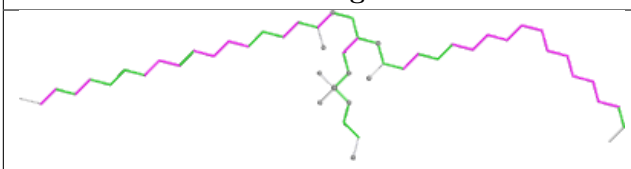
Rings

Ligand PEE Q 501

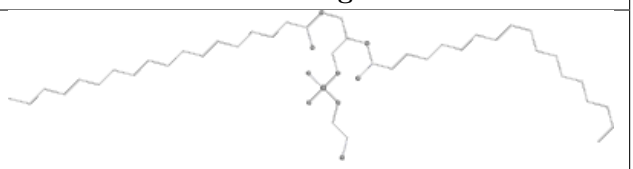
Bond lengths



Bond angles

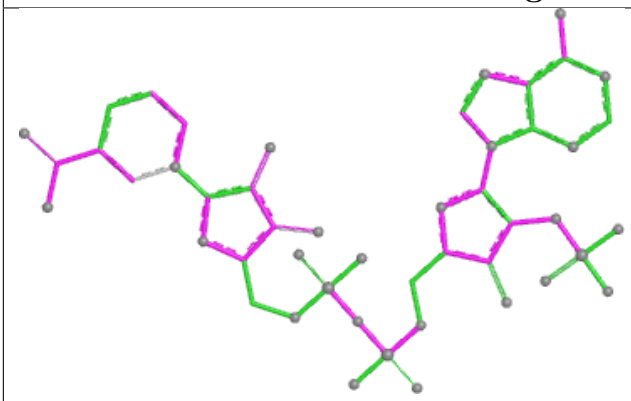


Torsions

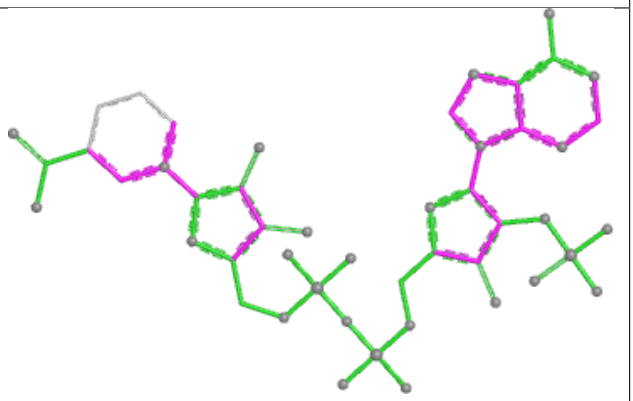


Rings

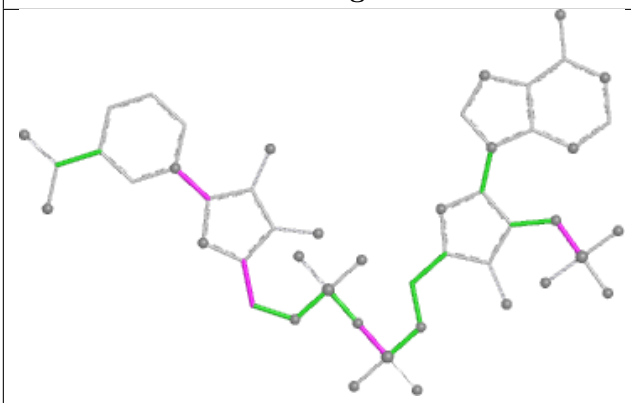
Ligand NDP J 401



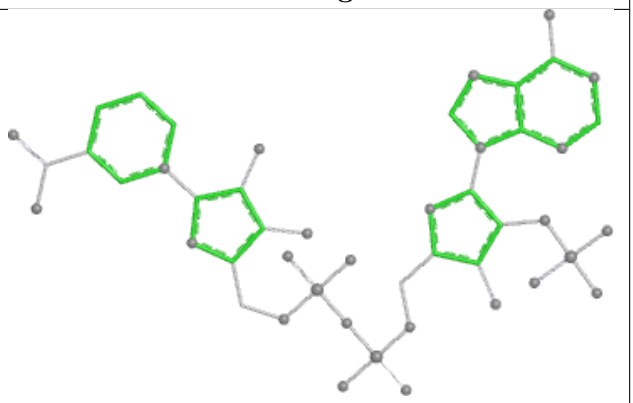
Bond lengths



Bond angles



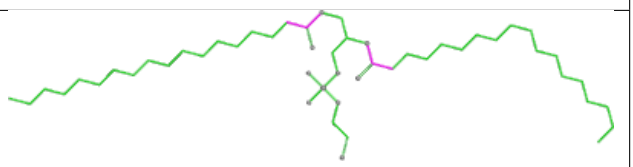
Torsions



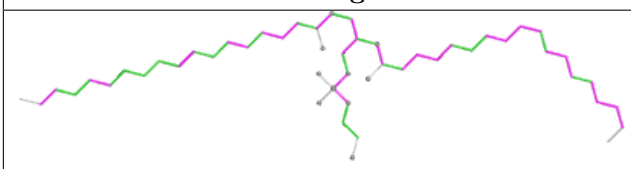
Rings

Ligand PEE r 501

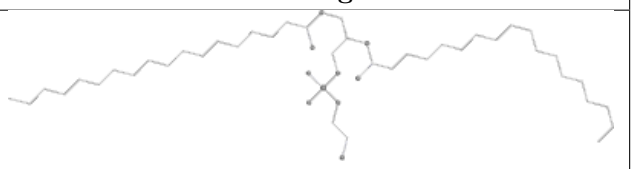
Bond lengths



Bond angles

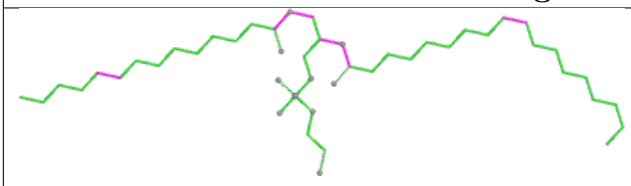


Torsions

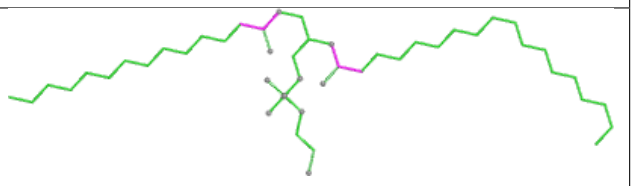


Rings

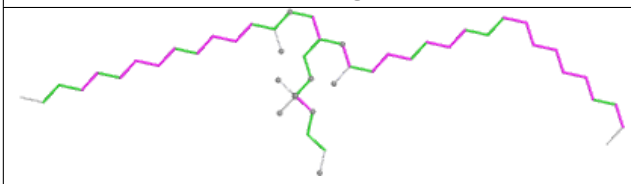
Ligand PEE i 402



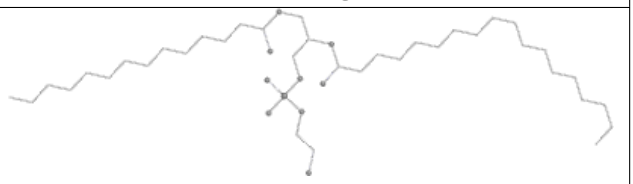
Bond lengths



Bond angles

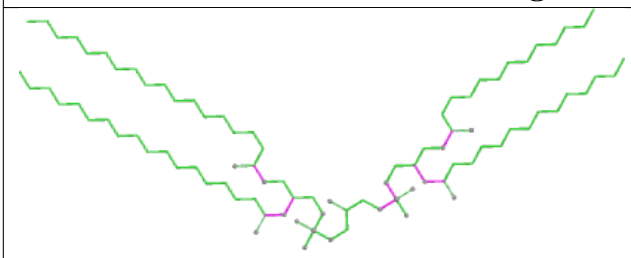


Torsions

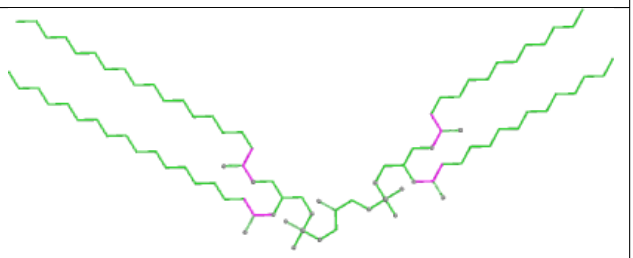


Rings

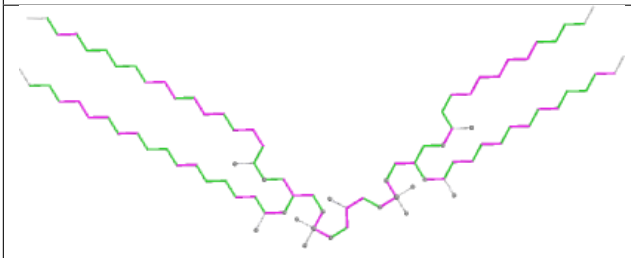
Ligand CDL a 201



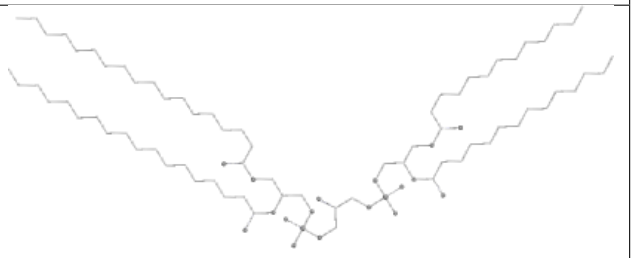
Bond lengths



Bond angles



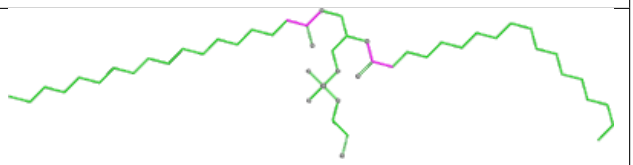
Torsions



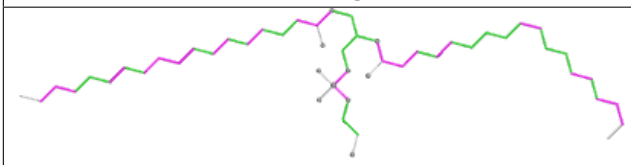
Rings

Ligand PEE s 401

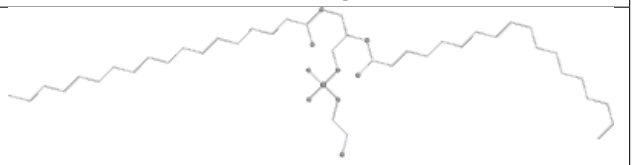
Bond lengths



Bond angles

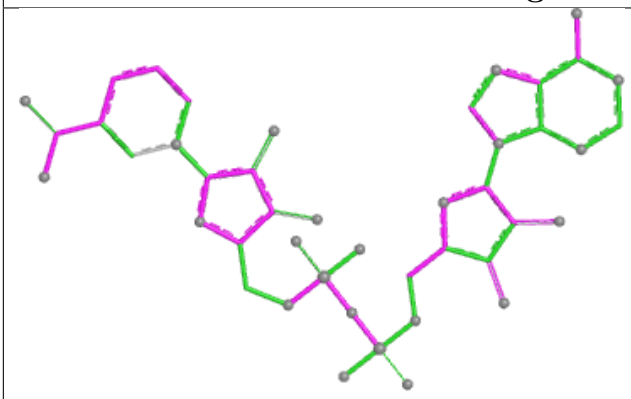


Torsions

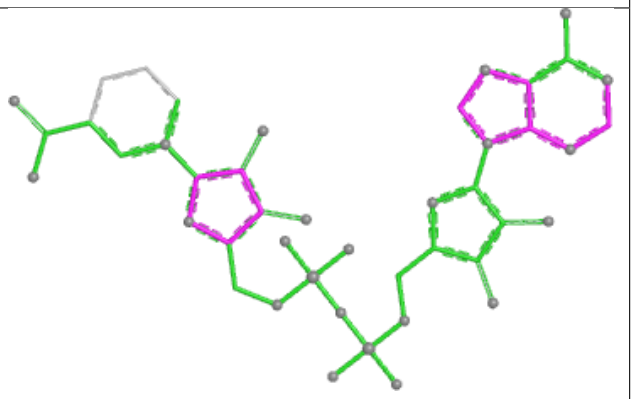


Rings

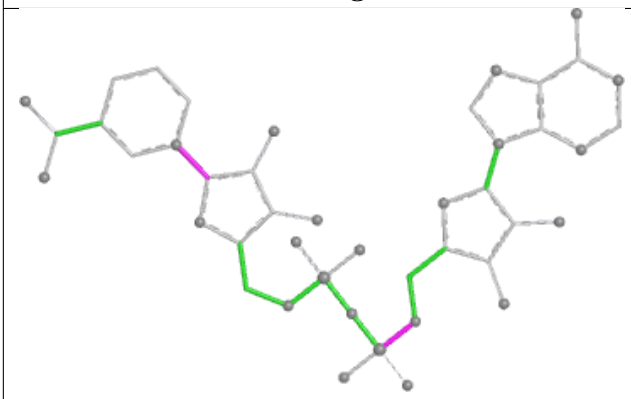
Ligand NAI A 503



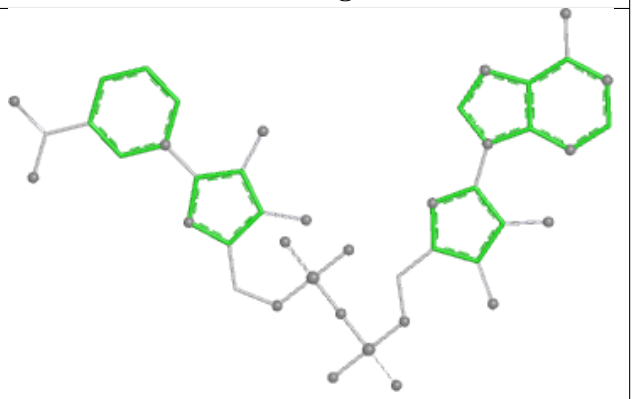
Bond lengths



Bond angles

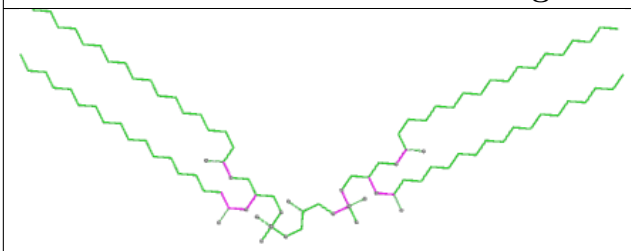


Torsions

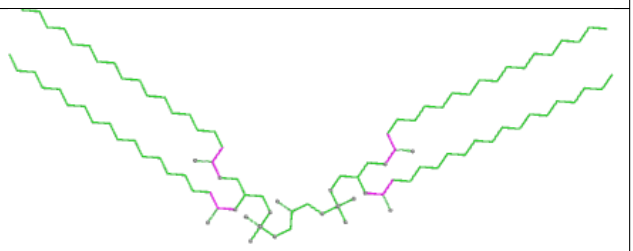


Rings

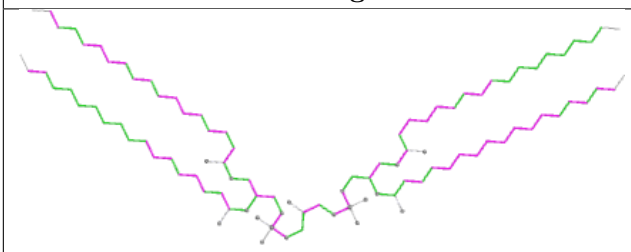
Ligand CDL l 701



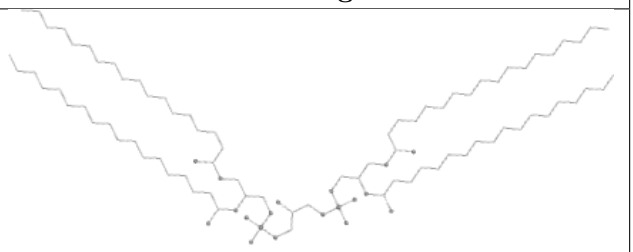
Bond lengths



Bond angles

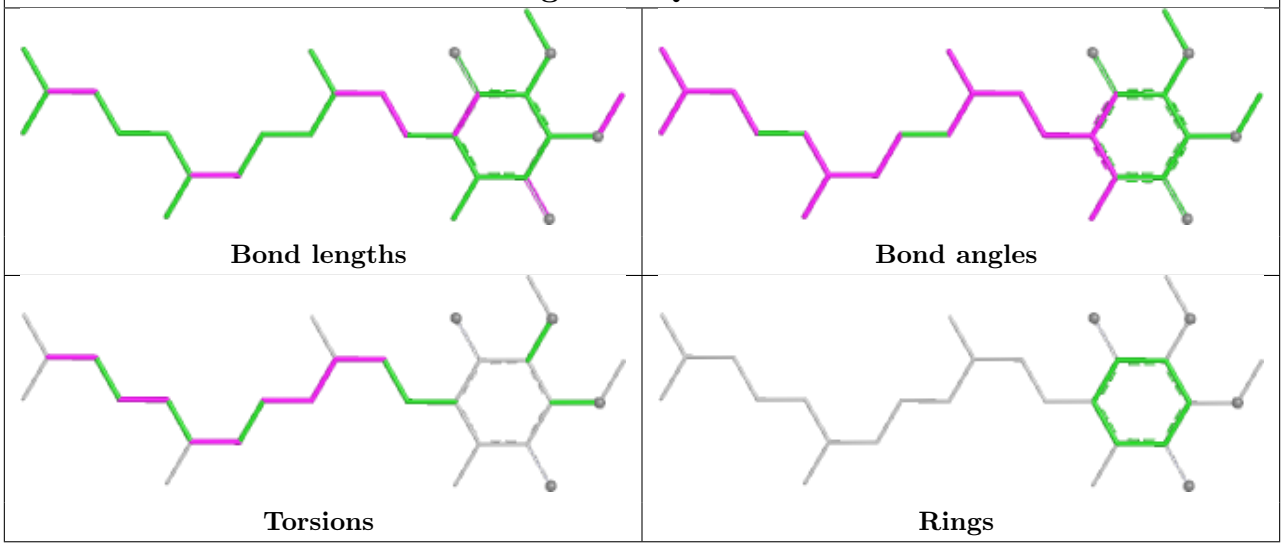


Torsions

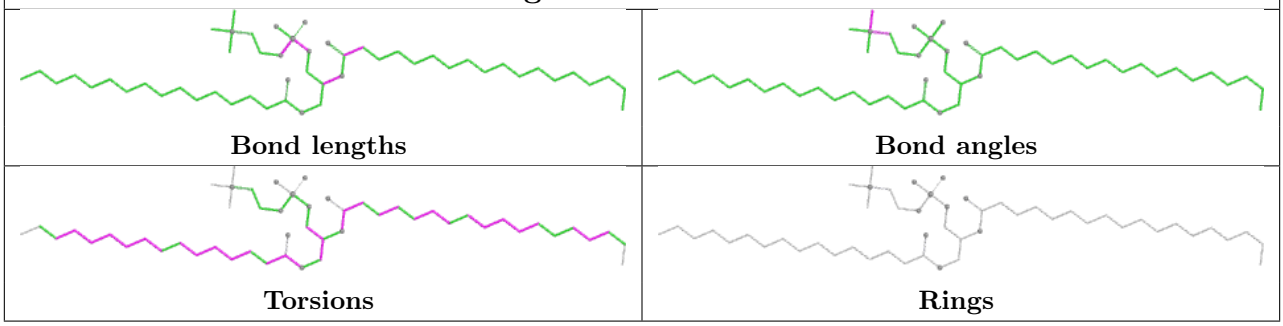


Rings

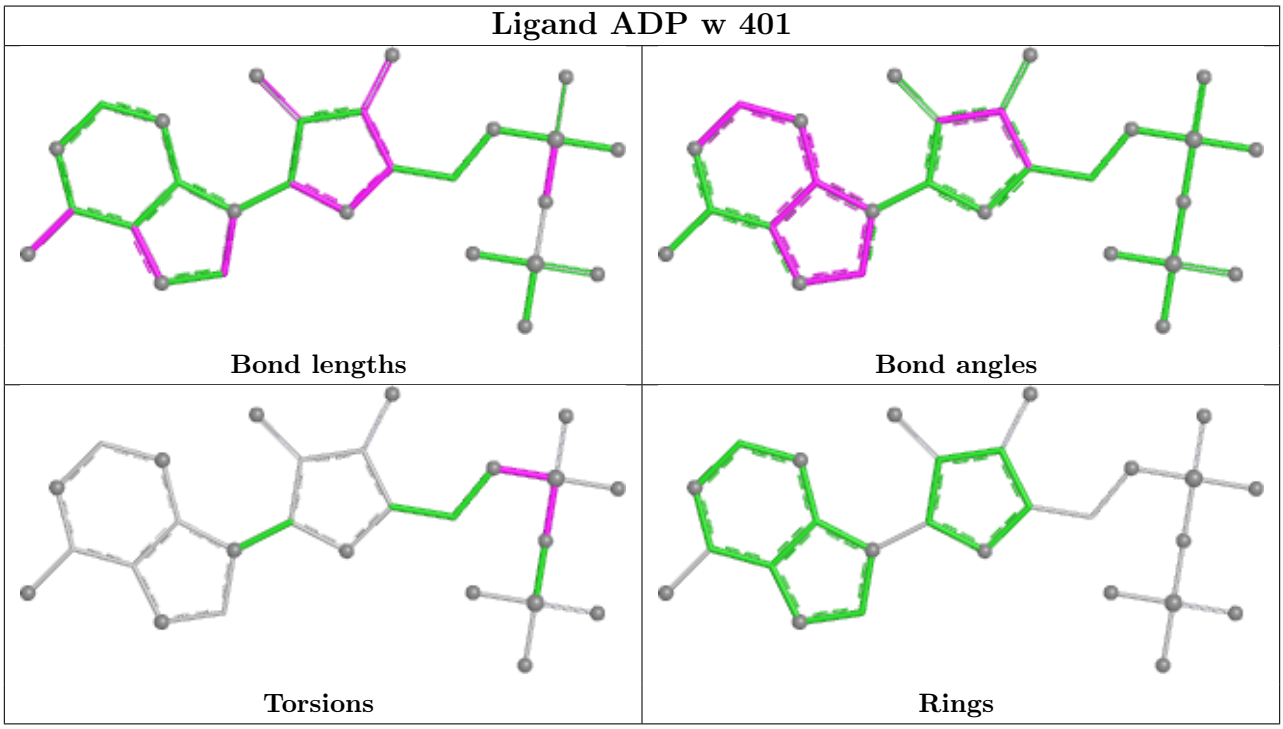
Ligand UQ s 402



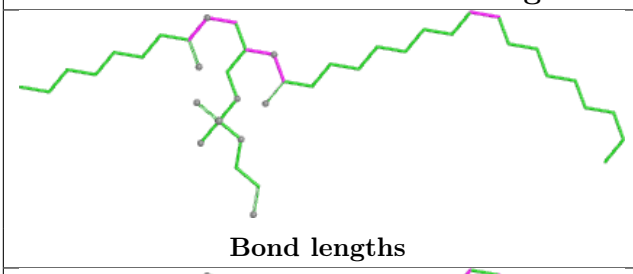
Ligand PLX m 201



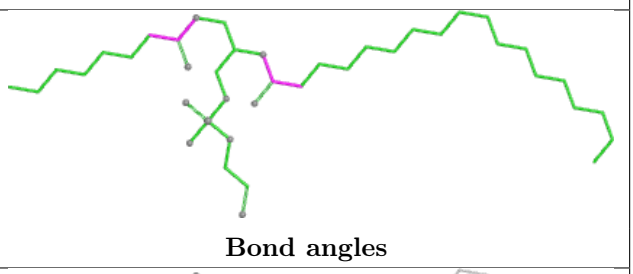
Ligand ADP w 401



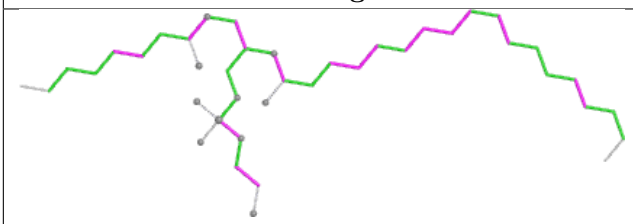
Ligand PEE m 202



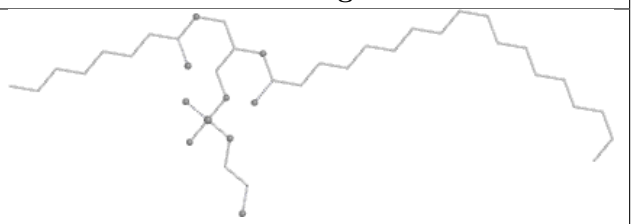
Bond lengths



Bond angles

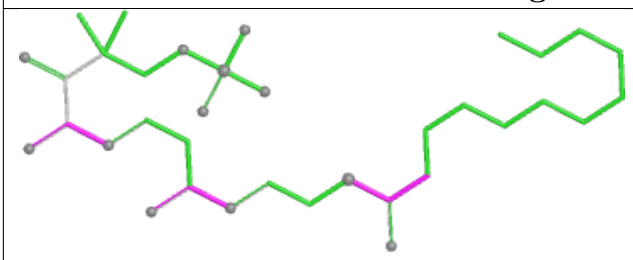


Torsions

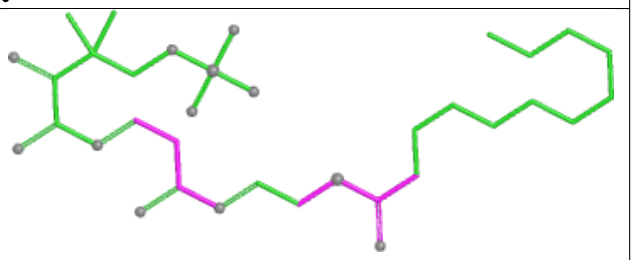


Rings

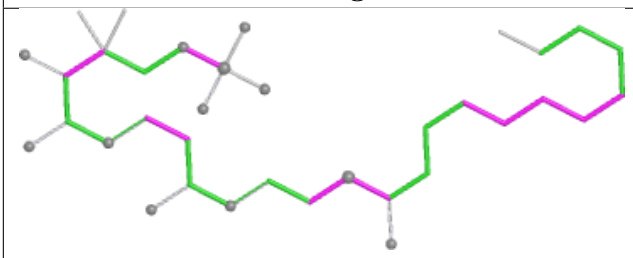
Ligand 8Q1 G 201



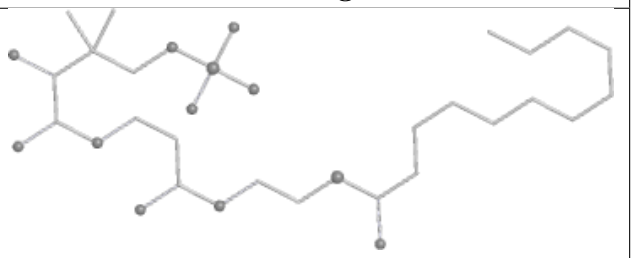
Bond lengths



Bond angles

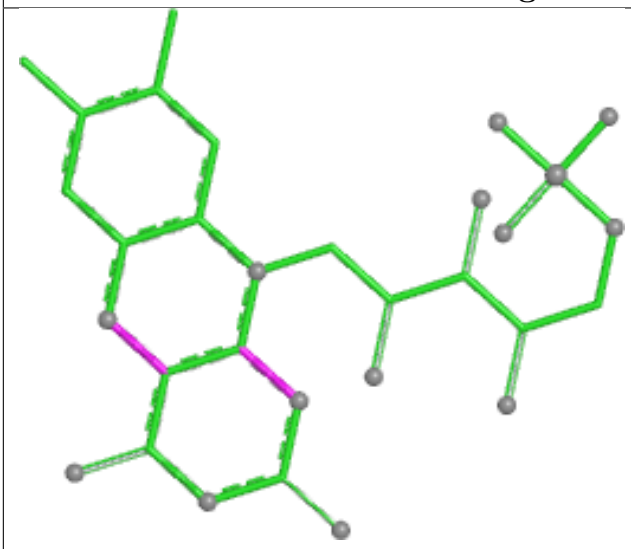


Torsions

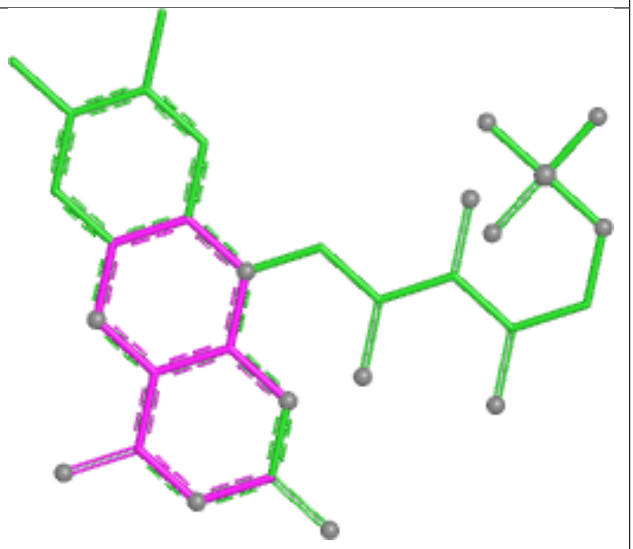


Rings

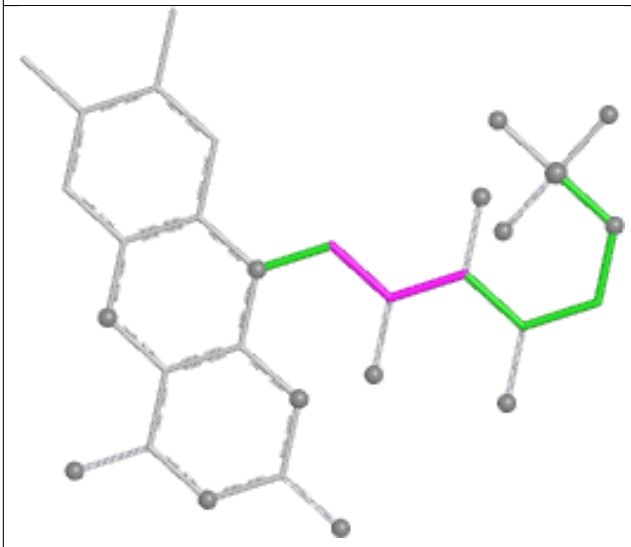
Ligand FMN A 502



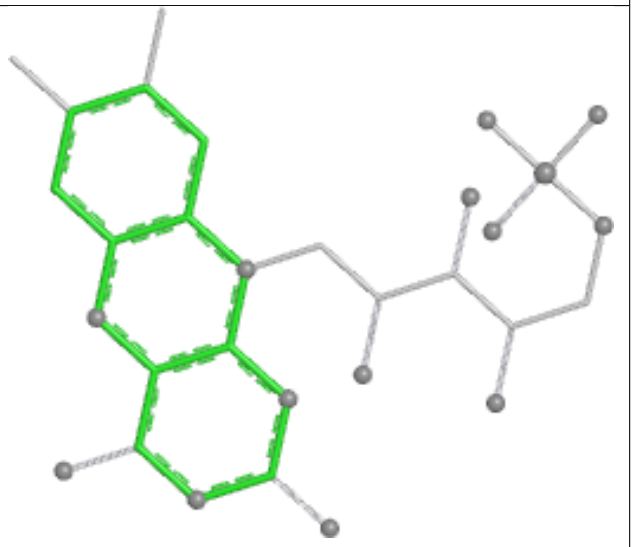
Bond lengths



Bond angles

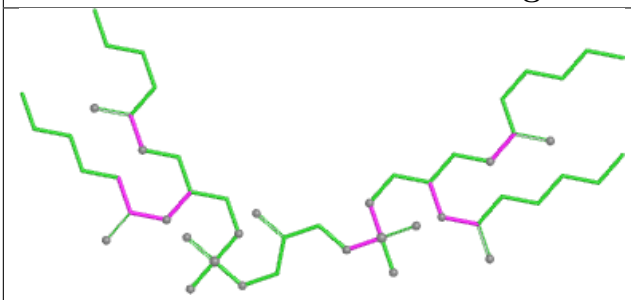


Torsions

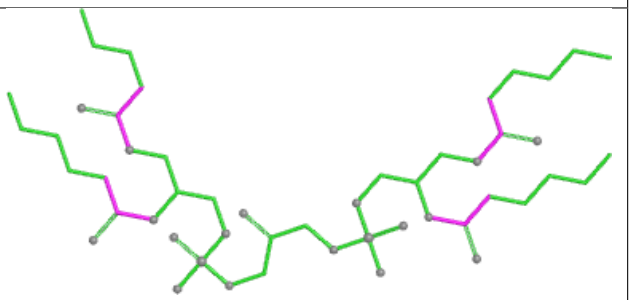


Rings

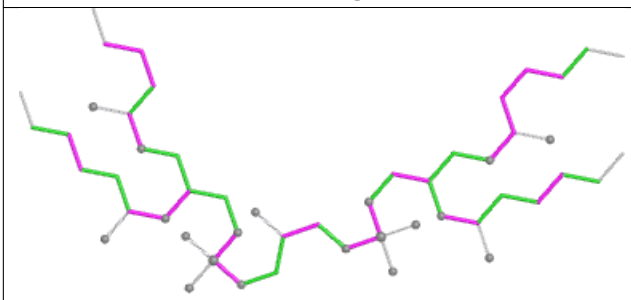
Ligand CDL N 201



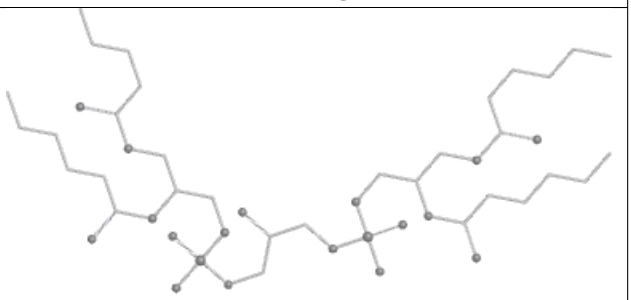
Bond lengths



Bond angles

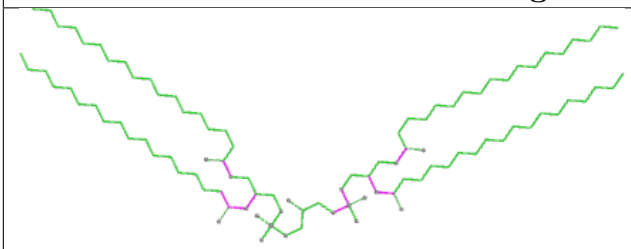


Torsions

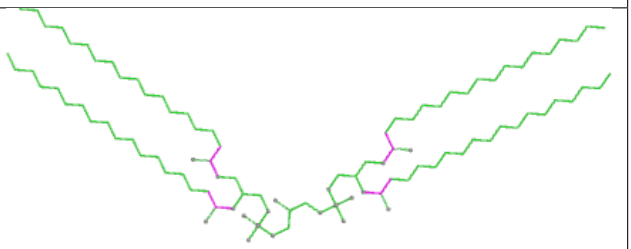


Rings

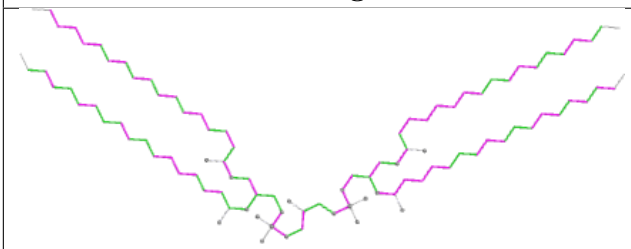
Ligand CDL r 504



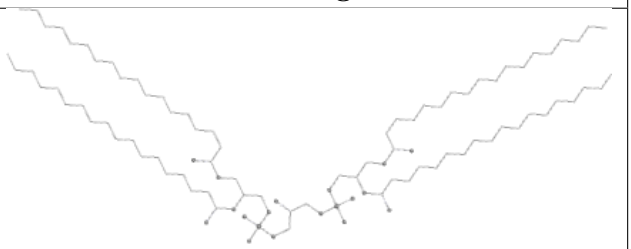
Bond lengths



Bond angles

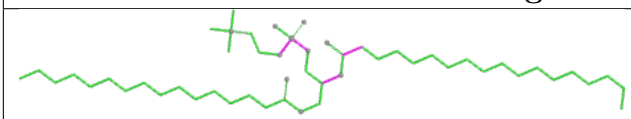


Torsions

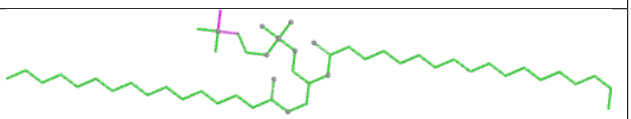


Rings

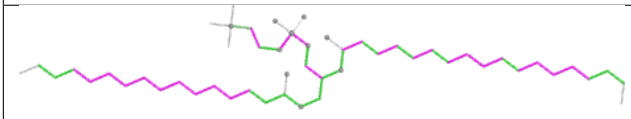
Ligand PLX C 302



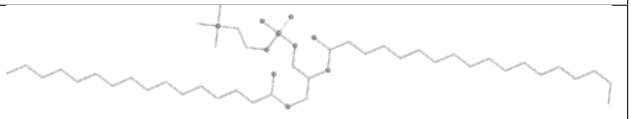
Bond lengths



Bond angles

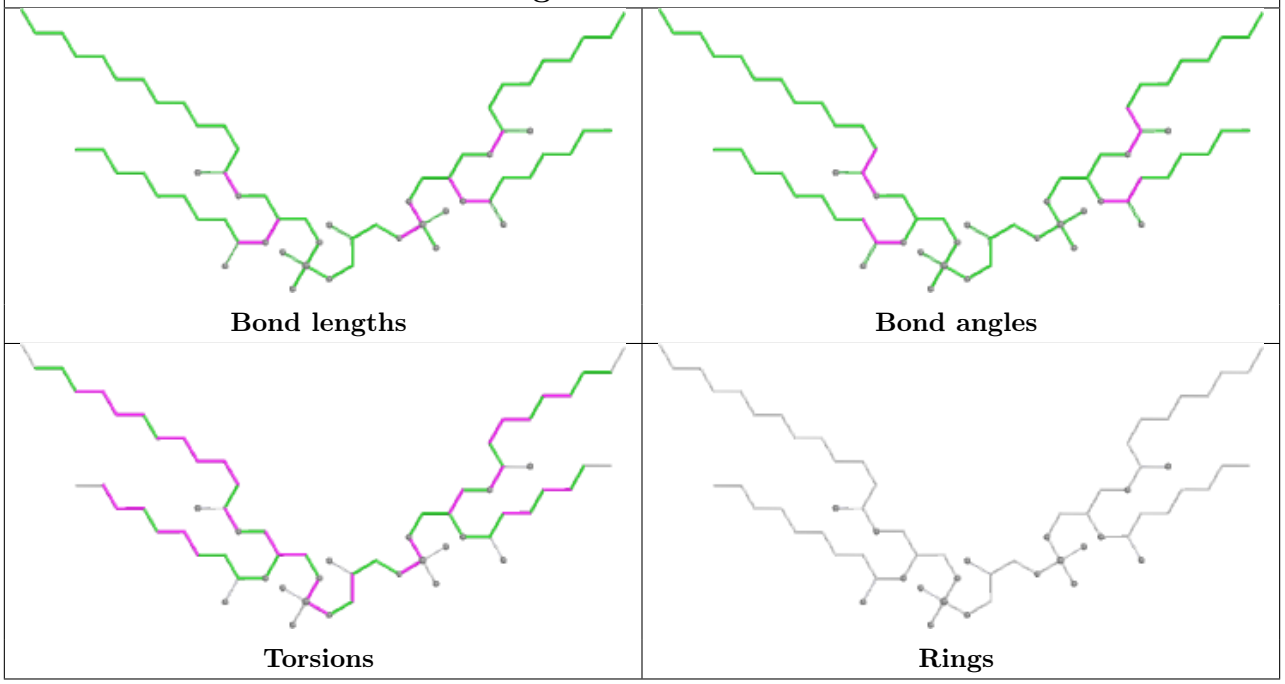


Torsions

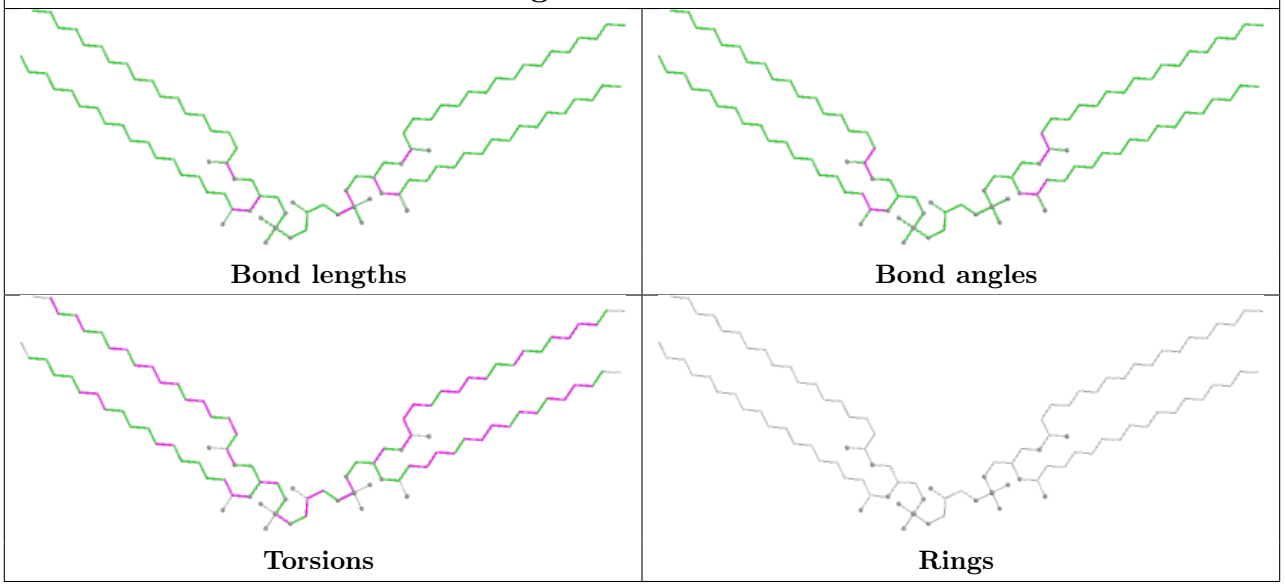


Rings

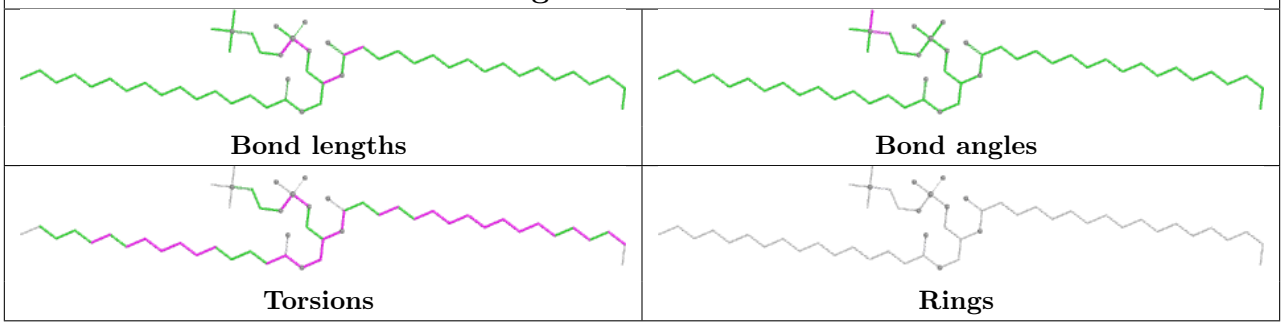
Ligand CDL i 401

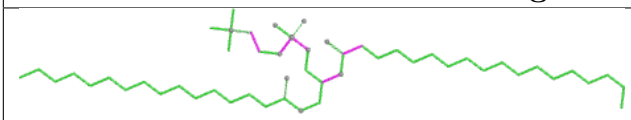
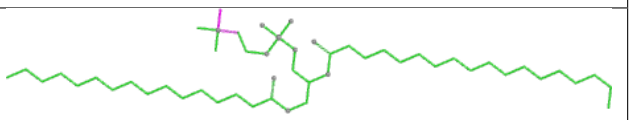
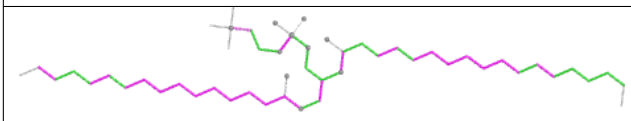
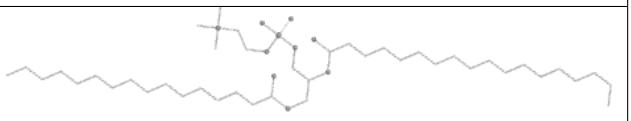


Ligand CDL r 503



Ligand PLX r 502



Ligand PLX e 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

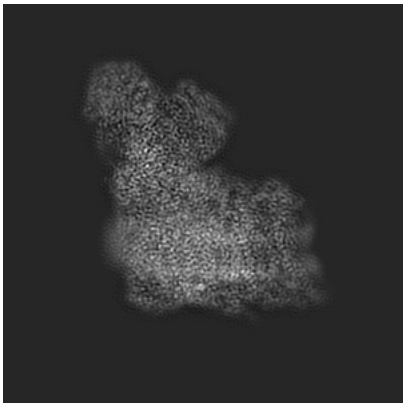
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32270. These allow visual inspection of the internal detail of the map and identification of artifacts.

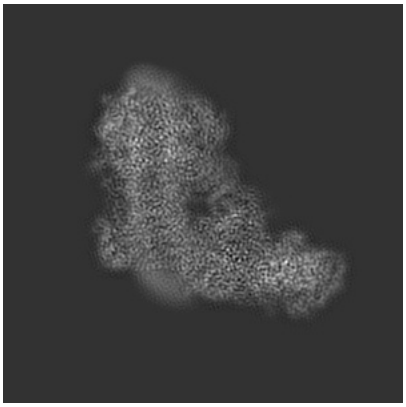
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

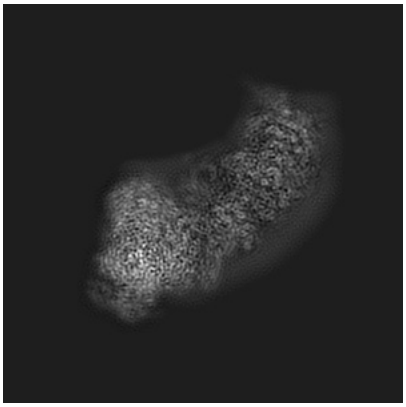
6.1.1 Primary map



X



Y

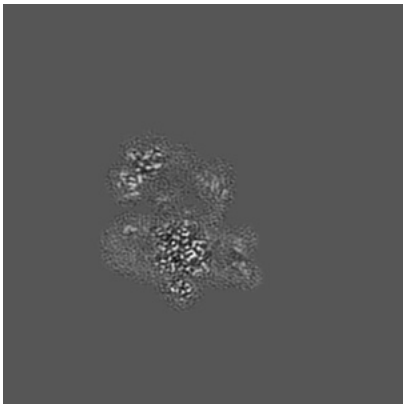


Z

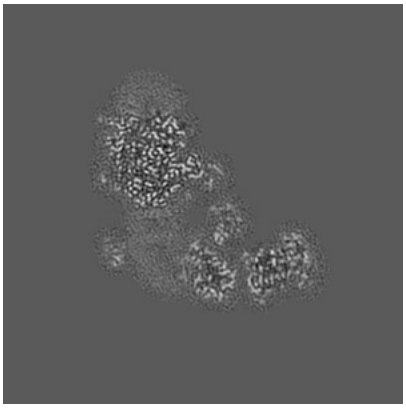
The images above show the map projected in three orthogonal directions.

6.2 Central slices

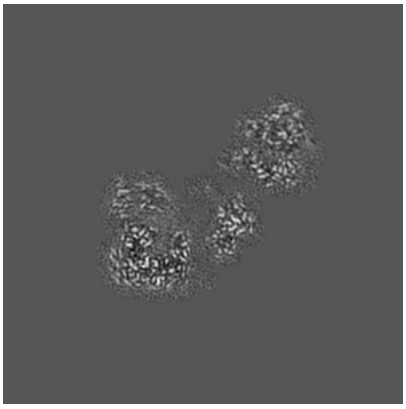
6.2.1 Primary map



X Index: 155



Y Index: 155

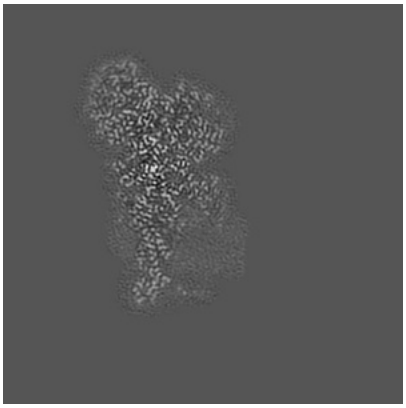


Z Index: 155

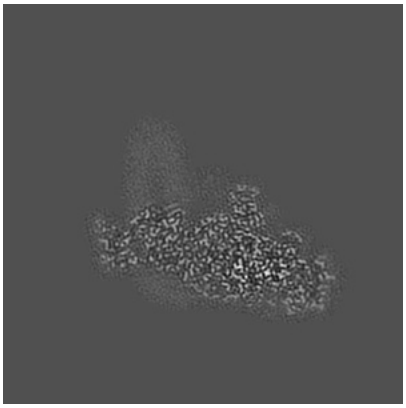
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

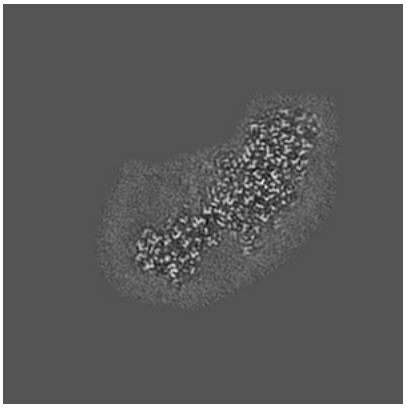
6.3.1 Primary map



X Index: 106



Y Index: 111

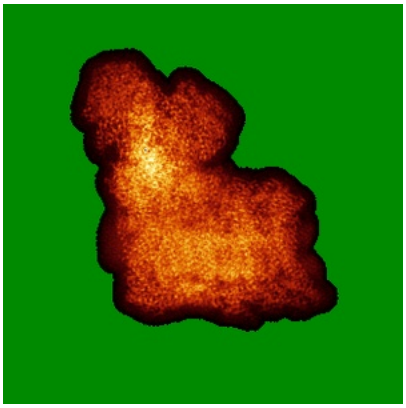


Z Index: 126

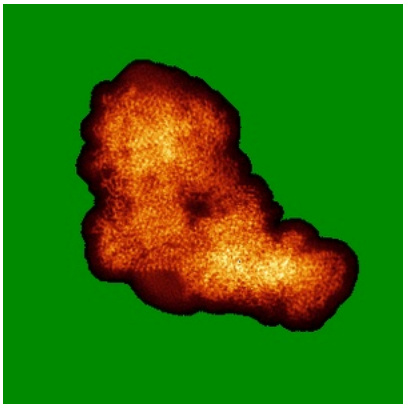
The images above show the largest variance slices of the map in three orthogonal directions.

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

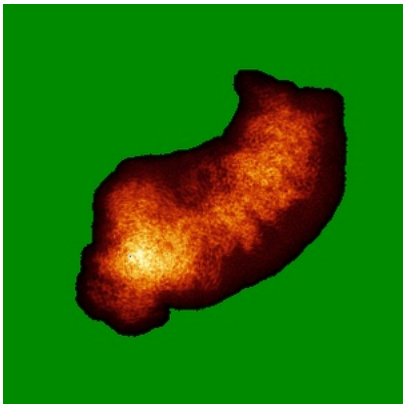
6.4.1 Primary map



X



Y

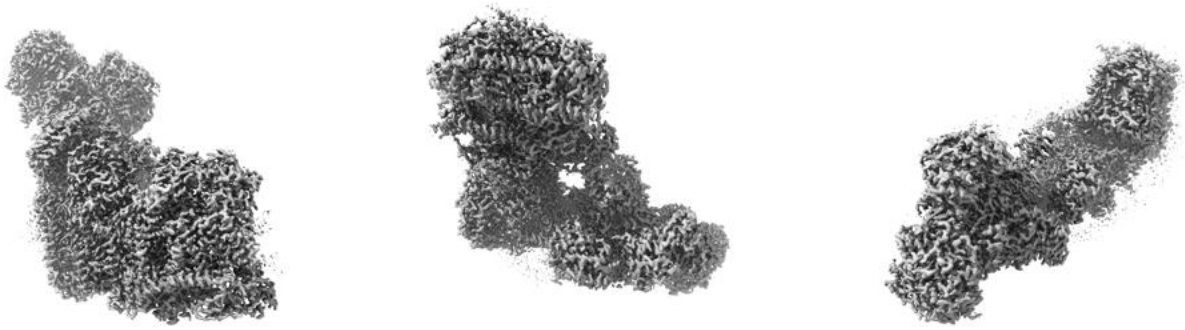


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0254. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

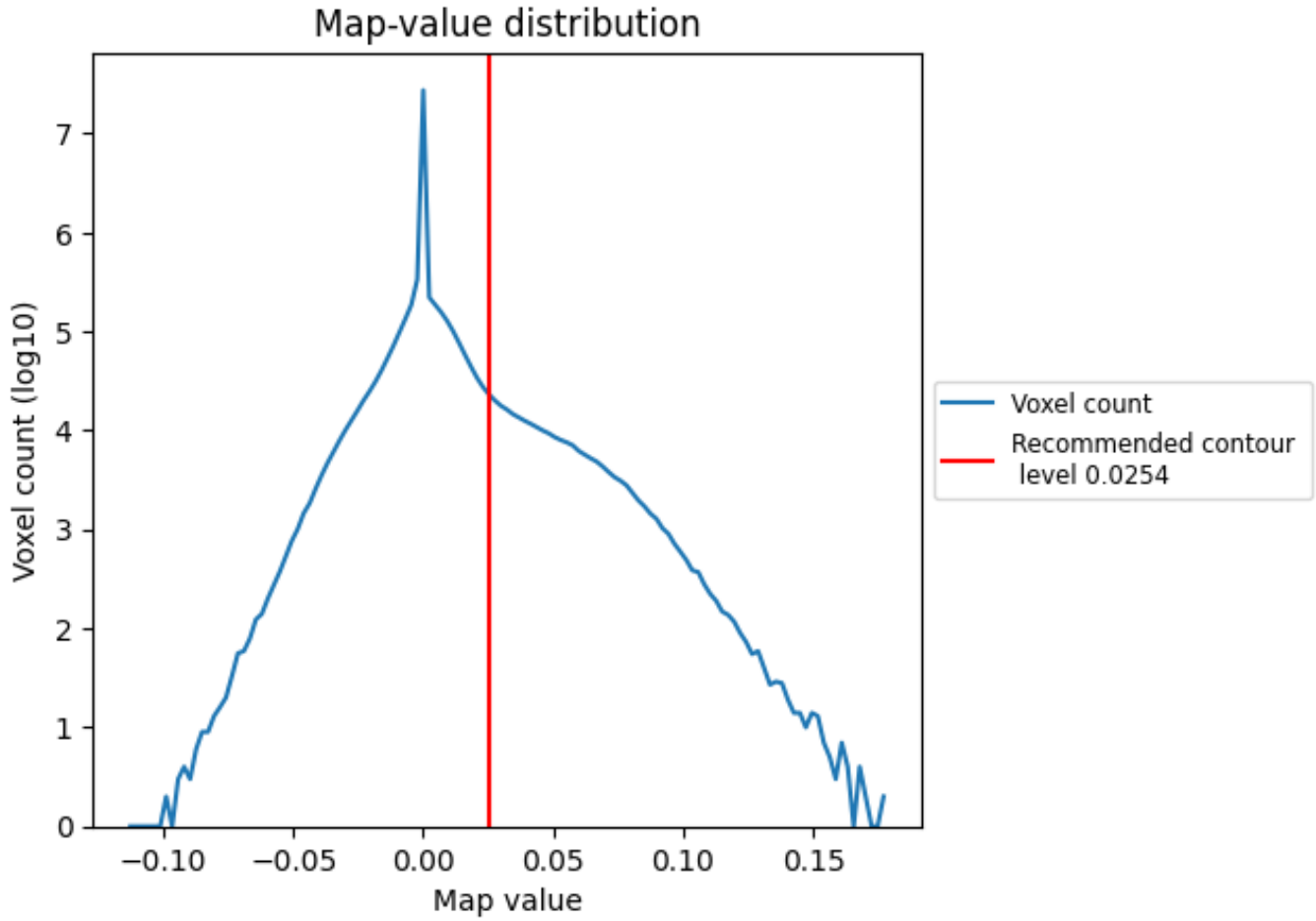
6.6 Mask visualisation (i)

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

7 Map analysis

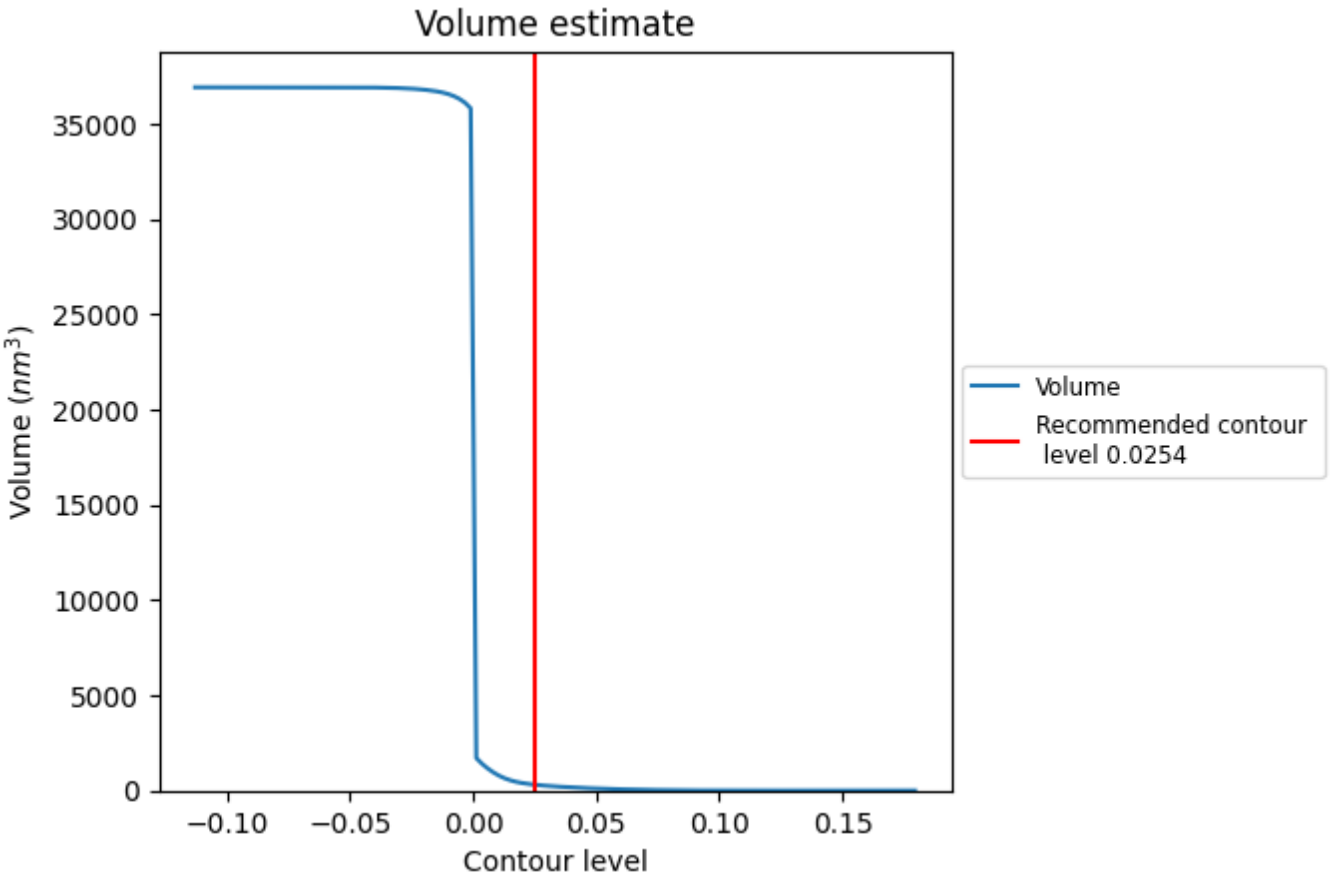
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

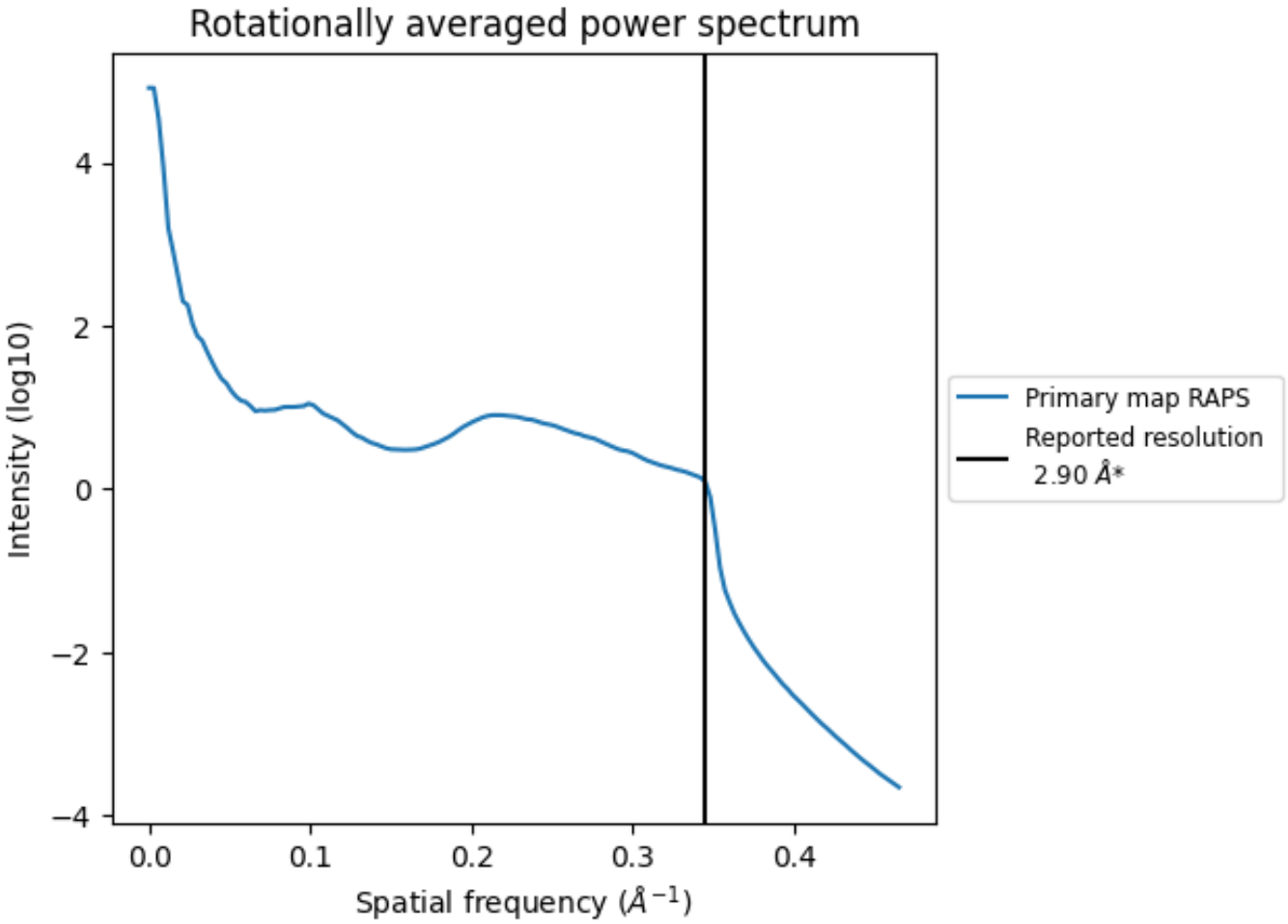
7.2 Volume estimate



The volume at the recommended contour level is 303 nm^3; this corresponds to an approximate mass of 274 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 0.345 $Å^{-1}$

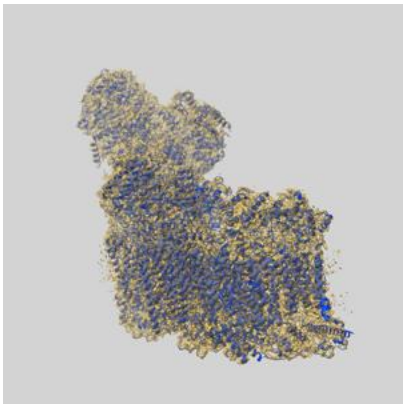
8 Fourier-Shell correlation

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

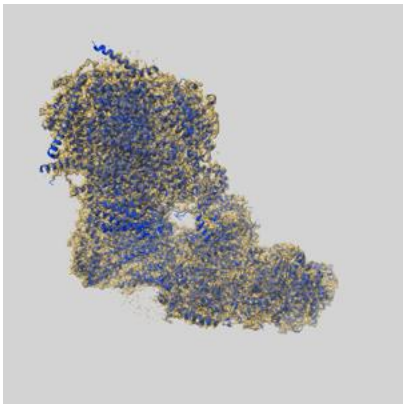
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32270 and PDB model 7W32. Per-residue inclusion information can be found in section 3 on page 20.

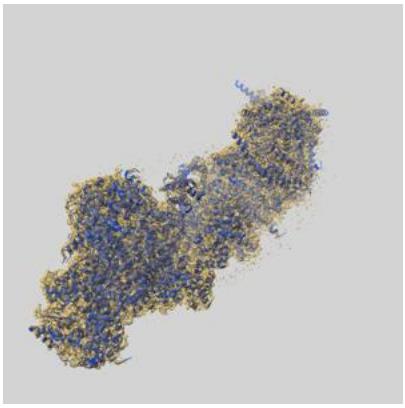
9.1 Map-model overlay



X



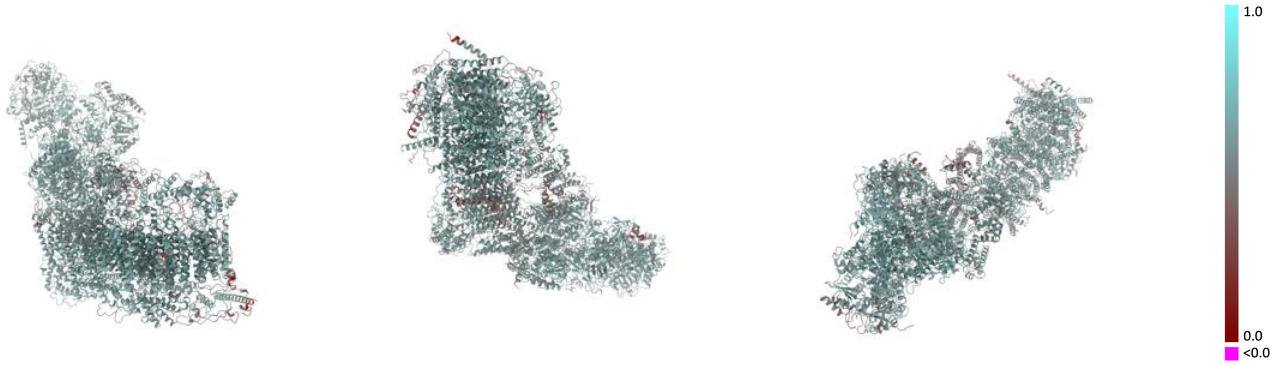
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0254 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

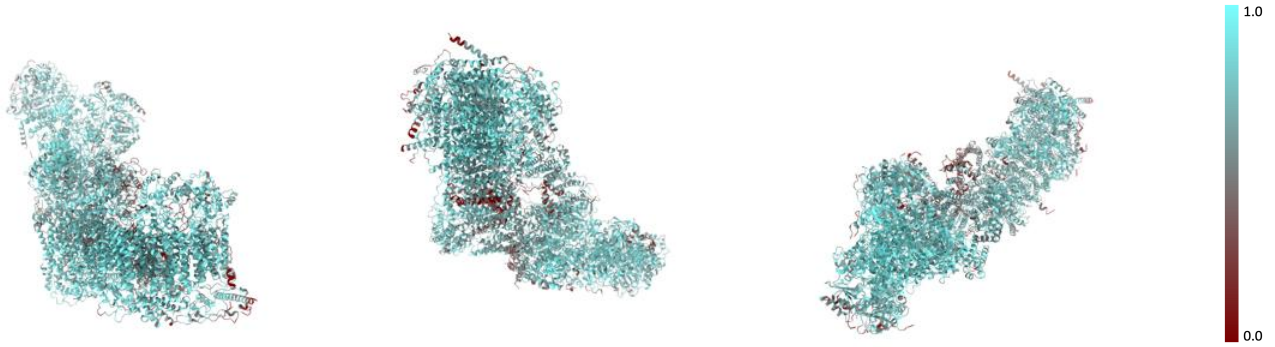
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

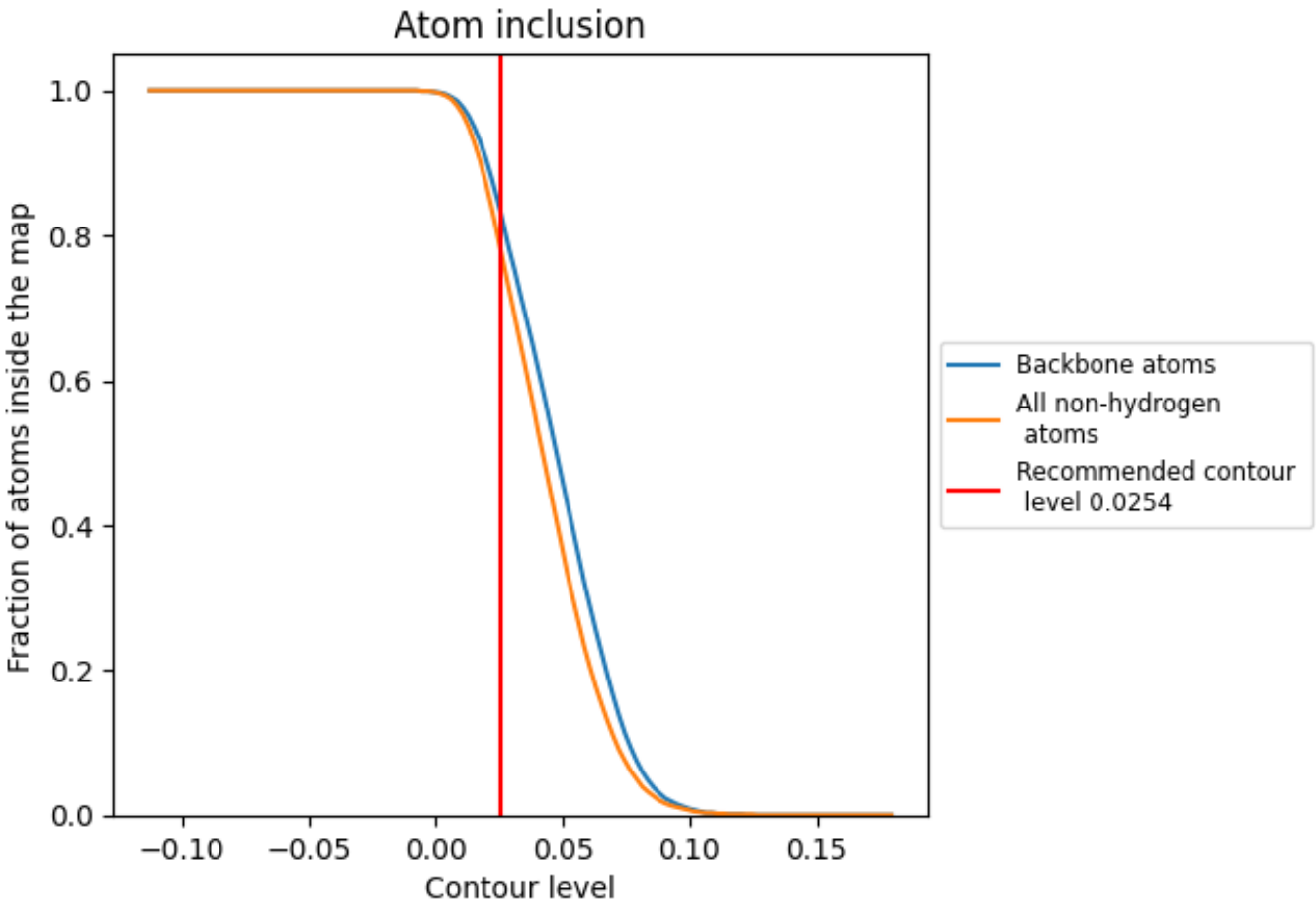
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0254).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 78% 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 (0.0254) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7830	0.5880
A	0.7740	0.5810
B	0.9320	0.6410
C	0.8780	0.6240
E	0.7570	0.5870
F	0.6670	0.5180
G	0.4170	0.4160
H	0.7500	0.5690
I	0.7200	0.5790
J	0.7220	0.5710
K	0.6540	0.5470
L	0.8460	0.6110
M	0.8500	0.6090
N	0.6850	0.5850
O	0.7180	0.5620
P	0.9200	0.6350
Q	0.8760	0.6290
S	0.8570	0.6090
T	0.7440	0.6000
U	0.7980	0.5890
V	0.3960	0.4500
W	0.8120	0.5990
X	0.7200	0.5530
Y	0.6190	0.5160
Z	0.5810	0.4890
a	0.8120	0.6060
b	0.6600	0.5240
c	0.7930	0.5860
d	0.7560	0.5820
e	0.7330	0.5650
f	0.6920	0.5480
g	0.8300	0.6060
h	0.8120	0.5990
i	0.8570	0.6190
j	0.6970	0.5560

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
k	0.6700	0.5630
l	0.8100	0.6000
m	0.6540	0.5580
n	0.6770	0.5650
o	0.7810	0.5890
p	0.7780	0.5840
r	0.8690	0.6200
s	0.8370	0.6010
u	0.8230	0.5970
v	0.6500	0.5220
w	0.7540	0.5790