Full wwPDB EM Validation Report

Mar 5, 2026 – 10:01 PM UTC

PDB ID	:	8UEU / pdb_00008ueu
EMDB ID	:	EMD-42171
Title	:	In-situ complex I, Deactive class03
Authors	:	Zheng, W.; Zhu, J.; Zhang, K.
Deposited on	:	2023-10-02
Resolution	:	3.60 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:

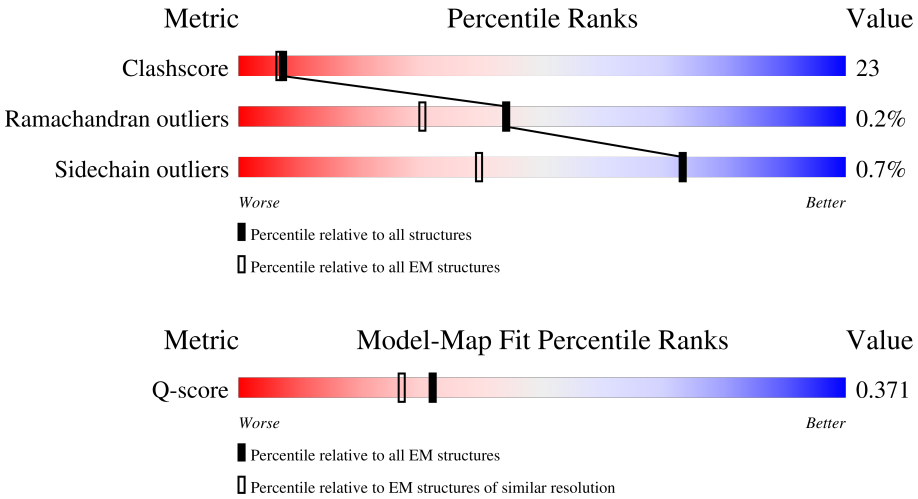
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 3.60 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.



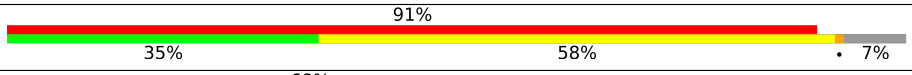
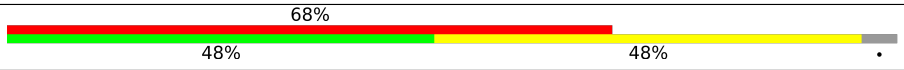
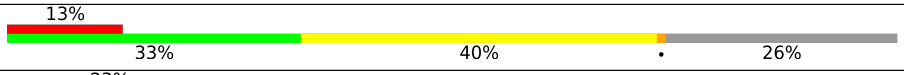
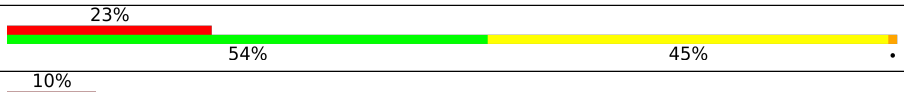
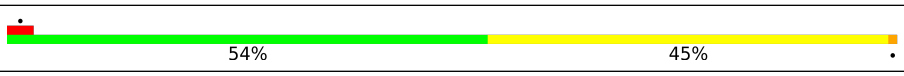
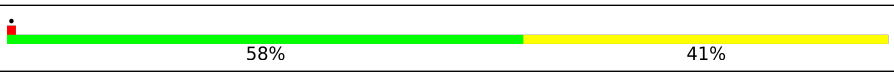
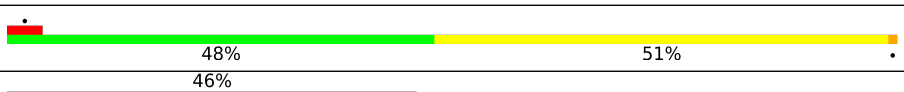
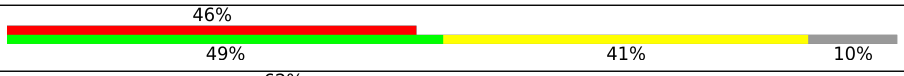
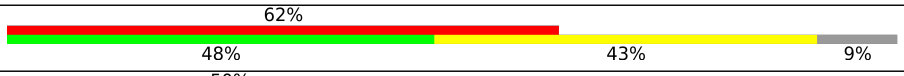
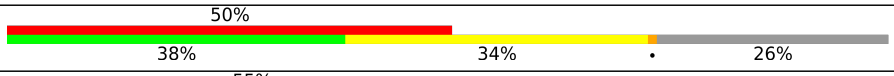
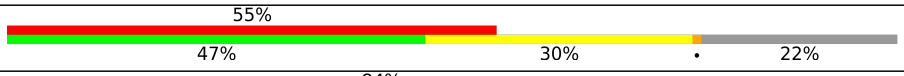
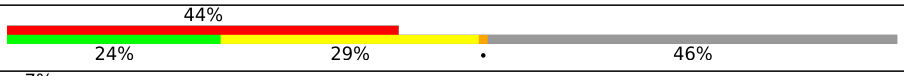
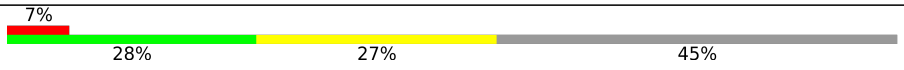
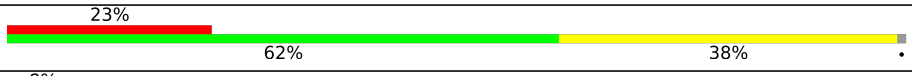
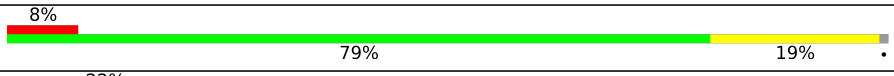
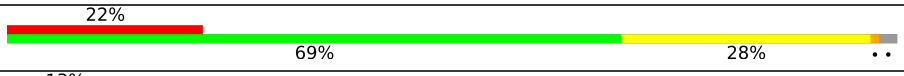
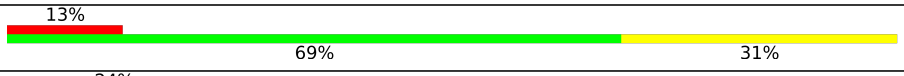
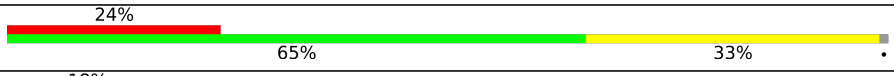
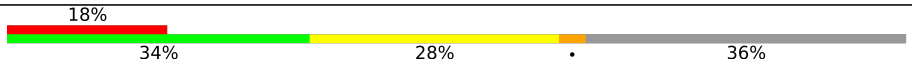
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	1A	115	17% 36% 40% · 23%
2	1B	258	17% 30% 30% 40%
3	1C	264	43% 35% 44% 21%
4	1D	476	30% 52% 38% 10%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	1Y	141	
25	1Z	144	
26	1a	70	
27	1b	84	
28	1c	76	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	1d	123	9% 69% 28%
30	1e	106	14% 53% 40% 7%
31	1f	135	15% 28% 14% 58%
32	1g	154	12% 40% 24% 35%
33	1h	189	9% 41% 32% 27%
34	1i	128	45% 55% 45%
35	1j	105	24% 31% 36% 32%
36	1k	98	32% 58% 24% 17%
37	1l	186	16% 54% 30% 16%
38	1m	129	9% 69% 30%
39	1n	179	12% 55% 41%
40	1o	137	28% 45% 45% 11%
41	1p	176	26% 67% 31%
42	1q	145	46% 63% 36%
43	1r	114	47% 56% 27% 16%
44	1s	471	10% 6% 90%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	SF4	1B	201	-	-	X	-
46	SF4	1F	502	-	-	X	-
46	SF4	1I	202	-	-	X	-
47	FES	1E	301	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67263 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1A	88	707	484	101	117	5	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1B	155	1242	791	226	211	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	1C	209	1740	1125	297	316	2	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1C	104	GLN	ARG	conflict	UNP A0A286ZNN4
1C	154	GLY	ASP	conflict	UNP A0A286ZNN4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	1D	429	3452	2207	593	628	24	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1D	0	GLY	GLU	conflict	UNP A0A8D0QM68

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	1E	214	Total	C	N	O	S	0	0
			1658	1058	278	312	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1F	432	Total	C	N	O	S	0	0
			3325	2100	592	613	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	1G	699	Total	C	N	O	S	0	0
			5362	3360	933	1029	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1H	318	Total	C	N	O	S	0	0
			2504	1673	385	425	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	1I	176	Total	C	N	O	S	0	0
			1412	887	243	269	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	1J	175	Total	C	N	O	S	0	0
			1339	898	190	238	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	98	Total	C	N	O	S	0	0
			750	494	113	129	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	606	Total	C	N	O	S	0	0
			4818	3195	746	826	51		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	459	Total	C	N	O	S	0	0
			3632	2411	572	610	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	347	Total	C	N	O	S	0	0
			2712	1783	420	463	46		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	1O	320	Total	C	N	O	S	0	0
			2590	1649	440	491	10		

- Molecule 16 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	1P	342	Total	C	N	O	S	0	0
			2751	1783	481	478	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	1Q	129	Total	C	N	O	S	0	0
			1047	659	186	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	1S	87	Total	C	N	O	S	0	0
			700	440	131	127	2		

- Molecule 20 is a protein called NADH:ubiquinone oxidoreductase subunit AB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	1T	85	Total	C	N	O	S	0	0
			689	445	101	138	5		
20	1U	86	Total	C	N	O	S	0	0
			694	448	102	139	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	1V	115	Total	C	N	O	S	0	0
			927	599	157	168	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1W	115	Total	C	N	O	S	0	0
			971	619	179	168	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	1X	171	Total	C	N	O	S	0	0
			1398	887	250	251	10		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	1Y	139	Total	C	N	O	S	0	0
			1016	648	173	189	6		

- Molecule 25 is a protein called NADH:ubiquinone oxidoreductase subunit A13.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1Z	141	Total	C	N	O	S	0	0
			1168	752	202	205	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	1a	70	Total	C	N	O	S	0	0
			562	361	101	94	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	1b	83	Total	C	N	O	S	0	0
			643	417	110	115	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
28	1c	49	Total	C	N	O	0	0
			417	276	71	70		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	1d	121	Total	C	N	O	S	0	0
			996	648	172	170	6		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1d	-2	ACE	-	acetylation	UNP A0A480JRW3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1e	99	Total	C	N	O	S	0	0
			816	519	151	140	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	1f	57	Total	C	N	O	S	0	0
			487	316	89	80	2		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1f	-77	MET	-	initiating methionine	UNP A0A8D1IZ33
1f	-76	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-75	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-74	ALA	-	expression tag	UNP A0A8D1IZ33
1f	-73	ILE	-	expression tag	UNP A0A8D1IZ33
1f	-72	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-71	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-70	LEU	-	expression tag	UNP A0A8D1IZ33
1f	-69	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-68	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-67	THR	-	expression tag	UNP A0A8D1IZ33
1f	-66	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-65	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-64	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-63	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-62	GLU	-	expression tag	UNP A0A8D1IZ33
1f	-61	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-60	CYS	-	expression tag	UNP A0A8D1IZ33
1f	-59	ASP	-	expression tag	UNP A0A8D1IZ33
1f	-58	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-57	ASN	-	expression tag	UNP A0A8D1IZ33
1f	-56	GLN	-	expression tag	UNP A0A8D1IZ33
1f	-55	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-54	VAL	-	expression tag	UNP A0A8D1IZ33
1f	-53	LYS	-	expression tag	UNP A0A8D1IZ33
1f	-52	GLY	-	expression tag	UNP A0A8D1IZ33
1f	-51	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-50	ARG	-	expression tag	UNP A0A8D1IZ33
1f	-49	PHE	-	expression tag	UNP A0A8D1IZ33

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	1g	100	Total	C	N	O	S	0	0
			835	535	138	158	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	1h	138	Total	C	N	O	S	0	0
			1151	754	195	199	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	1i	127	Total	C	N	O	S	0	0
			1100	723	194	181	2		

- Molecule 35 is a protein called NADH:ubiquinone oxidoreductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	1j	71	Total	C	N	O	S	0	0
			601	394	99	107	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	1k	81	Total	C	N	O	S	0	0
			649	422	110	116	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	1l	156	Total	C	N	O	S	0	0
			1310	847	213	242	8		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	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	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	1o	122	Total	C	N	O	S	0	0
			1045	650	198	187	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1p	173	Total	C	N	O	S	0	0
			1449	908	263	270	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
42	1q	145	Total	C	N	O	S	0	0
			1212	775	219	213	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	96	Total	C	N	O	S	0	0
			767	483	144	137	3		

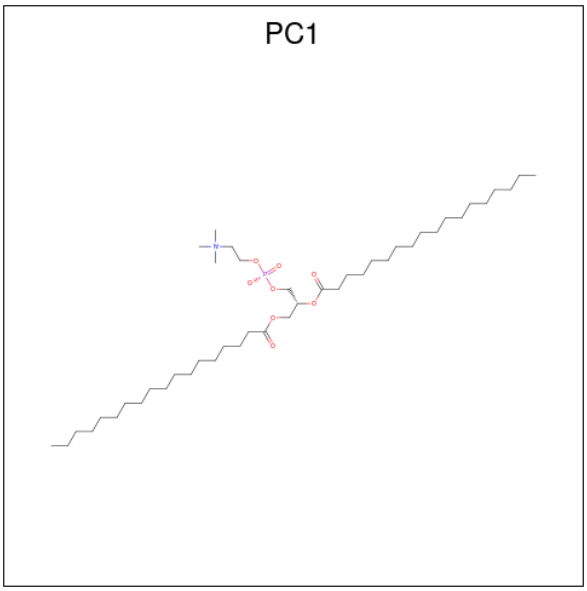
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1r	0	ACE	-	insertion	UNP A0A8W4F7N8

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

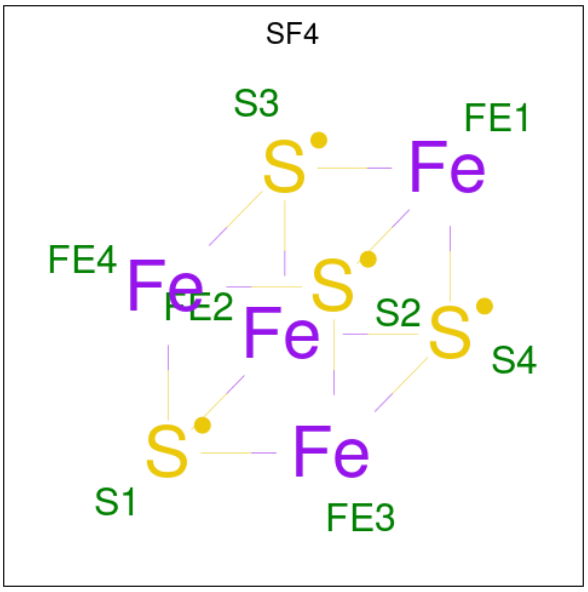
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



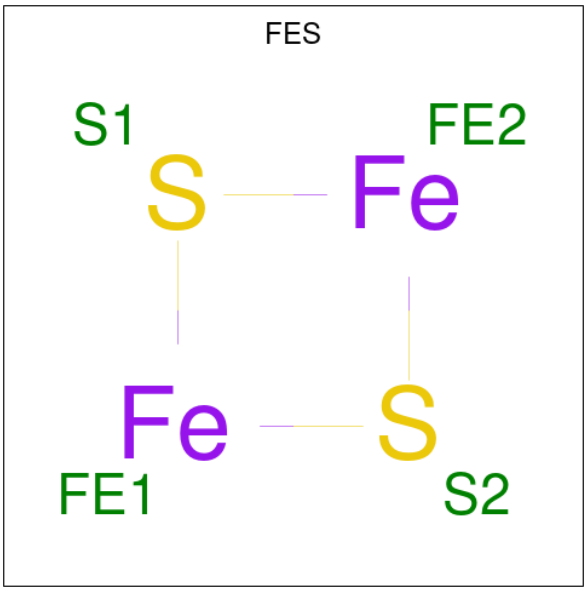
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	1H	1	Total	C	N	O	P	0
			44	34	1	8	1	
45	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
45	1M	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1g	1	Total	C	N	O	P	0
			44	34	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



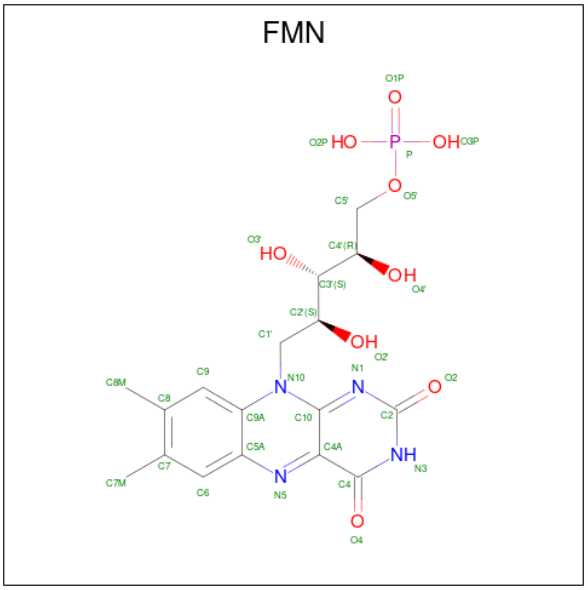
Mol	Chain	Residues	Atoms	AltConf
46	1B	1	Total Fe S 8 4 4	0
46	1F	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1G	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0
46	1I	1	Total Fe S 8 4 4	0

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



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

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

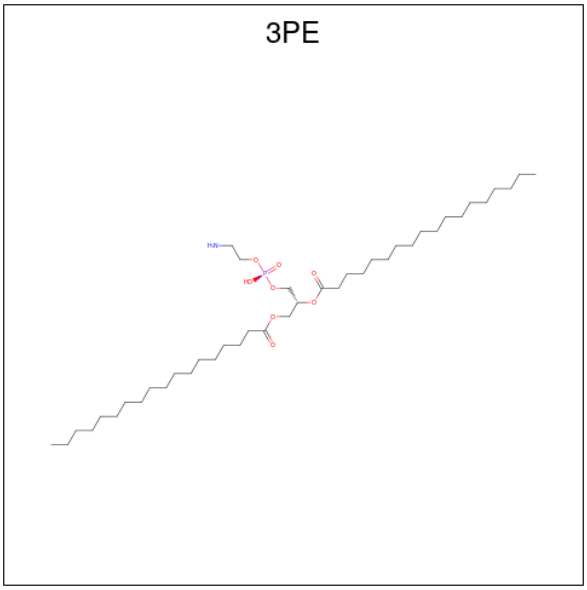


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is POTASSIUM ION (CCD ID: K) (formula: K).

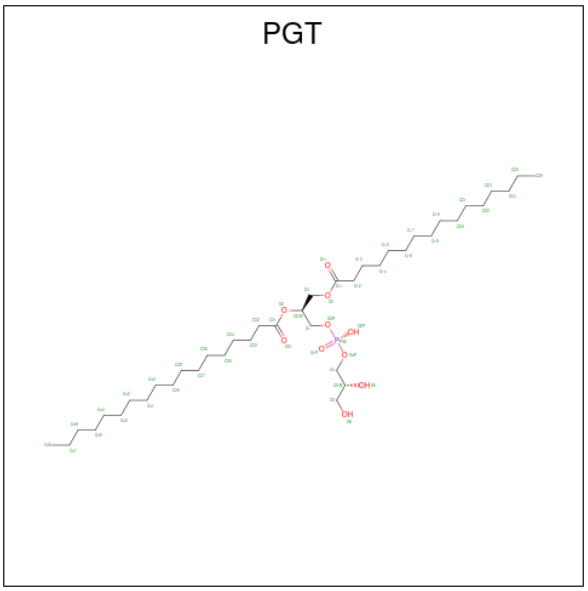
Mol	Chain	Residues	Atoms	AltConf
49	1G	1	Total K 1 1	0

- Molecule 50 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



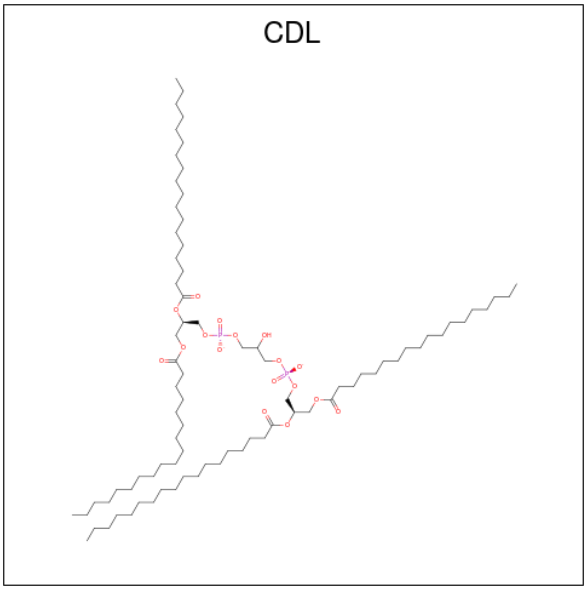
Mol	Chain	Residues	Atoms	AltConf
50	1L	1	Total C N O P 46 36 1 8 1	0
50	1L	1	Total C N O P 42 32 1 8 1	0
50	1N	1	Total C N O P 51 41 1 8 1	0
50	1Y	1	Total C N O P 31 21 1 8 1	0
50	1Y	1	Total C N O P 51 41 1 8 1	0
50	1b	1	Total C N O P 47 37 1 8 1	0

- Molecule 51 is (1S)-2-{[{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: $C_{40}H_{79}O_{10}P$).



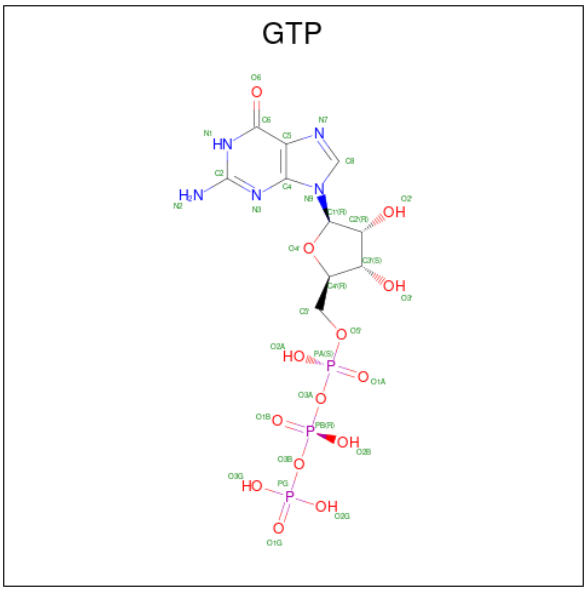
Mol	Chain	Residues	Atoms				AltConf
51	1M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	1N	1	Total	C	O	P	0
			77	58	17	2	
52	1r	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 53 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

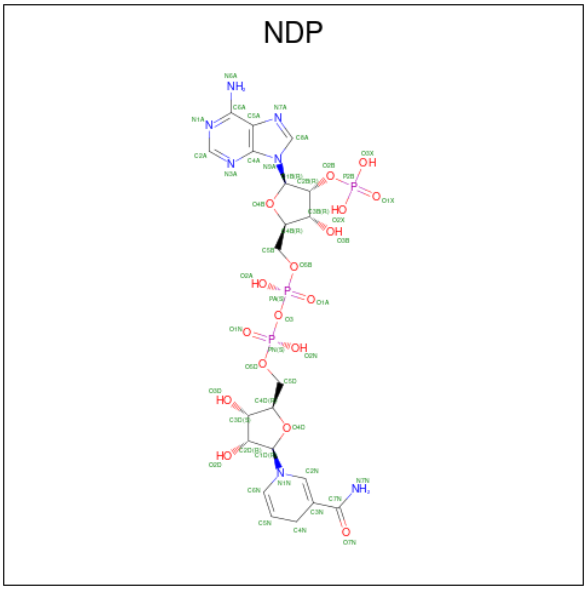


Mol	Chain	Residues	Atoms					AltConf
53	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 54 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
54	1O	1	Total	Mg	0
			1	1	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

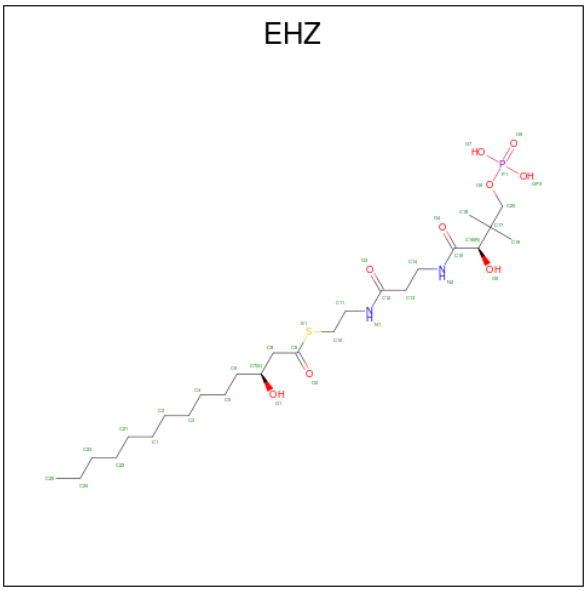


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

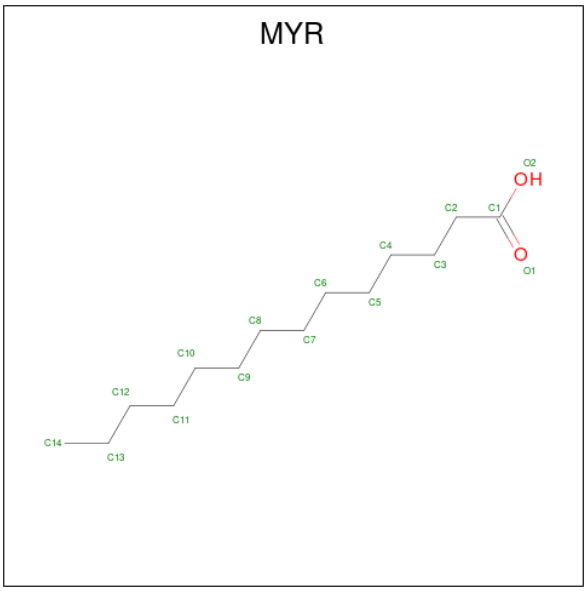
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

- Molecule 57 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



Mol	Chain	Residues	Atoms						AltConf
57	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



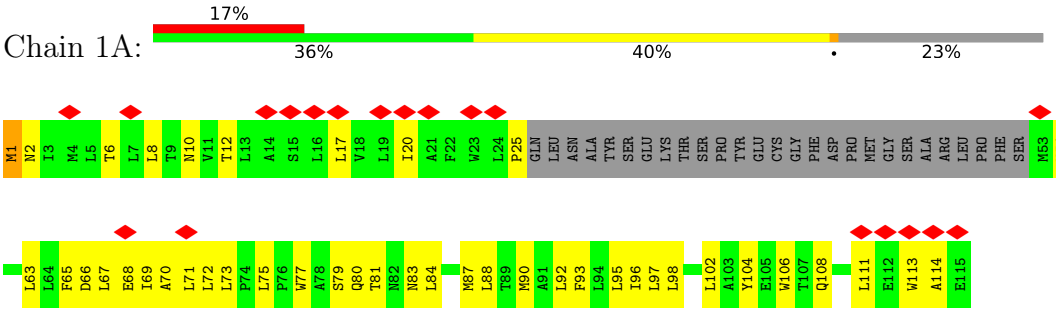
Mol	Chain	Residues	Atoms			AltConf
58	1l	1	Total	C	O	0
			15	14	1	

3 Residue-property plots (i)

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

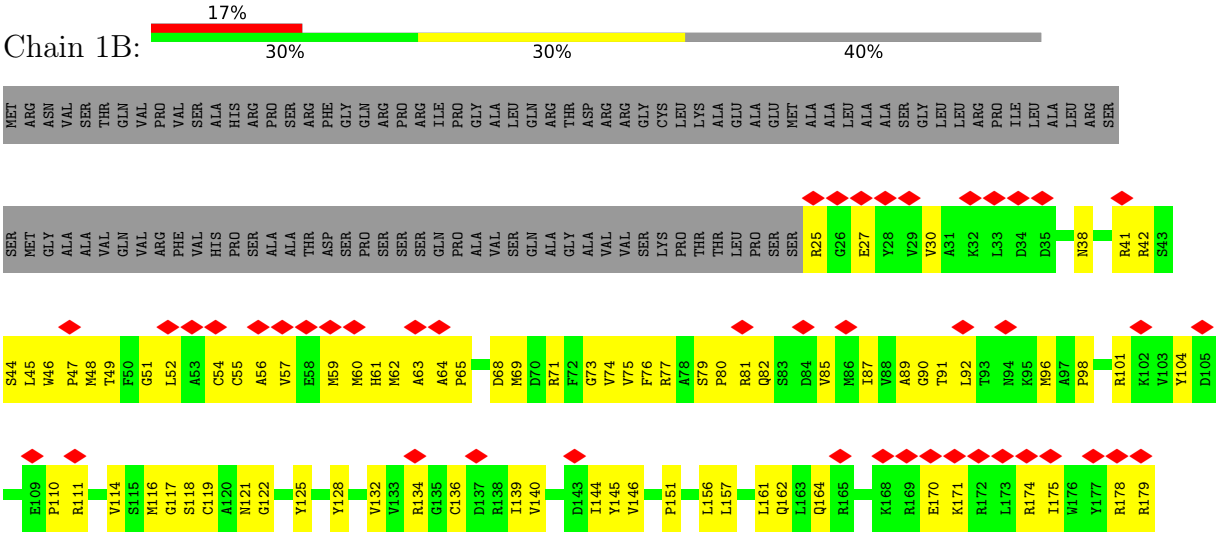
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain 1A:



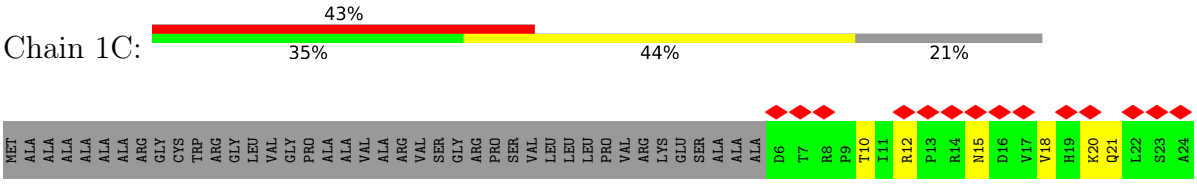
• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

Chain 1B:



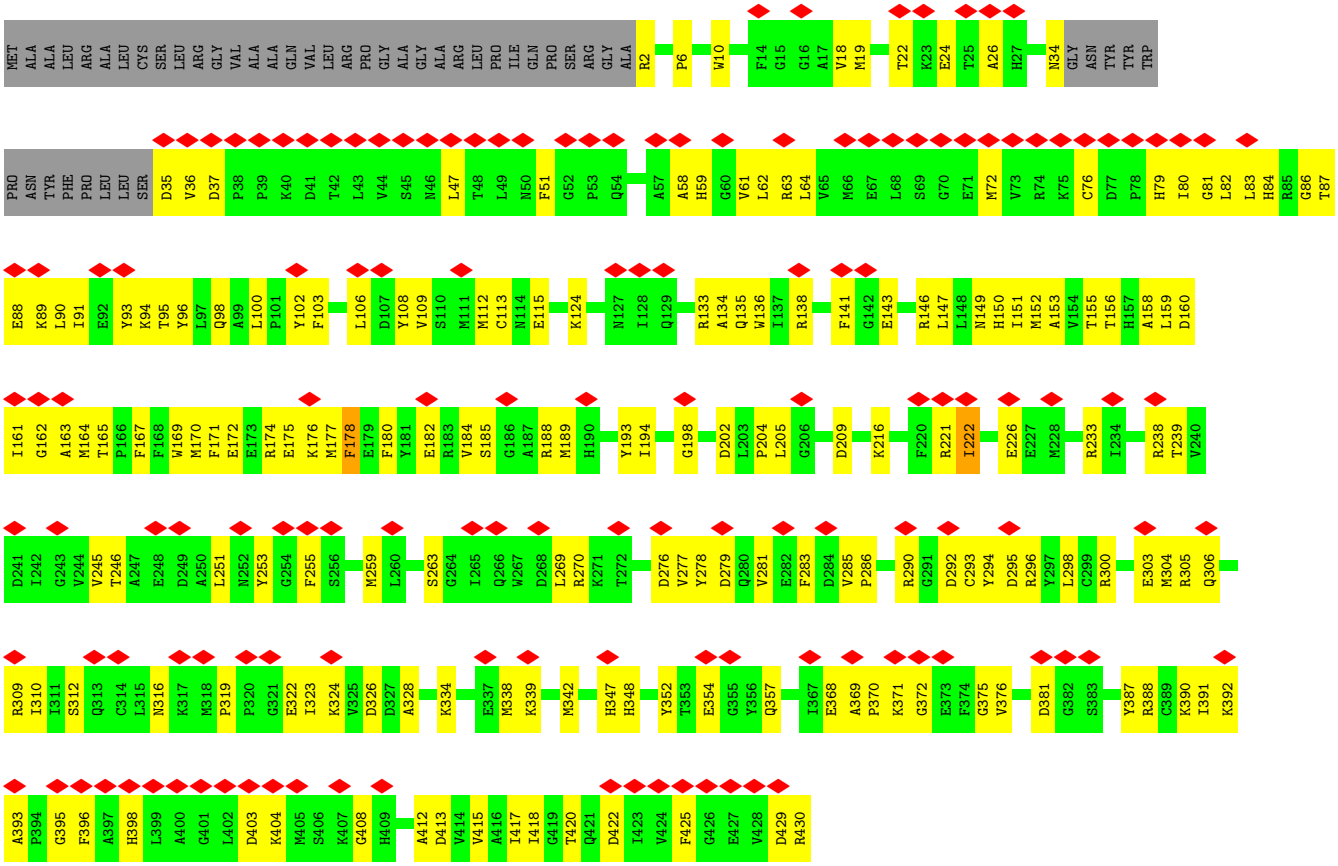
• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain 1C:



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

Chain 1D:

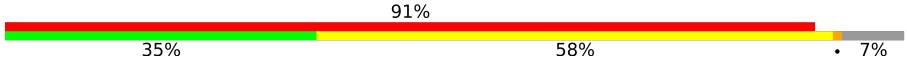


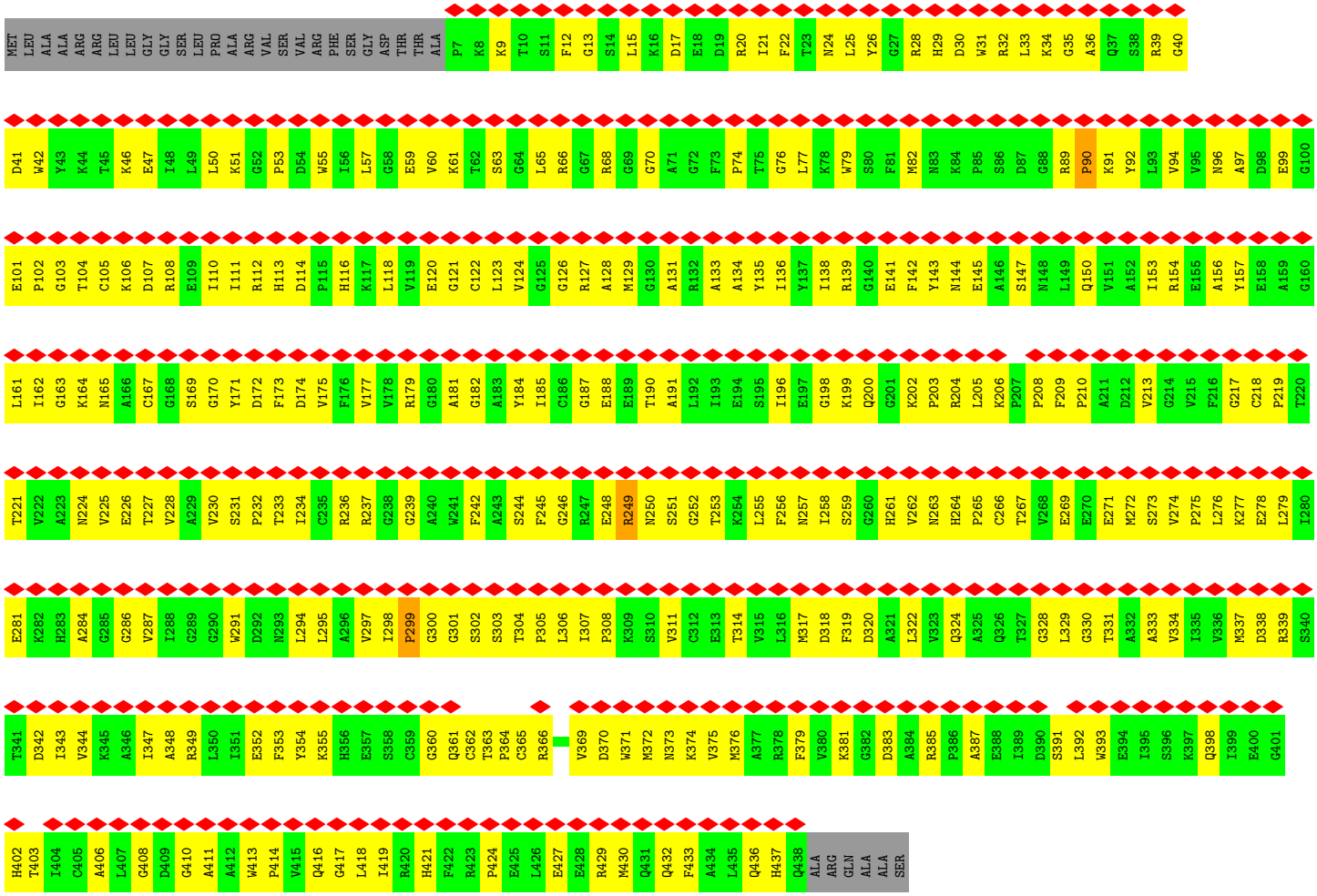
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 1E:

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

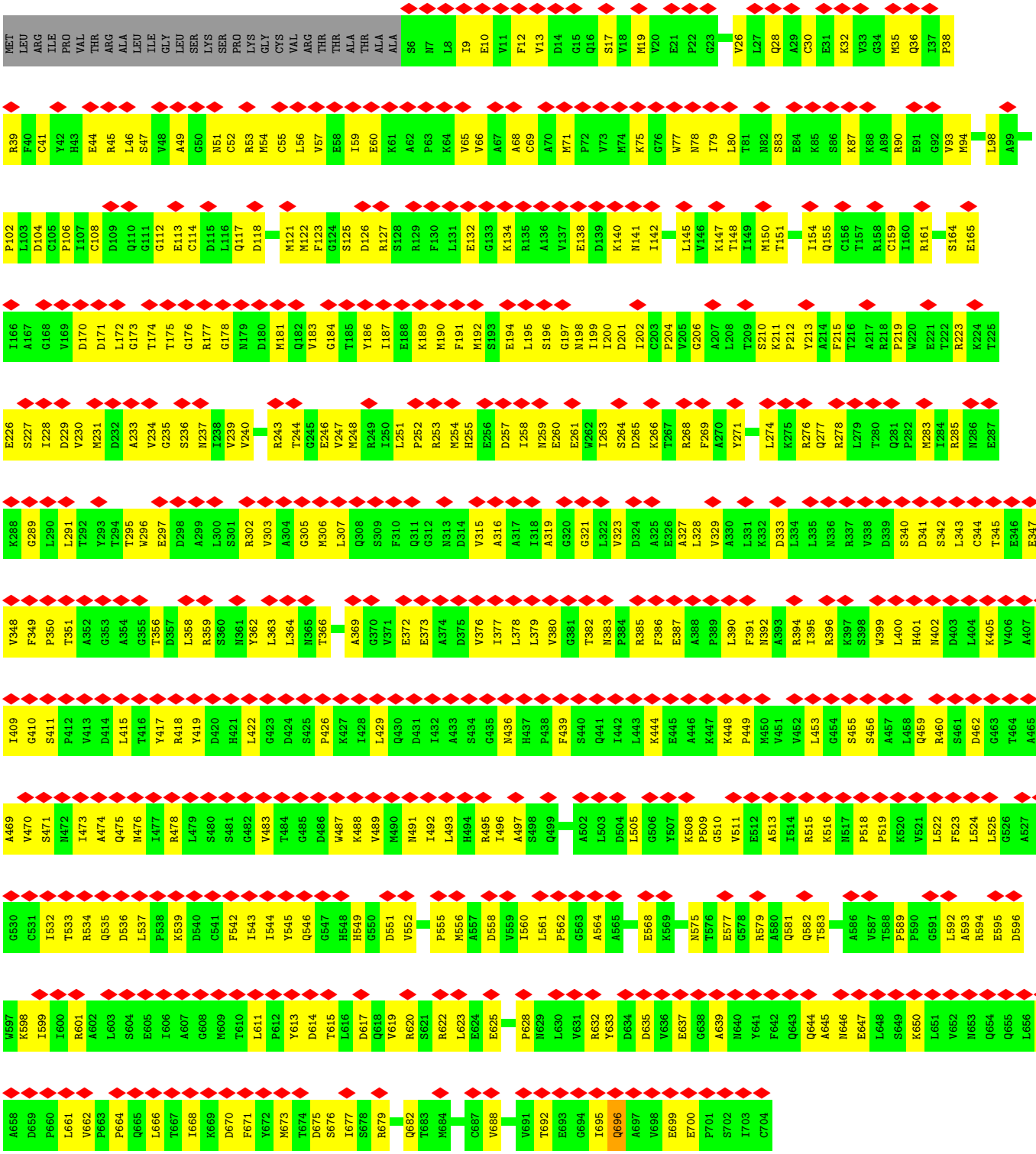
Chain 1F:





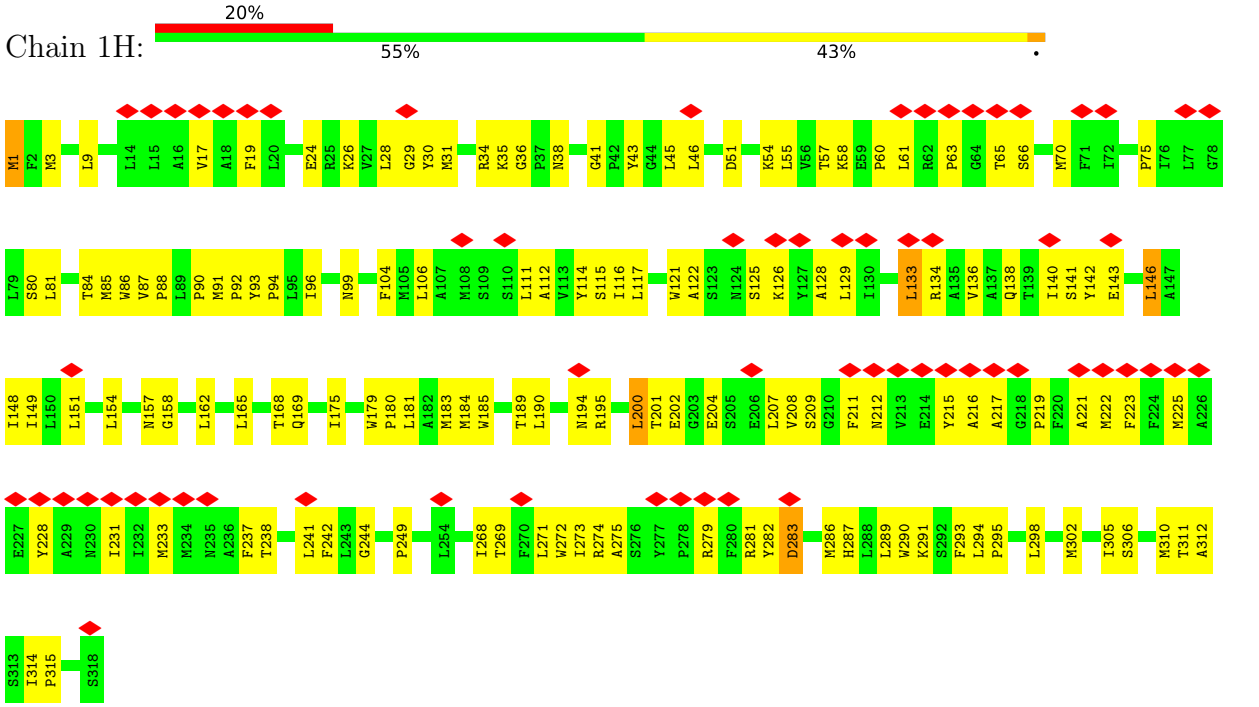
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G:



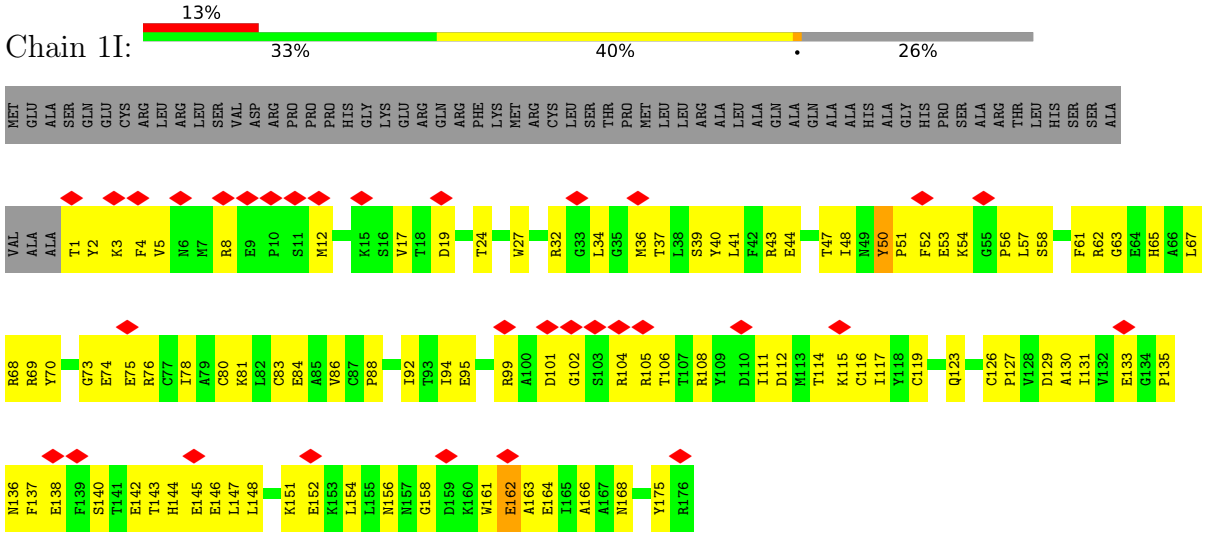
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H:



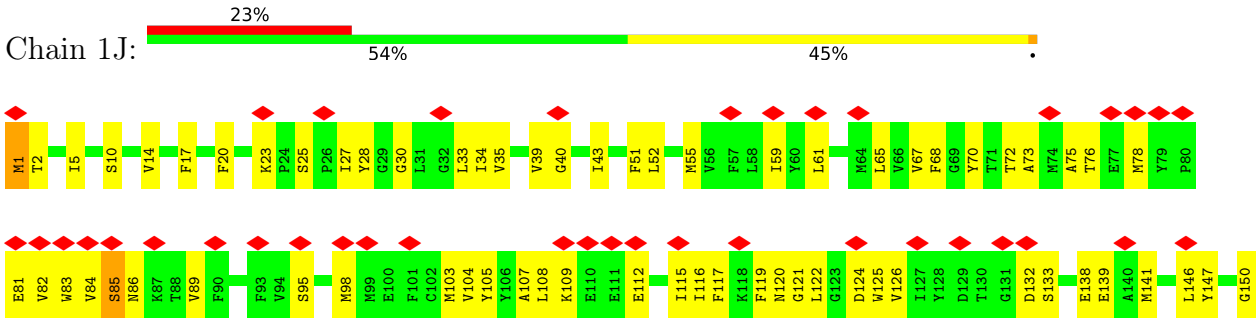
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I:



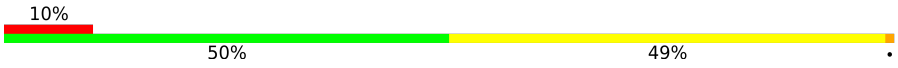
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

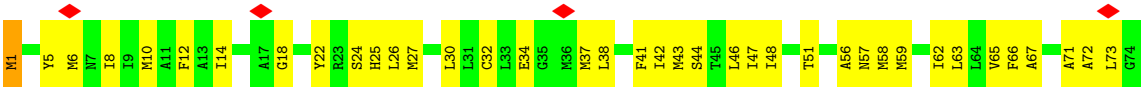
Chain 1J:

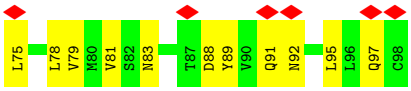


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K:

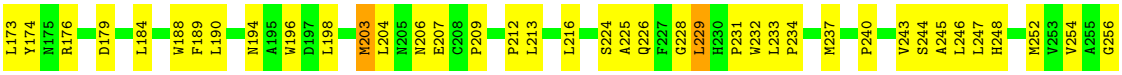


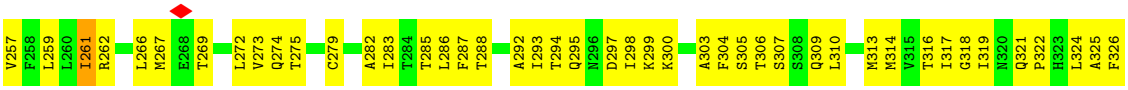


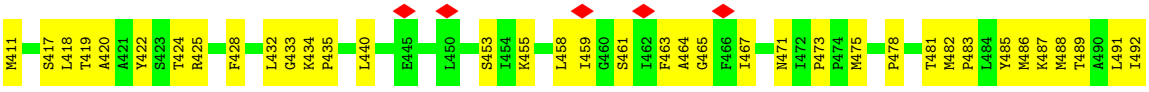


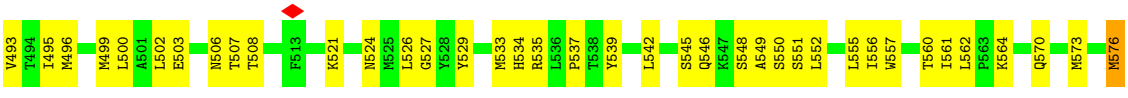
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

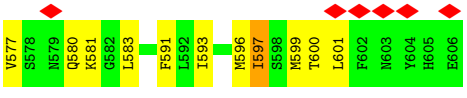
Chain 1L:





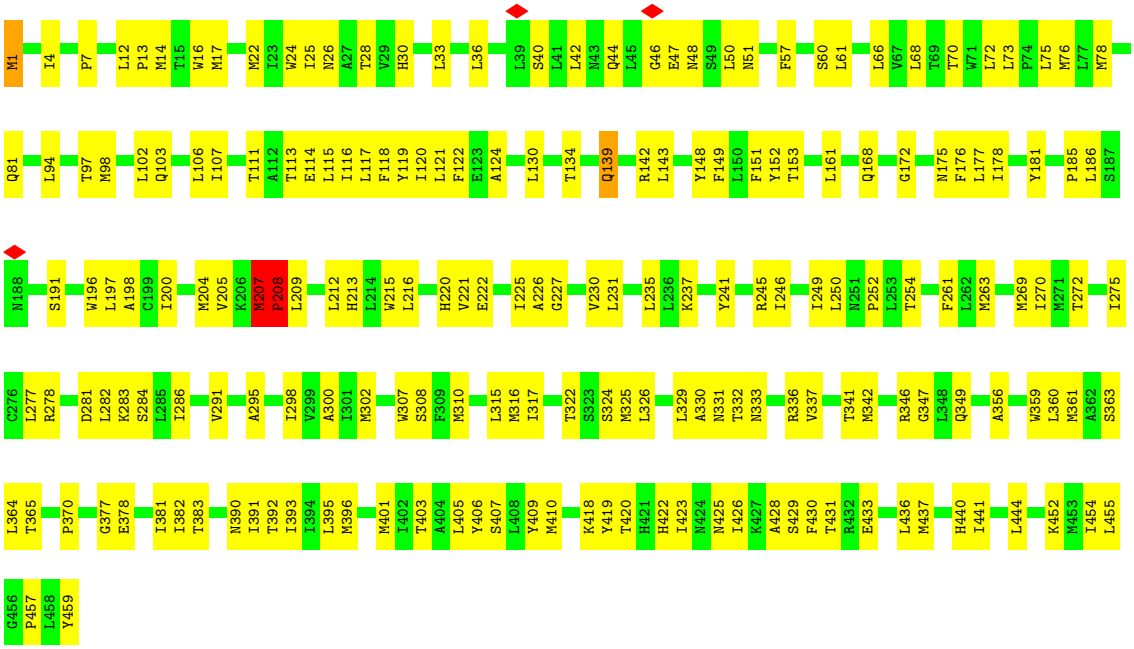






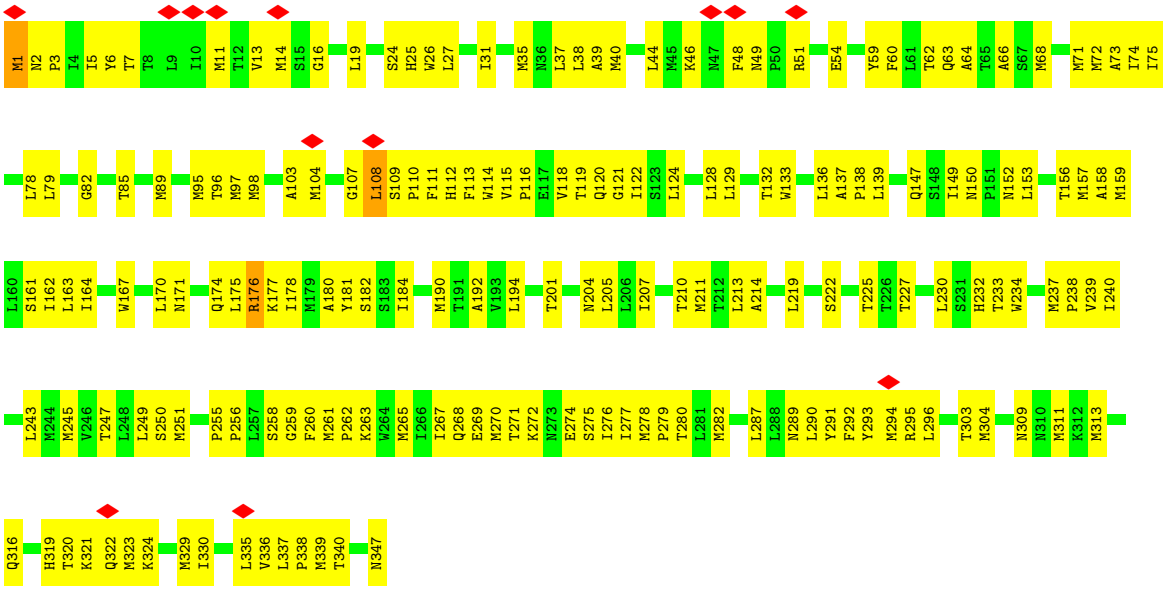
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain 1M:



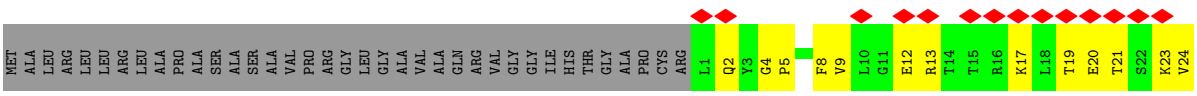
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

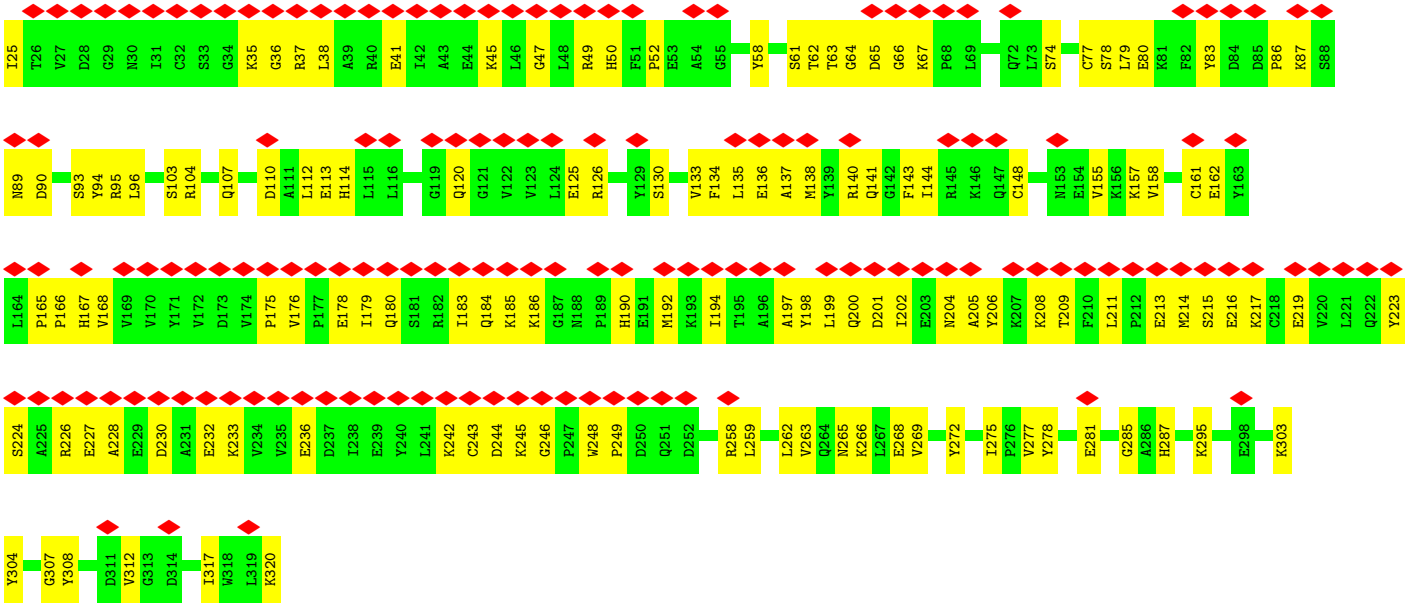
Chain 1N:



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

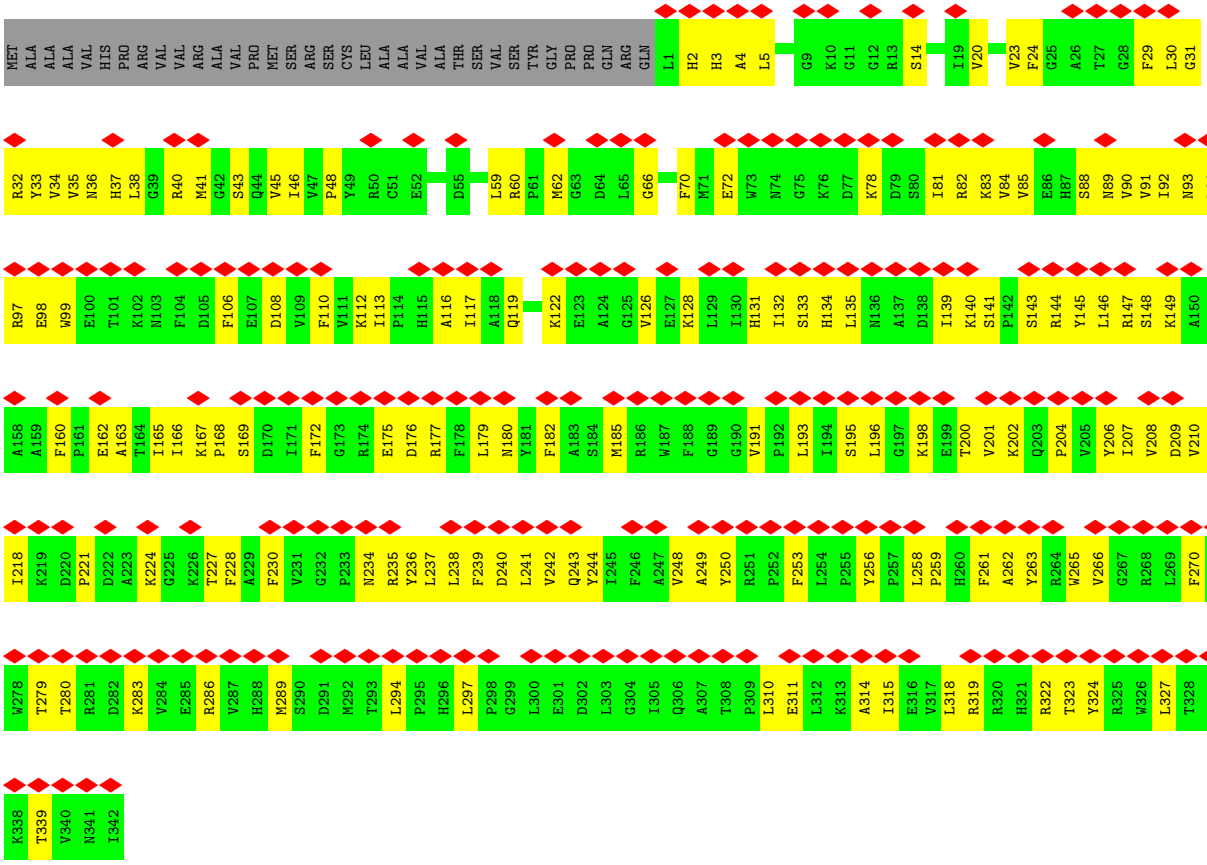
Chain 1O:





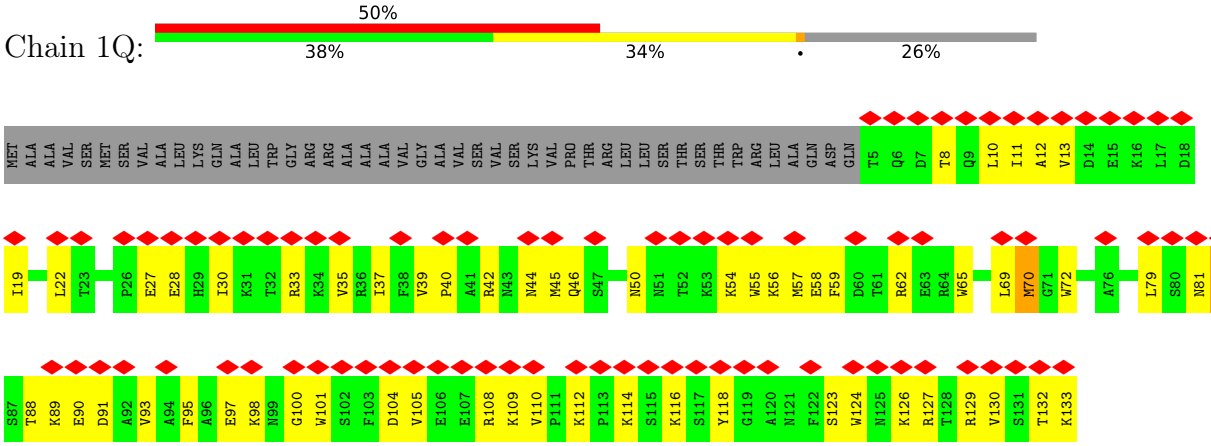
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

Chain 1P:



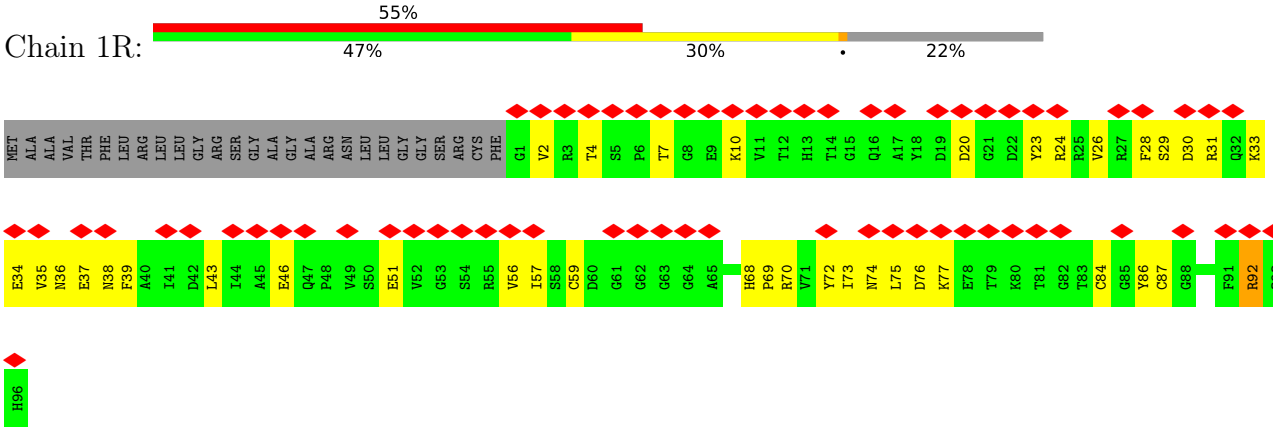
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

Chain 1Q:



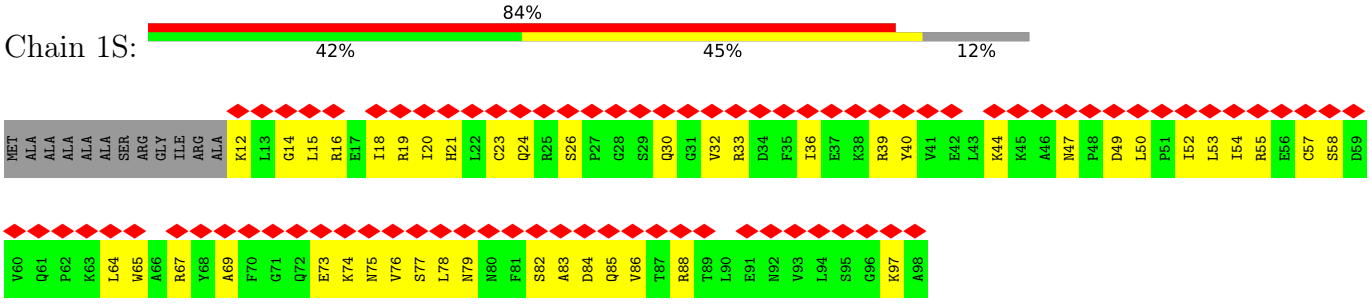
• Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

Chain 1R:



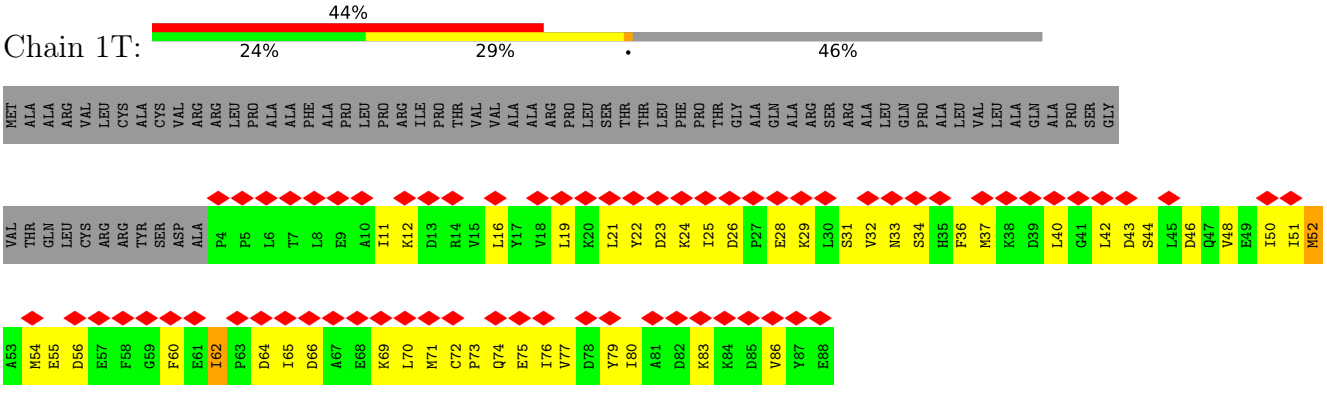
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain 1S:



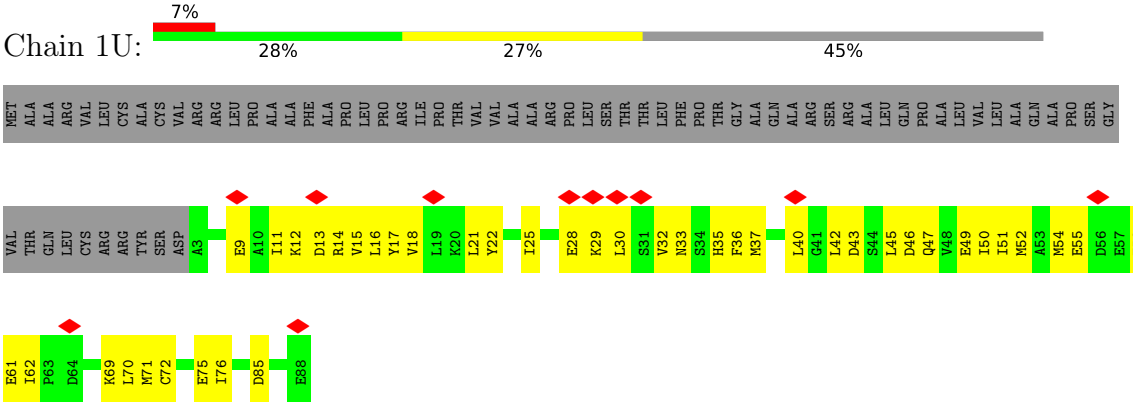
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1T:



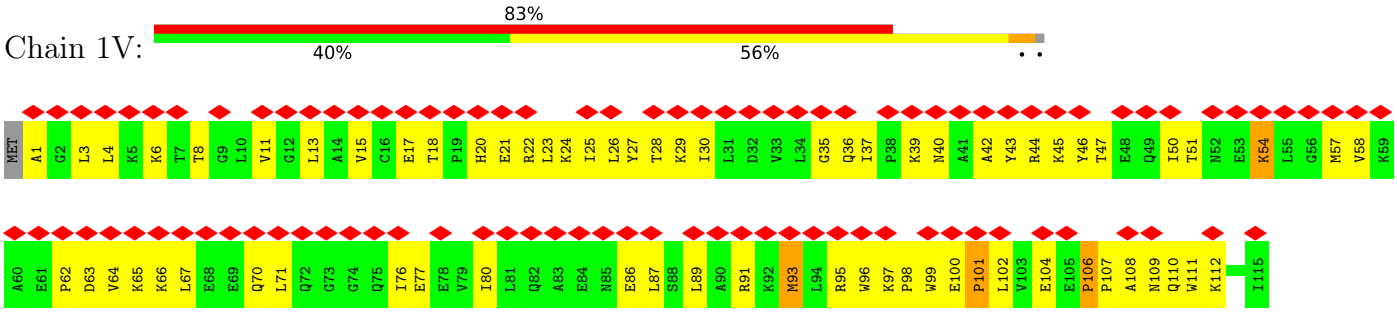
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

Chain 1U:



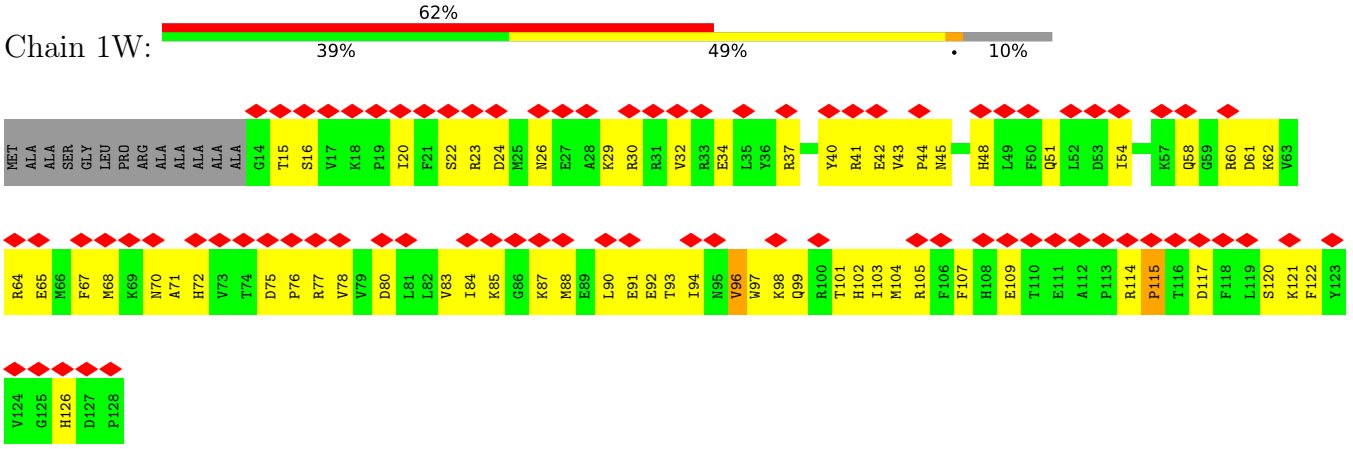
• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V:



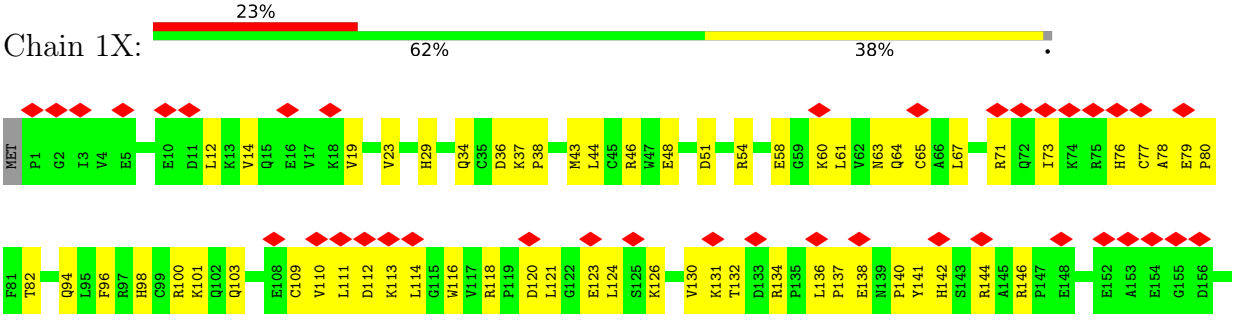
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

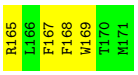
Chain 1W:



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

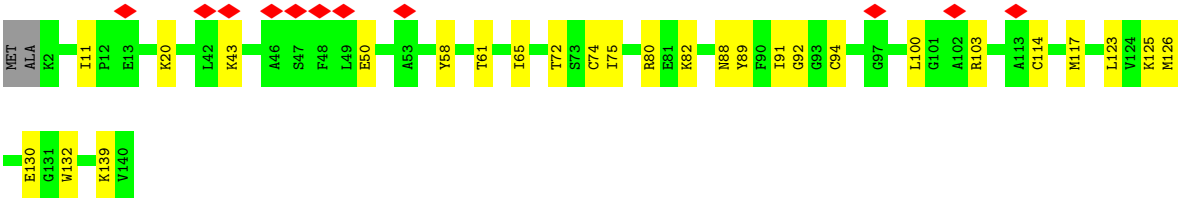
Chain 1X:





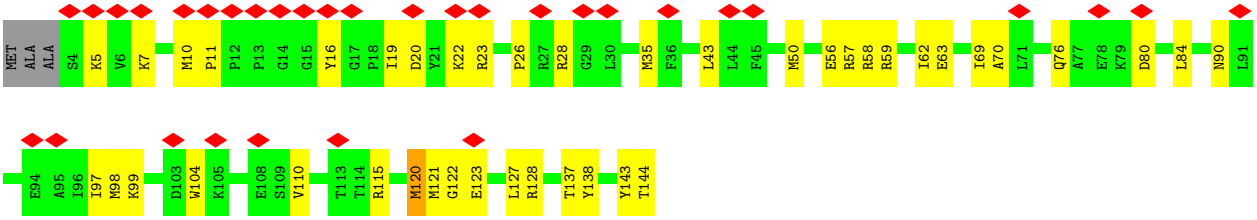
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y:



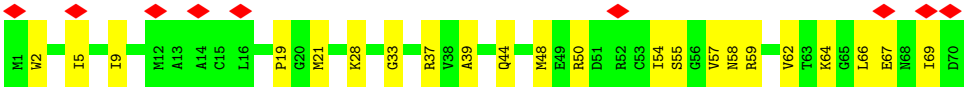
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z:



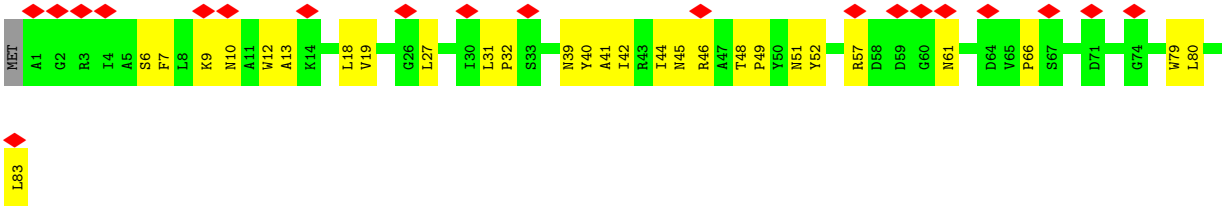
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a:



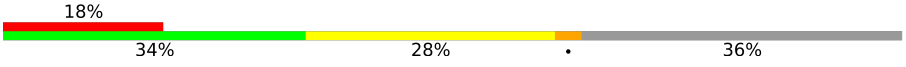
• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b:



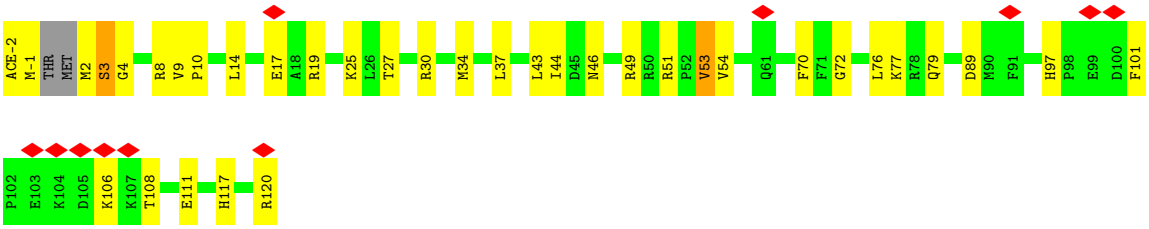
• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain 1c:



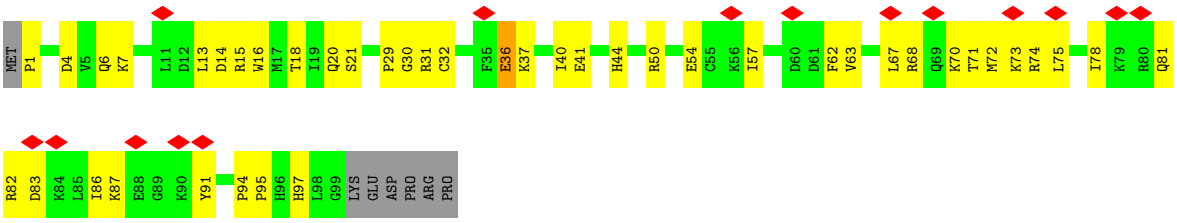
• Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain 1d:



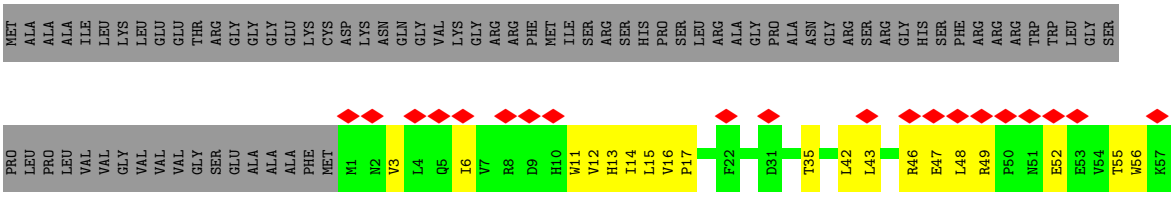
• Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e:



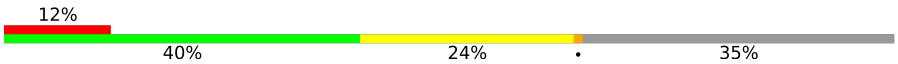
• Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

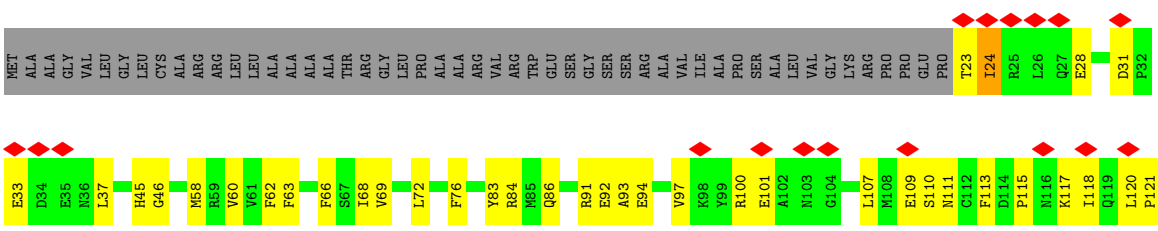
Chain 1f:



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

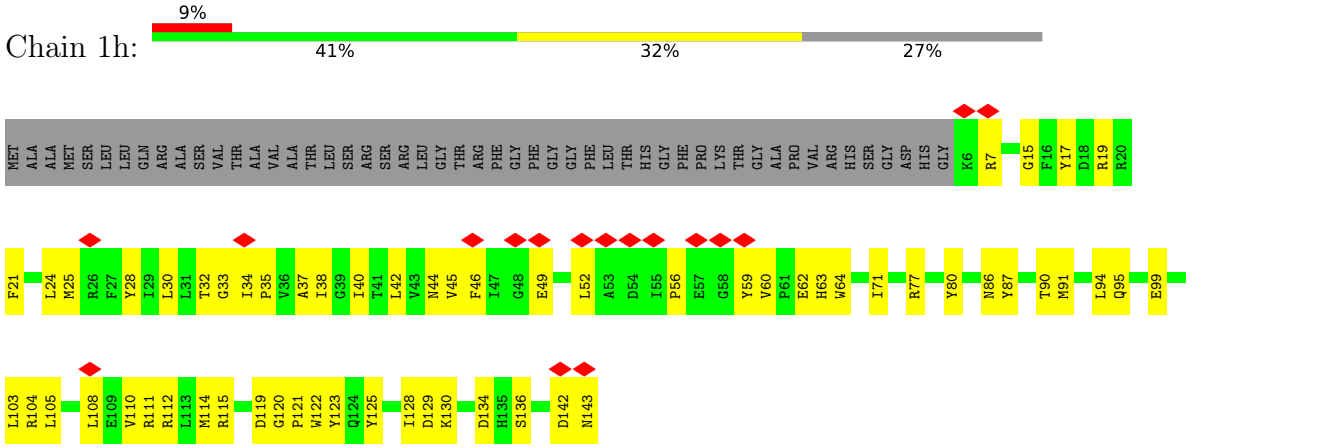
Chain 1g:





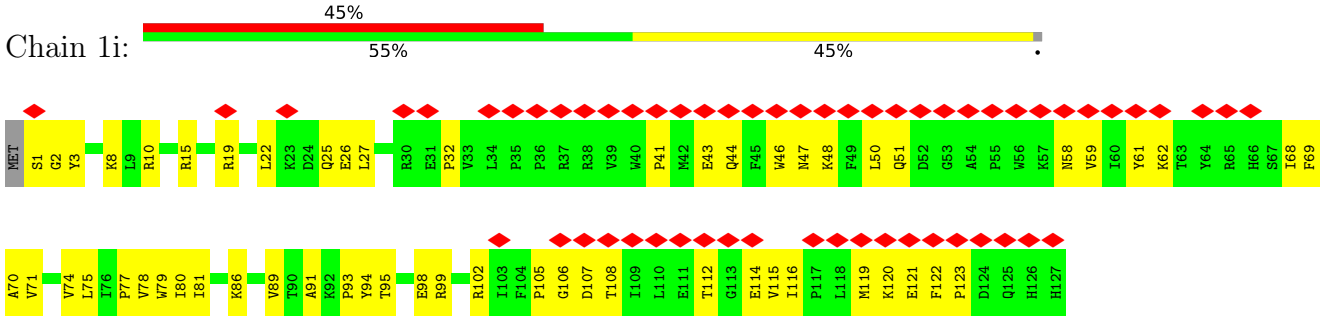
• Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h:



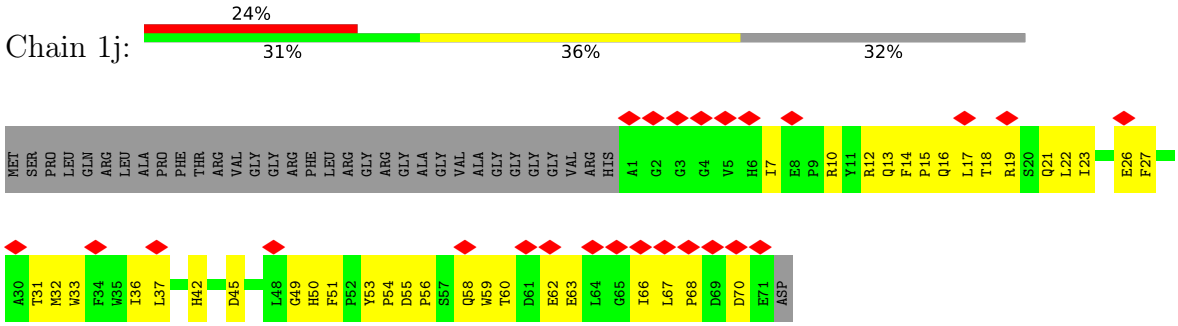
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:



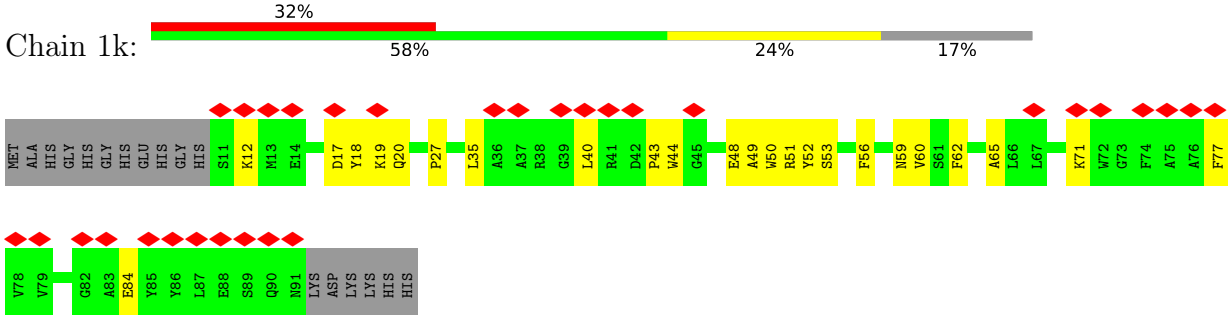
• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

Chain 1j:



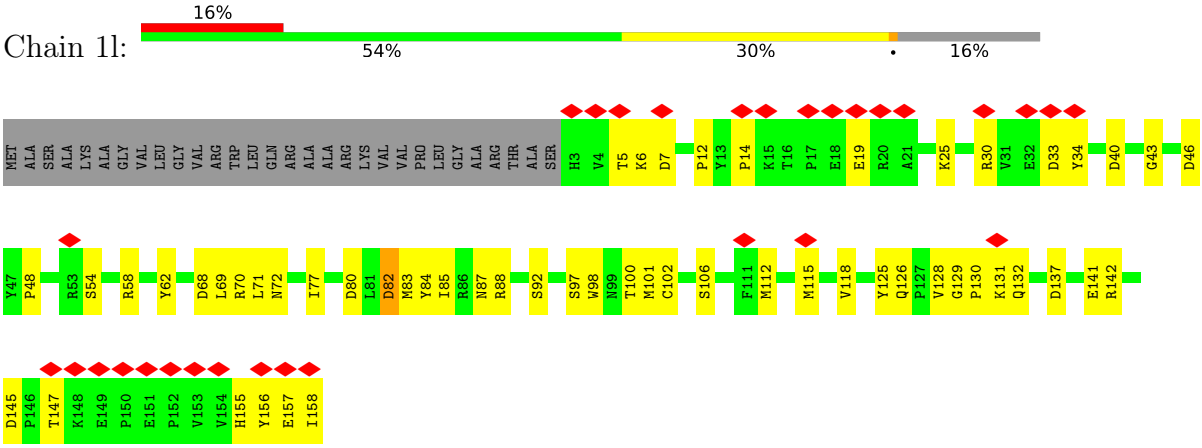
• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain 1k:



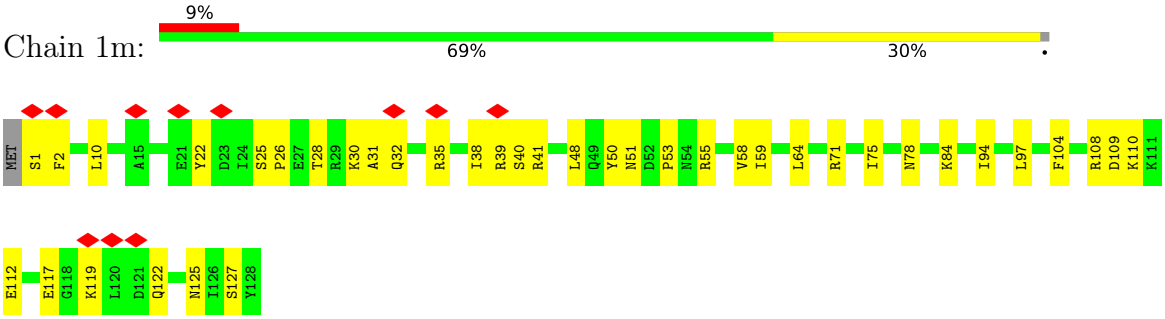
• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain 1l:



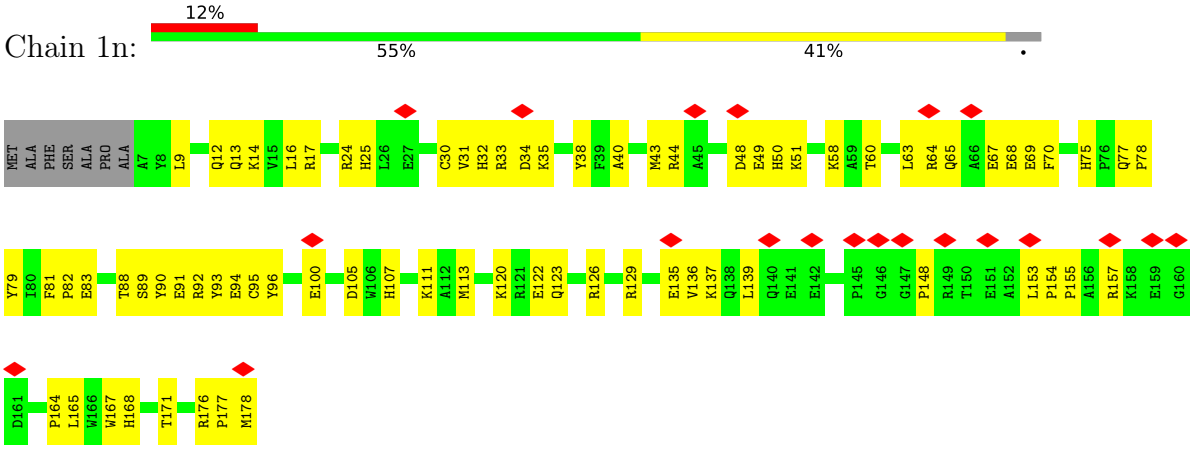
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m:



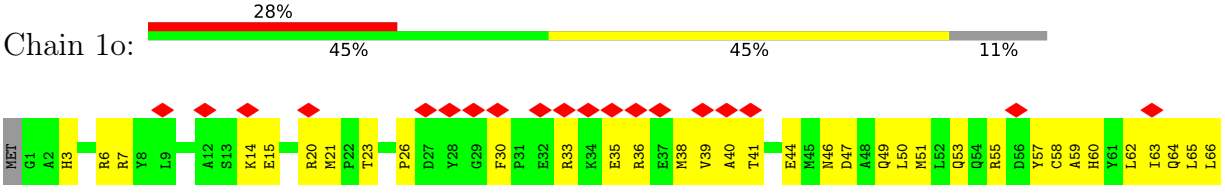
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

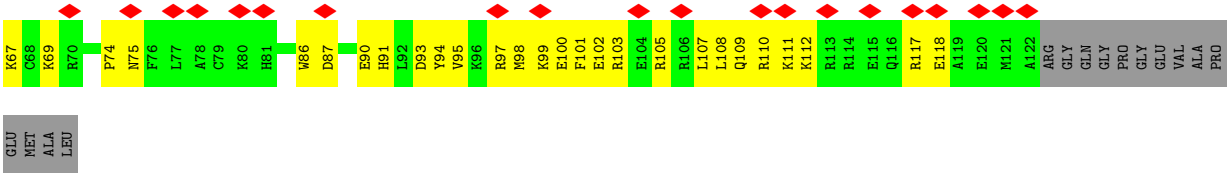
Chain 1n:



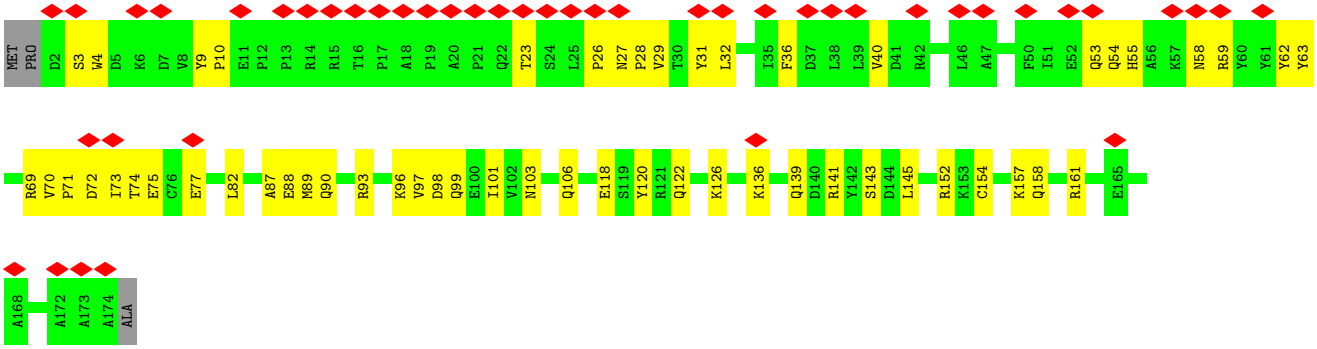
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o:

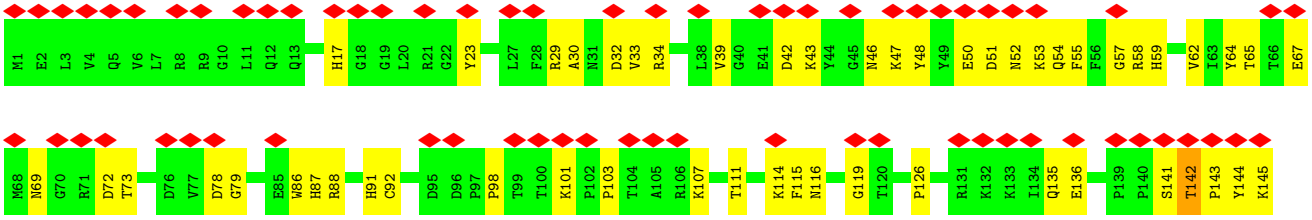




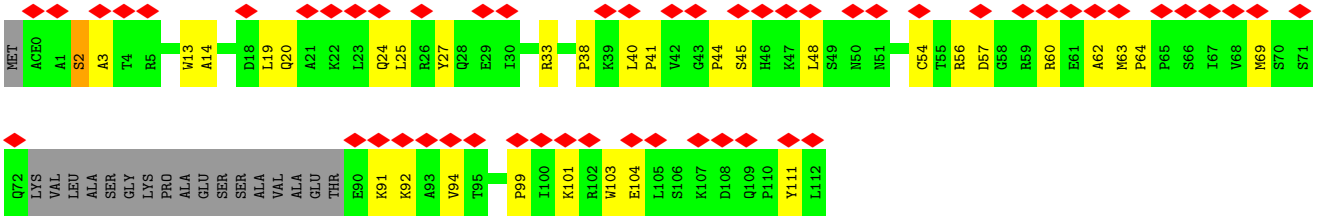
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



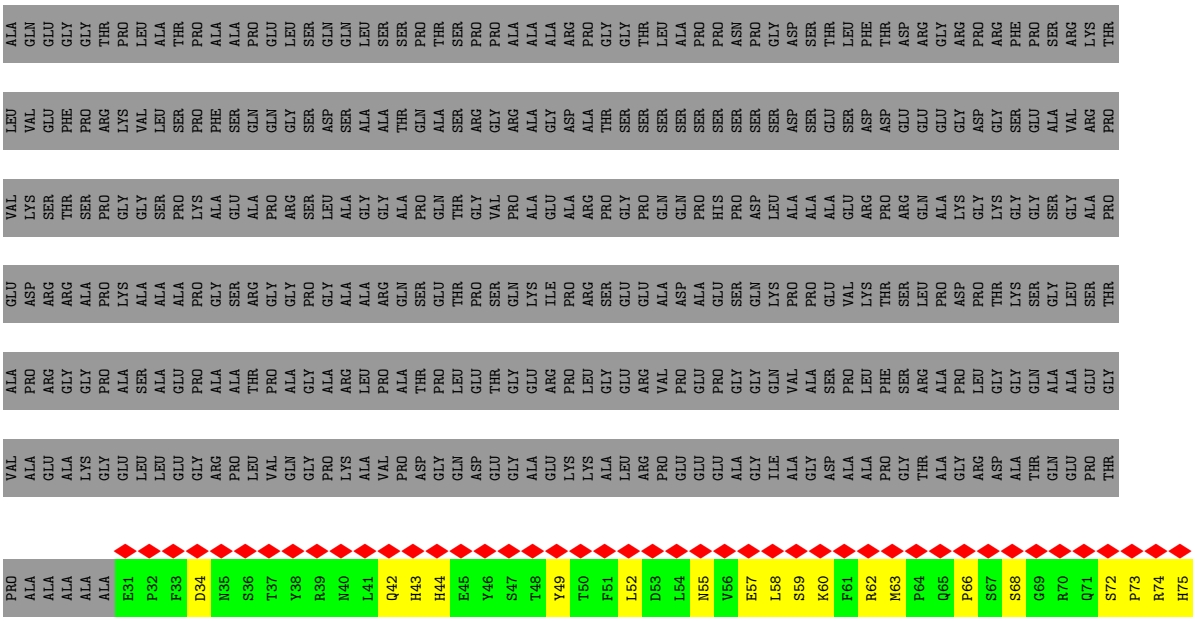
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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


ALA GLN GLU GLY GLY THR PRO LEU ALA THR PRO ALA ALA PRO GLU LEU SER GLN GLN LEU SER SER PRO THR SER PRO PRO ALA ALA ALA ARG PRO GLY GLY THR LEU ALA PRO PRO ASN PRO GLY ASP SER THR LEU PHE THR ASP ARG GLY ARG PRO ARG PHE PRO SER ARG LYS THR
LEU VAL GLU PHE PRO ARG LYS VAL LEU SER PRO PHE SER GLN GLN GLY SER ASP SER ALA ALA THR GLN ALA SER ARG GLY ARG ALA GLY ASP ALA THR GLY PRO SER SER SER SER SER SER SER ASP SER GLU SER ASP ASP GLU GLU GLU GLY ASP GLY SER GLU ALA VAL ARG PRO
VAL LYS SER THR SER PRO GLY GLY SER PRO LYS ALA GLU ALA PRO ARG SER LEU ALA ALA GLY GLY ALA PRO GLN THR GLY VAL PRO ALA GLU GLY ALA ARG PRO GLY PRO GLN GLN HIS PRO ASP LEU ALA ALA GLU ARG PRO ARG GLN ALA LYS GLY LYS GLY GLY SER GLY LEU SER PRO
GLU ASP ARG ARG ALA PRO LYS ALA ALA PRO GLY SER ARG GLY GLY PRO GLY ALA ALA ARG GLN SER GLU THR PRO SER GLN LYS ILE PRO ARG SER GLU GLU ALA ASP ALA GLU SER GLN LYS PRO PRO GLU VAL LYS THR SER LEU PRO ASP PRO THR LYS SER GLY LEU SER THR
ALA PRO ARG GLY GLY PRO ALA SER ALA GLU PRO ALA ALA THR PRO LEU GLU GLU THR GLY GLU ARG PRO LEU GLY GLU ARG VAL PRO GLU PRO GLY GLY GLY GLN VAL ALA SER PRO LEU PHE SER ARG ALA PRO LEU GLY GLN ALA GLY GLY GLN ALA ALA GLU GLY
VAL ALA GLU ALA LYS GLY GLU LEU LEU GLU GLY ARG PRO LEU VAL GLN GLY PRO LYS ALA VAL PRO ASP GLY GLN ASP GLU GLY GLY ALA GLU LYS LYS ALA LEU ARG PRO GLU GLU GLU ALA GLY ILE ALA GLY ASP ALA ALA PRO GLY THR ALA GLY ARG ASP ALA THR GLN GLU PRO THR
PRO ALA ALA ALA ALA E31 P32 F33 D34 N35 S36 T37 Y38 R39 N40 L41 Q42 H43 H44 E45 Y46 S47 T48 Y49 T50 F51 L52 D53 L54 N55 V56 E57 L58 S59 K60 F61 R62 M63 P64 Q65 P66 S67 S68 G69 R70 Q71 S72 P73 R74 H75

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	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)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.941	Depositor
Minimum map value	-0.401	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGT, FME, SAC, ACE, PC1, K, EHZ, NDP, ZN, GTP, MG, MYR, FES, SF4, CDL, 3PE, FMN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	1A	0.16	0/713	0.38	0/975
2	1B	0.18	0/1273	0.46	0/1722
3	1C	0.18	0/1791	0.46	0/2439
4	1D	0.16	0/3545	0.38	0/4806
5	1E	0.16	0/1698	0.46	0/2311
6	1F	0.30	2/3401 (0.1%)	0.55	5/4595 (0.1%)
7	1G	0.17	0/5451	0.45	2/7387 (0.0%)
8	1H	0.15	0/2566	0.41	0/3509
9	1I	0.17	0/1443	0.43	0/1952
10	1J	0.15	0/1364	0.43	0/1850
11	1K	0.14	0/751	0.41	0/1018
12	1L	0.16	0/4939	0.41	1/6718 (0.0%)
13	1M	0.15	0/3713	0.41	2/5063 (0.0%)
14	1N	0.16	0/2765	0.44	0/3758
15	1O	0.13	0/2650	0.37	0/3588
16	1P	0.14	0/2828	0.41	0/3834
17	1Q	0.15	0/1070	0.45	0/1446
18	1R	0.16	0/755	0.72	2/1018 (0.2%)
19	1S	0.18	0/711	0.52	0/956
20	1T	0.18	0/701	0.52	0/946
20	1U	0.17	0/706	0.48	0/954
21	1V	0.31	0/946	0.75	5/1281 (0.4%)
22	1W	1.15	3/995 (0.3%)	1.12	5/1340 (0.4%)
23	1X	0.13	0/1436	0.37	0/1938
24	1Y	0.10	0/1037	0.29	0/1404
25	1Z	0.15	0/1199	0.38	0/1617
26	1a	0.15	0/577	0.38	0/777
27	1b	0.14	0/664	0.39	0/912
28	1c	0.27	0/430	0.65	2/581 (0.3%)
29	1d	0.14	0/1024	0.36	0/1383
30	1e	0.16	0/836	0.41	1/1118 (0.1%)
31	1f	0.14	0/499	0.38	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
32	1g	0.16	0/858	0.43	0/1165
33	1h	0.15	0/1184	0.35	0/1603
34	1i	0.12	0/1131	0.33	0/1541
35	1j	0.13	0/627	0.37	0/858
36	1k	0.15	0/668	0.36	0/903
37	1l	0.15	0/1365	0.37	0/1867
38	1m	0.12	0/1092	0.35	0/1481
39	1n	0.10	0/1549	0.29	0/2098
40	1o	0.12	0/1069	0.36	0/1430
41	1p	0.12	0/1481	0.32	0/1997
42	1q	0.18	0/1253	0.47	0/1704
43	1r	0.16	0/782	0.46	0/1057
44	1s	0.17	0/394	0.45	0/533
All	All	0.22	5/67930 (0.0%)	0.45	25/92106 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	1M	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1W	115	PRO	CG-CD	-33.16	0.38	1.50
6	1F	299	PRO	CG-CD	-10.87	1.13	1.50
22	1W	115	PRO	N-CD	9.05	1.60	1.47
22	1W	115	PRO	CB-CG	7.68	1.88	1.49
6	1F	299	PRO	N-CD	6.54	1.56	1.47

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	1W	115	PRO	N-CD-CG	-30.04	58.15	103.20
22	1W	115	PRO	CA-CB-CG	-13.05	79.70	104.50
18	1R	92	ARG	CA-C-N	12.68	141.61	121.83
18	1R	92	ARG	C-N-CA	12.68	141.61	121.83
6	1F	90	PRO	CA-N-CD	-12.61	94.35	112.00
6	1F	299	PRO	N-CD-CG	-12.54	84.40	103.20
6	1F	299	PRO	CA-N-CD	-12.25	94.85	112.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	1G	426	PRO	CA-N-CD	-11.70	95.62	112.00
22	1W	115	PRO	CA-N-CD	-11.12	96.43	112.00
28	1c	7	PRO	CA-N-CD	-10.35	97.51	112.00
21	1V	106	PRO	CA-N-CD	-9.57	98.60	112.00
21	1V	62	PRO	CA-N-CD	-9.34	98.92	112.00
22	1W	115	PRO	N-CA-CB	-8.32	95.59	103.33
7	1G	426	PRO	N-CD-CG	-7.66	91.71	103.20
6	1F	90	PRO	N-CD-CG	-7.34	92.18	103.20
6	1F	299	PRO	CA-CB-CG	-7.24	90.75	104.50
13	1M	208	PRO	CA-N-CD	-6.79	102.50	112.00
21	1V	101	PRO	CA-N-CD	-6.21	103.31	112.00
13	1M	207	MET	C-N-CD	-6.14	99.82	125.00
30	1e	95	PRO	CA-N-CD	-5.73	103.98	112.00
21	1V	106	PRO	N-CA-CB	-5.58	100.32	103.22
12	1L	203	MET	CB-CG-SD	5.30	128.60	112.70
21	1V	108	ALA	CB-CA-C	-5.18	110.59	116.54
28	1c	7	PRO	N-CD-CG	-5.08	95.58	103.20
22	1W	115	PRO	CB-CG-CD	-5.03	90.00	106.10

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	1M	207	MET	Peptide
13	1M	208	PRO	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	707	0	757	52	0
2	1B	1242	0	1249	83	0
3	1C	1740	0	1691	136	0
4	1D	3452	0	3389	186	0
5	1E	1658	0	1662	134	0
6	1F	3325	0	3288	259	0
7	1G	5362	0	5388	318	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	1H	2504	0	2602	133	0
9	1I	1412	0	1366	114	0
10	1J	1339	0	1337	76	0
11	1K	750	0	798	47	0
12	1L	4818	0	4956	261	0
13	1M	3632	0	3834	186	0
14	1N	2712	0	2873	158	0
15	1O	2590	0	2556	118	0
16	1P	2751	0	2776	155	0
17	1Q	1047	0	1042	67	0
18	1R	741	0	704	33	0
19	1S	700	0	719	46	0
20	1T	689	0	687	53	0
20	1U	694	0	691	40	0
21	1V	927	0	972	63	0
22	1W	971	0	975	83	0
23	1X	1398	0	1378	65	0
24	1Y	1016	0	1019	19	0
25	1Z	1168	0	1161	52	0
26	1a	562	0	557	17	0
27	1b	643	0	644	23	0
28	1c	417	0	425	19	0
29	1d	996	0	990	37	0
30	1e	816	0	823	42	0
31	1f	487	0	498	18	0
32	1g	835	0	794	48	0
33	1h	1151	0	1164	64	0
34	1i	1100	0	1106	56	0
35	1j	601	0	546	35	0
36	1k	649	0	626	28	0
37	1l	1310	0	1204	59	0
38	1m	1062	0	1075	45	0
39	1n	1495	0	1434	64	0
40	1o	1045	0	1018	64	0
41	1p	1449	0	1416	62	0
42	1q	1212	0	1172	53	0
43	1r	767	0	790	39	0
44	1s	382	0	351	26	0
45	1A	35	0	44	2	0
45	1H	44	0	60	5	0
45	1I	54	0	88	4	0
45	1M	46	0	69	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1g	44	0	61	0	0
46	1B	8	0	0	2	0
46	1F	8	0	0	2	0
46	1G	16	0	0	1	0
46	1I	16	0	0	2	0
47	1E	4	0	0	3	0
47	1G	4	0	0	0	0
48	1F	31	0	19	2	0
49	1G	1	0	0	0	0
50	1L	88	0	125	5	0
50	1N	51	0	82	9	0
50	1Y	82	0	113	4	0
50	1b	47	0	69	1	0
51	1M	51	0	78	9	0
52	1N	77	0	96	4	0
52	1r	61	0	65	4	0
53	1O	32	0	12	1	0
54	1O	1	0	0	0	0
55	1P	48	0	26	5	0
56	1R	1	0	0	0	0
57	1W	37	0	0	1	0
57	1n	37	0	0	2	0
58	1l	15	0	27	1	0
All	All	67263	0	67537	3148	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 23.

All (3148) 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)
5:1E:144:CYS:HB2	47:1E:301:FES:S1	2.06	0.95
7:1G:41:CYS:HB3	7:1G:52:CYS:SG	2.07	0.93
7:1G:366:THR:H	7:1G:491:ASN:HD21	1.19	0.90
15:1O:138:MET:HG2	15:1O:144:ILE:HG12	1.54	0.90
14:1N:261:MET:HE1	14:1N:340:THR:HA	1.55	0.88
13:1M:208:PRO:HG3	13:1M:291:VAL:HA	1.57	0.87
14:1N:109:SER:HB3	14:1N:157:MET:HG3	1.56	0.86
43:1r:63:MET:HE3	43:1r:64:PRO:HD2	1.57	0.86
7:1G:283:MET:HG3	7:1G:291:LEU:HD12	1.58	0.85
12:1L:283:ILE:HD13	37:1l:112:MET:HG3	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:393:ALA:HB3	4:1D:396:PHE:HB2	1.59	0.84
29:1d:53:VAL:HG23	29:1d:54:VAL:H	1.42	0.84
1:1A:98:LEU:HB3	8:1H:298:LEU:HD21	1.60	0.83
35:1j:54:PRO:HB2	35:1j:59:TRP:HE1	1.43	0.83
12:1L:69:MET:HE3	12:1L:70:THR:H	1.43	0.83
3:1C:132:ARG:HG2	3:1C:149:ARG:H	1.41	0.82
7:1G:283:MET:HB3	7:1G:560:ILE:HB	1.62	0.81
7:1G:113:GLU:HG3	7:1G:219:PRO:HG3	1.62	0.81
12:1L:306:THR:HG22	12:1L:336:LYS:HD2	1.63	0.81
15:1O:194:ILE:HD13	15:1O:199:LEU:HD13	1.63	0.80
7:1G:349:PHE:HB3	7:1G:509:PRO:HB2	1.63	0.80
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.63	0.80
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.63	0.80
5:1E:124:LEU:HD11	5:1E:137:PHE:HD2	1.46	0.80
10:1J:120:ASN:H	11:1K:1:FME:H	1.30	0.79
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	1.64	0.79
2:1B:79:SER:HG	8:1H:209:SER:HG	1.30	0.79
3:1C:77:ASP:HA	3:1C:130:TYR:HE1	1.47	0.79
7:1G:453:LEU:HB3	7:1G:492:ILE:HG22	1.63	0.79
22:1W:42:GLU:OE1	22:1W:45:ASN:ND2	2.15	0.79
19:1S:74:LYS:HD3	19:1S:75:ASN:H	1.48	0.79
21:1V:13:LEU:HD11	21:1V:77:GLU:HB3	1.64	0.78
5:1E:36:LYS:HG2	44:1s:62:ARG:HE	1.49	0.78
22:1W:115:PRO:HB2	22:1W:121:LYS:HD2	1.64	0.78
6:1F:337:MET:HE1	6:1F:343:ILE:HA	1.64	0.78
16:1P:315:ILE:H	16:1P:331:MET:HE1	1.48	0.78
39:1n:155:PRO:HG2	39:1n:157:ARG:HH12	1.49	0.78
6:1F:42:TRP:HE1	6:1F:116:HIS:HB2	1.49	0.78
32:1g:120:LEU:HD12	32:1g:121:PRO:HD2	1.66	0.78
37:1l:30:ARG:HH12	38:1m:35:ARG:HG2	1.48	0.78
5:1E:31:ILE:HA	5:1E:34:ILE:HG12	1.67	0.77
9:1I:63:GLY:H	9:1I:133:GLU:HB3	1.48	0.77
3:1C:12:ARG:HH12	4:1D:124:LYS:HG3	1.49	0.77
2:1B:48:MET:HE3	2:1B:80:PRO:HD3	1.65	0.77
6:1F:272:MET:SD	6:1F:273:SER:OG	2.43	0.77
18:1R:33:LYS:HD2	18:1R:35:VAL:HG22	1.65	0.77
15:1O:77:CYS:HB3	15:1O:95:ARG:HG2	1.67	0.76
7:1G:38:PRO:HG2	7:1G:90:ARG:HD3	1.67	0.76
12:1L:190:LEU:HD23	13:1M:383:THR:HG21	1.67	0.76
6:1F:213:VAL:HG13	6:1F:217:GLY:HA2	1.66	0.76
15:1O:205:ALA:O	15:1O:209:THR:OG1	2.04	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:52:MET:HA	20:1T:55:GLU:HG2	1.67	0.76
8:1H:24:GLU:OE2	8:1H:274:ARG:NH1	2.18	0.76
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	1.68	0.76
12:1L:90:ILE:HD12	12:1L:129:MET:HE3	1.68	0.75
6:1F:322:LEU:HD12	6:1F:329:LEU:HB2	1.66	0.75
6:1F:355:LYS:HD2	6:1F:370:ASP:HA	1.66	0.75
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	1.66	0.75
16:1P:146:LEU:HD11	16:1P:289:MET:HE2	1.68	0.74
5:1E:88:THR:OG1	6:1F:181:ALA:O	2.04	0.74
45:1A:201:PC1:H32	10:1J:151:THR:HG21	1.67	0.74
17:1Q:90:GLU:OE2	17:1Q:90:GLU:N	2.19	0.74
22:1W:62:LYS:HG2	22:1W:107:PHE:HE1	1.51	0.74
28:1c:7:PRO:HD2	28:1c:7:PRO:O	1.87	0.74
3:1C:116:PRO:HG3	22:1W:20:ILE:HD13	1.70	0.74
3:1C:130:TYR:OH	4:1D:392:LYS:NZ	2.18	0.74
16:1P:324:TYR:HA	16:1P:327:LEU:HD23	1.70	0.74
16:1P:250:TYR:HB2	16:1P:322:ARG:HH21	1.51	0.74
6:1F:295:LEU:HD22	6:1F:339:ARG:HA	1.70	0.74
16:1P:46:ILE:HD13	18:1R:26:VAL:HG21	1.69	0.74
40:1o:62:LEU:HD12	40:1o:65:LEU:HD13	1.70	0.74
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	1.68	0.74
42:1q:65:THR:O	42:1q:73:THR:OG1	2.06	0.74
13:1M:181:TYR:O	41:1p:152:ARG:NH2	2.21	0.74
2:1B:179:ARG:HH11	16:1P:97:ARG:HH22	1.35	0.74
5:1E:150:ASN:ND2	5:1E:151:ALA:O	2.20	0.74
7:1G:392:ASN:HA	7:1G:395:ILE:HD12	1.69	0.74
20:1U:36:PHE:HA	20:1U:40:LEU:HD23	1.69	0.74
16:1P:249:ALA:HB2	16:1P:318:LEU:HD12	1.70	0.73
12:1L:593:ILE:HG22	12:1L:597:ILE:HD11	1.70	0.73
3:1C:114:LEU:HB2	22:1W:77:ARG:HH21	1.54	0.73
37:1l:130:PRO:HD3	40:1o:21:MET:HE1	1.69	0.73
6:1F:391:SER:HB2	43:1r:48:LEU:HD13	1.70	0.73
12:1L:174:TYR:HD1	12:1L:229:LEU:HD23	1.54	0.73
15:1O:112:LEU:HD11	15:1O:248:TRP:HZ2	1.52	0.73
12:1L:488:MET:HE1	12:1L:491:LEU:HD12	1.69	0.73
13:1M:237:LYS:HD2	13:1M:316:MET:HB3	1.71	0.73
40:1o:105:ARG:HG2	40:1o:109:GLN:HE22	1.54	0.73
1:1A:75:LEU:HD21	8:1H:305:ILE:HD12	1.69	0.73
8:1H:209:SER:HB3	8:1H:212:ASN:HB2	1.71	0.72
19:1S:85:GLN:OE1	19:1S:88:ARG:NH2	2.22	0.72
5:1E:148:CYS:HA	5:1E:153:MET:HE1	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:83:CYS:HB3	46:1I:202:SF4:S4	2.29	0.72
19:1S:18:ILE:HD11	19:1S:64:LEU:HD21	1.70	0.72
6:1F:110:ILE:O	6:1F:114:ASP:N	2.19	0.72
8:1H:3:MET:H	8:1H:3:MET:HE3	1.55	0.72
8:1H:1:FME:HB3	8:1H:3:MET:HE1	1.71	0.72
16:1P:182:PHE:HA	16:1P:185:MET:HE2	1.70	0.72
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.70	0.72
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.69	0.72
7:1G:239:VAL:HB	7:1G:251:LEU:HB2	1.71	0.72
14:1N:85:THR:HG22	30:1e:18:THR:HB	1.72	0.72
14:1N:245:MET:HE2	50:1N:401:3PE:H3A2	1.70	0.72
19:1S:12:LYS:HG3	19:1S:14:GLY:H	1.55	0.72
43:1r:101:LYS:NZ	43:1r:104:GLU:OE1	2.23	0.72
7:1G:268:ARG:HD2	7:1G:269:PHE:HE1	1.53	0.71
10:1J:34:ILE:HG23	10:1J:61:LEU:HD21	1.71	0.71
10:1J:166:VAL:HG21	14:1N:5:ILE:HD11	1.71	0.71
3:1C:196:LYS:HZ3	7:1G:223:ARG:HH21	1.38	0.71
5:1E:148:CYS:N	6:1F:105:CYS:SG	2.62	0.71
6:1F:162:ILE:HG13	6:1F:174:ASP:HA	1.70	0.71
7:1G:261:GLU:HB2	17:1Q:44:ASN:HD21	1.55	0.71
12:1L:533:MET:HA	12:1L:533:MET:HE3	1.71	0.71
4:1D:276:ASP:CG	4:1D:277:VAL:H	1.97	0.71
16:1P:35:VAL:HG13	16:1P:45:VAL:HG21	1.72	0.71
3:1C:93:VAL:HG13	3:1C:108:LYS:HG2	1.73	0.71
12:1L:411:MET:HE3	37:1l:112:MET:HE1	1.70	0.71
13:1M:14:MET:HB2	31:1f:15:LEU:HD13	1.72	0.71
16:1P:139:ILE:HA	16:1P:147:ARG:HA	1.72	0.71
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	1.72	0.71
13:1M:422:HIS:HB2	38:1m:59:ILE:HD12	1.73	0.71
38:1m:94:ILE:HD12	38:1m:94:ILE:H	1.56	0.71
3:1C:63:PHE:HA	21:1V:89:LEU:HD21	1.71	0.71
4:1D:312:SER:HB2	25:1Z:19:ILE:HD11	1.71	0.71
7:1G:386:PHE:HB3	7:1G:671:PHE:HB2	1.71	0.71
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.72	0.71
12:1L:357:ARG:HG2	39:1n:31:VAL:HG22	1.72	0.71
4:1D:178:PHE:HZ	4:1D:189:MET:HG2	1.55	0.70
4:1D:376:VAL:HG12	4:1D:391:ILE:HG22	1.72	0.70
6:1F:277:LYS:HZ3	6:1F:314:THR:HA	1.55	0.70
39:1n:178:MET:HE2	39:1n:178:MET:H	1.56	0.70
4:1D:150:HIS:HB2	4:1D:304:MET:HE3	1.74	0.70
7:1G:594:ARG:NH1	22:1W:122:PHE:O	2.25	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:71:MET:HE2	14:1N:71:MET:HA	1.73	0.70
7:1G:276:ARG:HG3	7:1G:277:GLN:HG2	1.73	0.70
16:1P:97:ARG:NH1	55:1P:501:NDP:O3X	2.25	0.70
3:1C:162:PHE:CZ	4:1D:88:GLU:HG2	2.27	0.70
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.72	0.70
13:1M:393:ILE:HA	13:1M:396:MET:HB2	1.73	0.70
3:1C:35:LYS:NZ	21:1V:97:LYS:O	2.21	0.70
32:1g:100:ARG:HG2	32:1g:107:LEU:HA	1.74	0.70
1:1A:57:LEU:HD21	10:1J:172:THR:HG21	1.72	0.70
23:1X:67:LEU:HB3	23:1X:71:ARG:HH12	1.57	0.70
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.71	0.70
13:1M:231:LEU:HA	13:1M:235:LEU:HD12	1.71	0.70
13:1M:286:ILE:HD13	13:1M:326:LEU:HB3	1.74	0.70
3:1C:82:ASP:HB2	3:1C:138:PHE:HE1	1.56	0.70
7:1G:215:PHE:HD2	9:1I:104:ARG:HE	1.39	0.70
7:1G:252:PRO:HD3	7:1G:268:ARG:HH12	1.57	0.70
7:1G:533:THR:HG23	7:1G:535:GLN:H	1.56	0.70
2:1B:75:VAL:HG22	2:1B:76:PHE:H	1.57	0.69
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.10	0.69
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	1.74	0.69
6:1F:68:ARG:NH2	6:1F:224:ASN:OD1	2.25	0.69
6:1F:106:LYS:HE3	6:1F:257:ASN:HB2	1.75	0.69
7:1G:233:ALA:HA	7:1G:497:ALA:HA	1.73	0.69
9:1I:161:TRP:O	9:1I:163:ALA:N	2.25	0.69
12:1L:417:SER:HB2	12:1L:493:VAL:HG22	1.72	0.69
20:1T:51:ILE:HD13	20:1T:62:ILE:HD11	1.74	0.69
12:1L:542:LEU:HD21	37:1l:88:ARG:HD2	1.72	0.69
5:1E:144:CYS:CB	47:1E:301:FES:S1	2.80	0.69
15:1O:47:GLY:O	15:1O:120:GLN:NE2	2.26	0.69
33:1h:95:GLN:HB2	41:1p:82:LEU:HD21	1.74	0.69
13:1M:326:LEU:HA	13:1M:329:LEU:HD12	1.75	0.69
23:1X:94:GLN:HE22	26:1a:37:ARG:HD3	1.56	0.69
12:1L:170:GLN:HE21	12:1L:232:TRP:HA	1.58	0.69
15:1O:168:VAL:HG23	15:1O:219:GLU:HB2	1.75	0.69
20:1U:12:LYS:HB2	20:1U:16:LEU:HD23	1.74	0.69
6:1F:266:CYS:SG	6:1F:267:THR:N	2.65	0.69
12:1L:207:GLU:HB2	12:1L:269:THR:HG21	1.74	0.69
12:1L:86:SER:OG	12:1L:262:ARG:NH2	2.25	0.69
12:1L:482:MET:HE1	12:1L:487:LYS:HD3	1.73	0.69
7:1G:196:SER:OG	7:1G:265:ASP:OD2	2.11	0.68
14:1N:211:MET:HE3	14:1N:251:MET:HA	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:82:ARG:NH1	16:1P:82:ARG:O	2.26	0.68
9:1I:8:ARG:HH12	43:1r:111:TYR:HB3	1.58	0.68
13:1M:295:ALA:HA	13:1M:298:ILE:HD12	1.75	0.68
6:1F:245:PHE:HB3	6:1F:271:GLU:HG3	1.76	0.68
2:1B:144:ILE:HD11	2:1B:162:GLN:HE21	1.58	0.68
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.76	0.68
6:1F:139:ARG:HD3	6:1F:182:GLY:HA2	1.74	0.68
8:1H:65:THR:HA	16:1P:324:TYR:HB2	1.76	0.68
9:1I:92:ILE:HG12	9:1I:111:ILE:HG12	1.74	0.68
1:1A:56:PHE:HZ	11:1K:75:LEU:HB3	1.59	0.68
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.11	0.68
5:1E:123:LYS:HD3	5:1E:173:ILE:HD11	1.75	0.68
9:1I:3:LYS:HD2	9:1I:4:PHE:N	2.09	0.68
17:1Q:33:ARG:HH21	17:1Q:59:PHE:HB3	1.58	0.68
6:1F:295:LEU:H	6:1F:338:ASP:HA	1.57	0.68
51:1M:501:PGT:H132	14:1N:277:ILE:HG13	1.76	0.68
37:1l:132:GLN:HG2	40:1o:97:ARG:HH12	1.58	0.68
7:1G:537:LEU:HD21	42:1q:145:LYS:HZ1	1.59	0.68
15:1O:89:ASN:O	32:1g:23:THR:N	2.27	0.68
21:1V:106:PRO:HD2	21:1V:106:PRO:O	1.92	0.68
22:1W:44:PRO:HD3	22:1W:60:ARG:HE	1.59	0.68
2:1B:61:HIS:CE1	4:1D:174:ARG:HH12	2.12	0.68
6:1F:60:VAL:HG21	6:1F:79:TRP:HD1	1.58	0.68
50:1L:701:3PE:H242	37:1l:88:ARG:HD3	1.76	0.68
3:1C:38:GLN:NE2	3:1C:110:TYR:OH	2.26	0.67
4:1D:306:GLN:HA	4:1D:309:ARG:HD3	1.74	0.67
5:1E:183:LYS:HB3	44:1s:44:HIS:HB3	1.75	0.67
33:1h:34:ILE:O	33:1h:38:ILE:HD12	1.95	0.67
2:1B:116:MET:HE3	2:1B:151:PRO:HD2	1.75	0.67
35:1j:67:LEU:HD22	35:1j:68:PRO:HD2	1.75	0.67
38:1m:26:PRO:O	38:1m:30:LYS:NZ	2.26	0.67
6:1F:82:MET:HB3	6:1F:129:MET:HB3	1.75	0.67
13:1M:423:ILE:HG22	38:1m:58:VAL:HG12	1.76	0.67
16:1P:93:ASN:HB3	16:1P:131:HIS:HA	1.76	0.67
35:1j:55:ASP:HB3	35:1j:58:GLN:HG2	1.75	0.67
2:1B:89:ALA:HA	2:1B:116:MET:HB3	1.77	0.67
5:1E:97:LYS:O	5:1E:157:ASN:ND2	2.28	0.67
7:1G:121:MET:HE2	7:1G:121:MET:HA	1.76	0.67
15:1O:138:MET:HG3	15:1O:143:PHE:HB2	1.77	0.67
1:1A:70:ALA:HB2	10:1J:59:ILE:HG21	1.76	0.67
3:1C:53:HIS:ND1	3:1C:55:ASP:OD1	2.24	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:58:ALA:HB1	4:1D:62:LEU:HB3	1.76	0.67
20:1T:37:MET:N	20:1T:37:MET:SD	2.68	0.67
4:1D:162:GLY:HA3	8:1H:279:ARG:HE	1.60	0.67
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.77	0.67
6:1F:227:THR:O	6:1F:231:SER:OG	2.12	0.67
8:1H:268:ILE:HD11	26:1a:9:ILE:HD11	1.75	0.67
20:1U:35:HIS:HE1	20:1U:37:MET:HB2	1.60	0.67
42:1q:78:ASP:OD1	42:1q:79:GLY:N	2.28	0.67
3:1C:35:LYS:HG2	3:1C:36:TYR:CD2	2.30	0.66
13:1M:277:LEU:O	37:1l:88:ARG:NH2	2.29	0.66
40:1o:26:PRO:HB3	40:1o:33:ARG:HH11	1.60	0.66
14:1N:7:THR:HG23	52:1N:402:CDL:H141	1.77	0.66
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.75	0.66
16:1P:72:GLU:O	16:1P:83:LYS:NZ	2.28	0.66
23:1X:110:VAL:O	23:1X:116:TRP:N	2.26	0.66
6:1F:106:LYS:HB2	6:1F:255:LEU:HD13	1.76	0.66
20:1T:43:ASP:H	20:1T:46:ASP:HB2	1.60	0.66
21:1V:20:HIS:HE1	21:1V:64:VAL:HG12	1.60	0.66
3:1C:88:ASN:HD21	21:1V:107:PRO:HG2	1.60	0.66
4:1D:395:GLY:HA2	4:1D:398:HIS:HB2	1.77	0.66
7:1G:138:GLU:N	7:1G:138:GLU:OE1	2.27	0.66
7:1G:255:HIS:HE1	7:1G:257:ASP:HB3	1.59	0.66
12:1L:432:LEU:HD13	36:1k:62:PHE:HA	1.78	0.66
42:1q:92:CYS:O	43:1r:33:ARG:NH1	2.29	0.66
3:1C:149:ARG:HB2	22:1W:88:MET:HE1	1.78	0.66
15:1O:135:LEU:HA	15:1O:138:MET:HB3	1.76	0.66
15:1O:275:ILE:HG22	15:1O:277:VAL:H	1.61	0.66
37:1l:115:MET:HA	37:1l:118:VAL:HG22	1.77	0.66
37:1l:125:TYR:OH	40:1o:7:ARG:NH1	2.29	0.66
25:1Z:127:LEU:HD13	30:1e:97:HIS:ND1	2.11	0.66
39:1n:89:SER:HB2	39:1n:92:ARG:HD2	1.78	0.66
42:1q:50:GLU:OE2	42:1q:50:GLU:N	2.29	0.66
6:1F:99:GLU:H	48:1F:501:FMN:HN3	1.44	0.66
6:1F:103:GLY:O	6:1F:257:ASN:ND2	2.28	0.66
7:1G:525:LEU:HA	7:1G:546:GLN:HE21	1.60	0.66
16:1P:240:ASP:HB3	16:1P:337:ALA:HB1	1.78	0.66
7:1G:165:GLU:OE1	7:1G:165:GLU:N	2.27	0.66
23:1X:138:GLU:N	23:1X:138:GLU:OE2	2.26	0.66
41:1p:158:GLN:HG3	41:1p:161:ARG:HH21	1.61	0.66
4:1D:259:MET:HA	4:1D:259:MET:HE3	1.78	0.66
7:1G:176:GLY:HA3	7:1G:181:MET:HA	1.76	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:323:VAL:HG21	7:1G:525:LEU:HD11	1.78	0.66
8:1H:211:PHE:HB2	8:1H:223:PHE:CE2	2.31	0.66
13:1M:78:MET:HG2	13:1M:436:LEU:HD12	1.77	0.66
40:1o:74:PRO:HD3	41:1p:27:ASN:HA	1.78	0.66
7:1G:55:CYS:SG	7:1G:69:CYS:HB2	2.35	0.65
12:1L:106:TRP:O	12:1L:109:HIS:ND1	2.29	0.65
13:1M:191:SER:HB2	51:1M:501:PGT:H31	1.79	0.65
3:1C:179:GLU:OE1	16:1P:40:ARG:NH2	2.30	0.65
5:1E:173:ILE:HA	5:1E:176:LEU:HD12	1.78	0.65
16:1P:81:ILE:H	16:1P:81:ILE:HD12	1.62	0.65
8:1H:35:LYS:HB2	9:1I:47:THR:HG21	1.78	0.65
51:1M:501:PGT:H362	14:1N:280:THR:HG21	1.79	0.65
16:1P:141:SER:O	16:1P:147:ARG:NH1	2.29	0.65
26:1a:67:GLU:OE2	26:1a:67:GLU:N	2.20	0.65
28:1c:44:ARG:HA	28:1c:49:GLU:HB3	1.78	0.65
39:1n:82:PRO:HB3	39:1n:88:THR:HG22	1.78	0.65
15:1O:285:GLY:HA3	32:1g:28:GLU:HG2	1.78	0.65
26:1a:57:VAL:HG13	26:1a:59:ARG:HG2	1.78	0.65
30:1e:31:ARG:HH22	30:1e:68:ARG:HE	1.43	0.65
13:1M:300:ALA:O	13:1M:308:SER:OG	2.14	0.65
38:1m:122:GLN:HB2	38:1m:125:ASN:HB3	1.78	0.65
10:1J:119:PHE:HE2	11:1K:5:TYR:HB2	1.62	0.65
12:1L:471:ASN:O	40:1o:69:LYS:NZ	2.29	0.65
17:1Q:39:VAL:HG21	17:1Q:108:ARG:HE	1.61	0.65
20:1T:11:ILE:HG22	20:1T:77:VAL:HG22	1.79	0.65
20:1T:65:ILE:H	20:1T:65:ILE:HD12	1.61	0.65
7:1G:274:LEU:HD13	7:1G:278:ARG:HH21	1.61	0.65
7:1G:351:THR:HG22	7:1G:509:PRO:HG2	1.79	0.65
7:1G:601:ARG:HH21	7:1G:614:ASP:HB3	1.62	0.65
11:1K:6:MET:HG3	11:1K:10:MET:HE3	1.77	0.65
2:1B:47:PRO:HD3	2:1B:74:VAL:HG12	1.79	0.64
2:1B:146:VAL:HG11	2:1B:156:LEU:HD12	1.79	0.64
4:1D:174:ARG:O	4:1D:178:PHE:HB2	1.97	0.64
4:1D:342:MET:HG3	7:1G:98:LEU:HG	1.79	0.64
38:1m:53:PRO:HB2	39:1n:129:ARG:HD2	1.79	0.64
3:1C:192:GLN:HG3	17:1Q:72:TRP:HB3	1.80	0.64
3:1C:205:ALA:HA	7:1G:122:MET:HE2	1.79	0.64
8:1H:207:LEU:O	8:1H:209:SER:N	2.29	0.64
13:1M:121:LEU:HA	13:1M:124:ALA:HB3	1.80	0.64
17:1Q:27:GLU:OE1	17:1Q:27:GLU:N	2.25	0.64
20:1U:46:ASP:OD1	39:1n:44:ARG:NH1	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:98:MET:HE3	30:1e:78:ILE:HD13	1.80	0.64
39:1n:88:THR:O	39:1n:92:ARG:NH1	2.30	0.64
43:1r:104:GLU:OE1	43:1r:104:GLU:N	2.30	0.64
5:1E:143:GLU:HG2	6:1F:353:PHE:HD1	1.61	0.64
7:1G:44:GLU:O	17:1Q:116:LYS:NZ	2.27	0.64
7:1G:456:SER:HB2	7:1G:664:PRO:HD2	1.79	0.64
15:1O:312:VAL:HG11	28:1c:2:PHE:HB2	1.80	0.64
7:1G:328:LEU:HB3	7:1G:505:LEU:HD12	1.79	0.64
12:1L:161:ARG:HG3	12:1L:164:ALA:H	1.62	0.64
20:1T:19:LEU:HB3	20:1T:25:ILE:HG21	1.78	0.64
32:1g:117:LYS:HE2	41:1p:75:GLU:HB3	1.79	0.64
6:1F:300:GLY:HA3	6:1F:304:THR:HG21	1.79	0.64
13:1M:307:TRP:HE1	38:1m:127:SER:HB2	1.63	0.64
16:1P:20:VAL:O	16:1P:88:SER:OG	2.15	0.64
25:1Z:22:LYS:HA	25:1Z:22:LYS:HE3	1.79	0.64
25:1Z:110:VAL:HG11	30:1e:71:THR:HB	1.79	0.64
32:1g:62:PHE:O	33:1h:28:TYR:OH	2.12	0.64
5:1E:79:ARG:NH1	7:1G:170:ASP:OD1	2.30	0.64
6:1F:101:GLU:OE2	6:1F:302:SER:N	2.24	0.64
37:1l:130:PRO:O	40:1o:97:ARG:NH1	2.30	0.64
39:1n:123:GLN:OE1	39:1n:126:ARG:NH2	2.31	0.64
4:1D:158:ALA:HB1	4:1D:163:ALA:HB3	1.80	0.64
6:1F:276:LEU:HA	6:1F:279:LEU:HD12	1.80	0.64
7:1G:455:SER:OG	7:1G:459:GLN:NE2	2.31	0.64
4:1D:88:GLU:OE2	4:1D:88:GLU:N	2.28	0.64
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.79	0.64
4:1D:136:TRP:CD1	4:1D:277:VAL:HG11	2.32	0.64
7:1G:673:MET:HE1	7:1G:679:ARG:HA	1.80	0.64
11:1K:37:MET:HB3	14:1N:68:MET:HE1	1.78	0.64
12:1L:237:MET:HE1	12:1L:244:SER:HB2	1.78	0.64
15:1O:213:GLU:O	15:1O:217:LYS:NZ	2.29	0.64
24:1Y:100:LEU:HD12	24:1Y:117:MET:HE1	1.80	0.64
9:1I:50:TYR:CD1	9:1I:51:PRO:HA	2.33	0.63
12:1L:206:ASN:HB2	12:1L:266:LEU:HD11	1.79	0.63
13:1M:452:LYS:HD2	32:1g:86:GLN:HE22	1.62	0.63
18:1R:51:GLU:OE2	18:1R:92:ARG:NH2	2.31	0.63
12:1L:560:THR:HA	12:1L:564:LYS:HB2	1.79	0.63
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.31	0.63
19:1S:16:ARG:HD3	19:1S:69:ALA:HB2	1.79	0.63
20:1U:35:HIS:CE1	20:1U:37:MET:HB2	2.33	0.63
20:1U:51:ILE:H	20:1U:51:ILE:HD12	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:62:LYS:HG2	22:1W:107:PHE:CE1	2.30	0.63
34:1i:10:ARG:NH2	39:1n:154:PRO:O	2.31	0.63
37:1l:5:THR:OG1	37:1l:7:ASP:OD1	2.17	0.63
6:1F:46:LYS:HB3	6:1F:167:CYS:HB3	1.79	0.63
14:1N:108:LEU:HB2	14:1N:161:SER:HB3	1.80	0.63
22:1W:75:ASP:HB3	22:1W:78:VAL:HG12	1.78	0.63
36:1k:18:TYR:HB3	36:1k:19:LYS:HE2	1.78	0.63
42:1q:65:THR:HG22	42:1q:67:GLU:H	1.63	0.63
4:1D:151:ILE:HG23	4:1D:170:MET:HE2	1.81	0.63
6:1F:90:PRO:HD2	6:1F:90:PRO:O	1.96	0.63
9:1I:2:TYR:HB3	43:1r:103:TRP:HE3	1.63	0.63
9:1I:3:LYS:NZ	43:1r:111:TYR:HA	2.13	0.63
13:1M:102:LEU:HD21	13:1M:230:VAL:HG11	1.81	0.63
15:1O:52:PRO:O	15:1O:107:GLN:NE2	2.32	0.63
26:1a:21:MET:N	26:1a:21:MET:SD	2.72	0.63
4:1D:161:ILE:HG23	4:1D:238:ARG:HH21	1.64	0.63
12:1L:440:LEU:HB2	20:1U:14:ARG:HH12	1.63	0.63
16:1P:78:LYS:HA	16:1P:78:LYS:HE3	1.80	0.63
16:1P:200:THR:O	16:1P:238:LEU:N	2.32	0.63
22:1W:62:LYS:HD2	22:1W:65:GLU:OE1	1.98	0.63
6:1F:163:GLY:HA2	6:1F:174:ASP:HB3	1.80	0.63
7:1G:252:PRO:HD2	17:1Q:44:ASN:HD22	1.63	0.63
7:1G:620:ARG:NH1	7:1G:633:TYR:OH	2.32	0.63
16:1P:113:ILE:HA	16:1P:116:ALA:HB3	1.81	0.63
7:1G:622:ARG:NH1	7:1G:625:GLU:OE2	2.32	0.63
10:1J:146:LEU:HA	11:1K:58:MET:HE1	1.81	0.63
16:1P:201:VAL:HB	16:1P:235:ARG:HH21	1.64	0.63
8:1H:204:GLU:OE2	8:1H:274:ARG:NH2	2.32	0.63
12:1L:59:GLN:NE2	34:1i:98:GLU:OE1	2.31	0.63
15:1O:180:GLN:O	15:1O:184:GLN:NE2	2.32	0.63
20:1U:52:MET:HA	20:1U:55:GLU:HB2	1.81	0.63
2:1B:79:SER:O	2:1B:82:GLN:N	2.31	0.63
7:1G:255:HIS:CE1	7:1G:257:ASP:HB3	2.34	0.63
9:1I:145:GLU:N	9:1I:145:GLU:OE1	2.30	0.63
14:1N:51:ARG:HB3	14:1N:121:GLY:HA2	1.81	0.63
43:1r:40:LEU:HD13	43:1r:41:PRO:HD2	1.79	0.63
5:1E:10:ARG:NH1	18:1R:76:ASP:O	2.30	0.62
7:1G:285:ARG:HG2	7:1G:291:LEU:HD22	1.81	0.62
17:1Q:88:THR:OG1	17:1Q:91:ASP:OD1	2.17	0.62
21:1V:1:ALA:N	21:1V:63:ASP:OD1	2.32	0.62
21:1V:110:GLN:NE2	21:1V:110:GLN:O	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:19:ARG:HD3	35:1j:23:ILE:HD13	1.81	0.62
2:1B:171:LYS:HB3	2:1B:174:ARG:HB3	1.82	0.62
5:1E:185:GLY:O	5:1E:187:ARG:NH1	2.32	0.62
6:1F:108:ARG:HD3	6:1F:112:ARG:HH12	1.64	0.62
7:1G:359:ARG:NH1	7:1G:637:GLU:O	2.31	0.62
10:1J:112:GLU:OE1	30:1e:73:LYS:NZ	2.32	0.62
12:1L:79:SER:O	12:1L:139:GLN:NE2	2.31	0.62
7:1G:453:LEU:HD12	7:1G:470:VAL:HG21	1.82	0.62
8:1H:157:ASN:HA	8:1H:168:THR:HG21	1.82	0.62
8:1H:211:PHE:HB2	8:1H:223:PHE:HE2	1.63	0.62
9:1I:63:GLY:N	9:1I:133:GLU:HB3	2.14	0.62
19:1S:77:SER:OG	19:1S:79:ASN:OD1	2.15	0.62
27:1b:51:ASN:OD1	27:1b:52:TYR:N	2.33	0.62
7:1G:373:GLU:OE1	7:1G:373:GLU:N	2.30	0.62
13:1M:329:LEU:HD22	13:1M:359:TRP:CD2	2.33	0.62
21:1V:26:LEU:HA	21:1V:29:LYS:HE2	1.80	0.62
23:1X:96:PHE:O	23:1X:100:ARG:NH1	2.33	0.62
4:1D:100:LEU:HD11	4:1D:115:GLU:HG2	1.79	0.62
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.32	0.62
10:1J:125:TRP:HE3	25:1Z:121:MET:HE1	1.65	0.62
16:1P:90:VAL:HG11	16:1P:218:ILE:HD12	1.82	0.62
20:1T:28:GLU:OE1	20:1T:28:GLU:N	2.28	0.62
21:1V:109:ASN:HB2	21:1V:112:LYS:HB2	1.80	0.62
25:1Z:59:ARG:NH1	27:1b:80:LEU:O	2.33	0.62
30:1e:20:GLN:NE2	30:1e:30:GLY:O	2.31	0.62
12:1L:38:THR:HB	34:1i:69:PHE:HE2	1.63	0.62
22:1W:26:ASN:O	22:1W:30:ARG:N	2.32	0.62
22:1W:42:GLU:HG2	22:1W:90:LEU:HD21	1.80	0.62
22:1W:84:ILE:HA	22:1W:87:LYS:HB3	1.81	0.62
6:1F:299:PRO:HA	6:1F:334:VAL:HA	1.82	0.62
6:1F:360:GLY:HA2	6:1F:366:ARG:HB2	1.82	0.62
7:1G:255:HIS:CE1	7:1G:258:ILE:HG13	2.34	0.62
16:1P:106:PHE:HE2	16:1P:145:TYR:HA	1.65	0.62
16:1P:311:GLU:OE1	16:1P:311:GLU:N	2.33	0.62
18:1R:36:ASN:ND2	18:1R:38:ASN:O	2.32	0.62
21:1V:30:ILE:HG22	21:1V:87:LEU:HD13	1.81	0.62
4:1D:375:GLY:H	4:1D:392:LYS:HB3	1.63	0.62
12:1L:343:SER:HA	12:1L:346:ILE:HD12	1.82	0.62
25:1Z:90:ASN:ND2	25:1Z:123:GLU:O	2.33	0.62
2:1B:71:ARG:HG3	8:1H:38:ASN:HB3	1.82	0.62
2:1B:179:ARG:NH2	55:1P:501:NDP:O2X	2.33	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:29:HIS:O	6:1F:39:ARG:NH1	2.33	0.62
6:1F:129:MET:N	6:1F:129:MET:SD	2.73	0.62
7:1G:534:ARG:HD2	42:1q:145:LYS:HA	1.82	0.62
10:1J:125:TRP:CE3	25:1Z:121:MET:HE1	2.35	0.62
12:1L:467:ILE:O	12:1L:471:ASN:ND2	2.33	0.62
15:1O:204:ASN:HB2	15:1O:208:LYS:NZ	2.14	0.62
26:1a:66:LEU:HD13	26:1a:69:ILE:HD11	1.82	0.62
3:1C:90:PHE:HE1	3:1C:113:GLU:HG3	1.64	0.61
4:1D:135:GLN:HA	4:1D:138:ARG:HD2	1.82	0.61
5:1E:202:LEU:HD22	6:1F:26:TYR:HB2	1.82	0.61
7:1G:688:VAL:O	7:1G:692:THR:OG1	2.17	0.61
18:1R:34:GLU:N	18:1R:34:GLU:OE2	2.33	0.61
4:1D:87:THR:OG1	4:1D:430:ARG:O	2.17	0.61
7:1G:356:THR:O	19:1S:55:ARG:NH2	2.33	0.61
8:1H:295:PRO:HB3	50:1b:101:3PE:H271	1.82	0.61
13:1M:457:PRO:O	32:1g:84:ARG:NH2	2.32	0.61
14:1N:96:THR:HA	14:1N:153:LEU:HD11	1.82	0.61
23:1X:121:LEU:HD13	25:1Z:62:ILE:HD11	1.83	0.61
6:1F:150:GLN:HE22	44:1s:58:LEU:HD13	1.65	0.61
10:1J:173:ARG:NH2	10:1J:175:ASN:O	2.33	0.61
11:1K:8:ILE:HG21	11:1K:43:MET:HB2	1.82	0.61
18:1R:20:ASP:N	18:1R:20:ASP:OD1	2.34	0.61
2:1B:60:MET:HE1	4:1D:152:MET:HE1	1.81	0.61
7:1G:319:ALA:HB3	7:1G:345:THR:HA	1.82	0.61
16:1P:36:ASN:OD1	16:1P:40:ARG:NH2	2.34	0.61
32:1g:117:LYS:HE3	41:1p:74:THR:HG23	1.83	0.61
4:1D:233:ARG:HH21	9:1I:24:THR:HA	1.65	0.61
15:1O:12:GLU:OE1	15:1O:17:LYS:NZ	2.26	0.61
32:1g:113:PHE:HB2	41:1p:158:GLN:HE22	1.65	0.61
2:1B:125:TYR:CD2	9:1I:117:ILE:HG21	2.35	0.61
3:1C:64:LEU:O	3:1C:72:PHE:N	2.34	0.61
4:1D:103:PHE:HA	4:1D:106:LEU:HG	1.83	0.61
5:1E:9:HIS:CD2	5:1E:63:ILE:HG12	2.36	0.61
6:1F:164:LYS:HA	6:1F:172:ASP:HA	1.81	0.61
13:1M:36:LEU:HD21	45:1M:502:PC1:H371	1.83	0.61
14:1N:103:ALA:O	14:1N:107:GLY:N	2.33	0.61
15:1O:95:ARG:NH1	15:1O:281:GLU:O	2.34	0.61
4:1D:381:ASP:HB3	4:1D:387:TYR:HD2	1.65	0.61
7:1G:145:LEU:HB2	7:1G:269:PHE:HE2	1.65	0.61
13:1M:12:LEU:HD21	13:1M:97:THR:HG23	1.82	0.61
20:1U:11:ILE:O	20:1U:15:VAL:HG23	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:10:ARG:HH21	35:1j:16:GLN:HB3	1.66	0.61
6:1F:256:PHE:HZ	6:1F:317:MET:HE3	1.65	0.61
6:1F:257:ASN:HB3	6:1F:333:ALA:HA	1.82	0.61
7:1G:199:ILE:H	7:1G:199:ILE:HD12	1.66	0.61
15:1O:200:GLN:NE2	15:1O:200:GLN:O	2.33	0.61
20:1T:65:ILE:HA	22:1W:30:ARG:HH12	1.64	0.61
3:1C:185:ALA:HB2	22:1W:105:ARG:HH21	1.66	0.61
12:1L:400:ASN:HA	12:1L:409:LEU:HD11	1.82	0.61
13:1M:78:MET:HA	13:1M:81:GLN:HE22	1.66	0.61
16:1P:249:ALA:HA	16:1P:322:ARG:HG2	1.83	0.61
16:1P:286:ARG:O	16:1P:286:ARG:NH1	2.32	0.61
17:1Q:22:LEU:HD21	22:1W:78:VAL:HG23	1.83	0.61
20:1T:70:LEU:HA	20:1T:75:GLU:HB3	1.83	0.61
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	1.81	0.61
4:1D:312:SER:O	4:1D:316:ASN:ND2	2.34	0.60
45:1H:401:PC1:H121	25:1Z:35:MET:HE1	1.81	0.60
12:1L:293:ILE:O	12:1L:425:ARG:NH1	2.34	0.60
6:1F:393:TRP:HB2	6:1F:419:ILE:HG21	1.83	0.60
7:1G:173:GLY:N	7:1G:184:GLY:O	2.34	0.60
7:1G:191:PHE:CE2	7:1G:196:SER:HB2	2.35	0.60
7:1G:564:ALA:HB1	7:1G:568:GLU:HB2	1.83	0.60
12:1L:581:LYS:HE2	24:1Y:43:LYS:HG2	1.81	0.60
23:1X:141:TYR:O	25:1Z:115:ARG:NH1	2.33	0.60
31:1f:49:ARG:HH12	33:1h:60:VAL:H	1.47	0.60
38:1m:117:GLU:OE1	38:1m:117:GLU:N	2.31	0.60
7:1G:341:ASP:OD2	19:1S:67:ARG:NH2	2.34	0.60
8:1H:24:GLU:HG3	8:1H:195:ARG:HH22	1.67	0.60
12:1L:203:MET:HE2	12:1L:203:MET:HA	1.82	0.60
16:1P:175:GLU:O	16:1P:177:ARG:NH2	2.34	0.60
19:1S:18:ILE:HG23	19:1S:52:ILE:HA	1.84	0.60
44:1s:59:SER:HA	44:1s:62:ARG:HG3	1.84	0.60
2:1B:122:GLY:N	9:1I:114:THR:OG1	2.35	0.60
5:1E:217:LEU:HD11	6:1F:236:ARG:HA	1.83	0.60
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.82	0.60
13:1M:72:LEU:HD23	13:1M:75:LEU:HD12	1.83	0.60
30:1e:6:GLN:NE2	30:1e:13:LEU:H	1.99	0.60
6:1F:206:LYS:HD3	6:1F:209:PHE:HA	1.83	0.60
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.65	0.60
50:1N:401:3PE:O14	15:1O:303:LYS:NZ	2.34	0.60
16:1P:167:LYS:NZ	16:1P:228:PHE:O	2.28	0.60
20:1U:29:LYS:HA	20:1U:29:LYS:HE3	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:47:LEU:HD11	8:1H:126:LYS:HD2	1.82	0.60
5:1E:110:LEU:HD11	6:1F:337:MET:HG3	1.83	0.60
2:1B:87:ILE:HG12	2:1B:114:VAL:HB	1.83	0.60
6:1F:264:HIS:H	6:1F:284:ALA:HB1	1.65	0.60
13:1M:175:ASN:HB3	13:1M:178:ILE:HG22	1.84	0.60
23:1X:136:LEU:HD12	23:1X:137:PRO:HD2	1.82	0.60
7:1G:575:ASN:ND2	7:1G:581:GLN:OE1	2.34	0.60
9:1I:43:ARG:HD2	43:1r:24:GLN:HE22	1.66	0.60
2:1B:139:ILE:HG22	2:1B:140:VAL:HG13	1.84	0.60
6:1F:30:ASP:HB3	6:1F:35:GLY:HA3	1.84	0.60
8:1H:185:TRP:NE1	8:1H:238:THR:OG1	2.34	0.60
18:1R:59:CYS:O	18:1R:68:HIS:NE2	2.35	0.60
20:1T:16:LEU:HA	20:1T:19:LEU:HD12	1.84	0.60
8:1H:80:SER:O	8:1H:84:THR:HG22	2.02	0.60
12:1L:237:MET:HE2	12:1L:299:LYS:HB3	1.83	0.60
12:1L:293:ILE:HG13	12:1L:294:THR:HG23	1.83	0.60
14:1N:294:MET:HE2	14:1N:294:MET:HA	1.84	0.60
7:1G:358:LEU:HD12	7:1G:645:ALA:HB2	1.83	0.59
7:1G:543:ILE:HG13	42:1q:145:LYS:HE2	1.84	0.59
10:1J:78:MET:N	10:1J:78:MET:SD	2.75	0.59
16:1P:237:LEU:HD13	16:1P:239:PHE:H	1.65	0.59
20:1T:44:SER:OG	22:1W:29:LYS:NZ	2.35	0.59
23:1X:19:VAL:HB	23:1X:23:VAL:HG11	1.84	0.59
32:1g:109:GLU:O	41:1p:141:ARG:NH1	2.34	0.59
34:1i:48:LYS:HA	34:1i:51:GLN:HG2	1.84	0.59
35:1j:12:ARG:HB3	36:1k:50:TRP:CG	2.37	0.59
36:1k:48:GLU:HA	36:1k:51:ARG:HD2	1.83	0.59
5:1E:89:MET:HG2	5:1E:90:TYR:H	1.66	0.59
6:1F:31:TRP:HB2	6:1F:113:HIS:HA	1.84	0.59
13:1M:209:LEU:HD23	13:1M:212:LEU:HD12	1.84	0.59
15:1O:83:TYR:HB2	15:1O:190:HIS:HB2	1.84	0.59
20:1T:74:GLN:HA	20:1T:77:VAL:HB	1.83	0.59
3:1C:32:ILE:HG23	21:1V:43:TYR:HB2	1.83	0.59
6:1F:25:LEU:O	6:1F:113:HIS:ND1	2.33	0.59
12:1L:570:GLN:OE1	14:1N:167:TRP:NE1	2.35	0.59
13:1M:204:MET:HE1	13:1M:261:PHE:HB3	1.82	0.59
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.18	0.59
42:1q:55:PHE:HE1	42:1q:58:ARG:HE	1.48	0.59
6:1F:61:LYS:HE2	6:1F:76:GLY:HA3	1.84	0.59
6:1F:190:THR:HB	6:1F:204:ARG:H	1.67	0.59
15:1O:35:LYS:NZ	53:1O:401:GTP:O1G	2.28	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:290:ARG:NH1	4:1D:292:ASP:OD2	2.36	0.59
12:1L:173:LEU:HD12	13:1M:405:LEU:HD11	1.85	0.59
14:1N:62:THR:HG21	14:1N:114:TRP:CD1	2.38	0.59
21:1V:65:LYS:HD3	21:1V:66:LYS:HG3	1.83	0.59
4:1D:245:VAL:O	4:1D:263:SER:OG	2.21	0.59
12:1L:254:VAL:HG23	12:1L:329:ILE:HD12	1.85	0.59
16:1P:113:ILE:H	16:1P:113:ILE:HD12	1.67	0.59
17:1Q:59:PHE:CD1	17:1Q:79:LEU:HB3	2.37	0.59
4:1D:115:GLU:OE1	4:1D:194:ILE:N	2.34	0.59
6:1F:298:ILE:HB	6:1F:306:LEU:HD13	1.85	0.59
7:1G:395:ILE:O	7:1G:399:TRP:N	2.33	0.59
9:1I:163:ALA:HB1	42:1q:103:PRO:HB2	1.85	0.59
13:1M:336:ARG:HH22	13:1M:429:SER:HA	1.65	0.59
16:1P:294:LEU:HD11	16:1P:297:LEU:HD12	1.84	0.59
40:1o:14:LYS:HG2	40:1o:112:LYS:HD2	1.85	0.59
4:1D:296:ARG:HH21	4:1D:420:THR:HG21	1.68	0.59
7:1G:235:GLY:O	7:1G:581:GLN:NE2	2.35	0.59
21:1V:15:VAL:HA	21:1V:77:GLU:HG2	1.85	0.59
4:1D:178:PHE:CZ	4:1D:189:MET:HG2	2.37	0.59
4:1D:281:VAL:HG21	4:1D:310:ILE:HG23	1.85	0.59
50:1L:702:3PE:H231	50:1L:702:3PE:H321	1.85	0.59
13:1M:278:ARG:NH2	37:1l:80:ASP:OD1	2.36	0.59
20:1U:32:VAL:HG13	20:1U:33:ASN:OD1	2.03	0.59
31:1f:46:ARG:HD3	33:1h:60:VAL:HG21	1.84	0.59
6:1F:274:VAL:HB	6:1F:279:LEU:HD11	1.85	0.59
7:1G:675:ASP:OD1	7:1G:676:SER:N	2.36	0.59
12:1L:556:ILE:HD11	38:1m:75:ILE:HG12	1.84	0.59
4:1D:63:ARG:HG2	4:1D:79:HIS:HB2	1.85	0.58
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.38	0.58
15:1O:8:PHE:O	15:1O:13:ARG:NH1	2.31	0.58
22:1W:23:ARG:NH1	22:1W:23:ARG:O	2.36	0.58
4:1D:147:LEU:O	4:1D:151:ILE:HG13	2.02	0.58
4:1D:239:THR:HG23	4:1D:293:CYS:HB2	1.84	0.58
7:1G:364:LEU:HD12	7:1G:491:ASN:HD22	1.67	0.58
12:1L:550:SER:HB2	13:1M:275:ILE:HG13	1.85	0.58
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.67	0.58
15:1O:36:GLY:HA2	15:1O:125:GLU:HG2	1.84	0.58
25:1Z:10:MET:HE3	25:1Z:11:PRO:HD2	1.84	0.58
1:1A:79:SER:HA	1:1A:87:MET:HE2	1.85	0.58
6:1F:416:GLN:HA	6:1F:419:ILE:HD12	1.84	0.58
9:1I:54:LYS:NZ	9:1I:138:GLU:OE1	2.27	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:508:THR:O	39:1n:35:LYS:NZ	2.32	0.58
13:1M:118:PHE:O	13:1M:122:PHE:HB3	2.04	0.58
6:1F:13:GLY:N	6:1F:271:GLU:OE1	2.29	0.58
34:1i:32:PRO:HB3	39:1n:113:MET:HE3	1.85	0.58
2:1B:25:ARG:HD2	2:1B:27:GLU:H	1.67	0.58
3:1C:147:ASP:OD2	3:1C:149:ARG:NH2	2.36	0.58
4:1D:35:ASP:OD2	14:1N:176:ARG:NH2	2.30	0.58
6:1F:22:PHE:HB2	6:1F:25:LEU:HB3	1.86	0.58
7:1G:28:GLN:NE2	17:1Q:114:LYS:O	2.26	0.58
10:1J:153:LEU:HD12	11:1K:62:ILE:HG13	1.85	0.58
13:1M:98:MET:HE1	50:1N:401:3PE:H3D1	1.85	0.58
14:1N:234:TRP:CE2	14:1N:304:MET:HB3	2.38	0.58
42:1q:32:ASP:OD2	42:1q:34:ARG:NH1	2.37	0.58
5:1E:159:ASN:ND2	5:1E:159:ASN:O	2.36	0.58
19:1S:53:LEU:HG	19:1S:55:ARG:HH21	1.68	0.58
35:1j:32:MET:O	35:1j:36:ILE:HG12	2.04	0.58
4:1D:34:ASN:HA	15:1O:272:TYR:CZ	2.39	0.58
7:1G:229:ASP:N	7:1G:236:SER:O	2.31	0.58
7:1G:418:ARG:HD2	44:1s:74:ARG:HH22	1.69	0.58
8:1H:194:ASN:OD1	8:1H:201:THR:OG1	2.21	0.58
9:1I:152:GLU:OE1	18:1R:36:ASN:N	2.31	0.58
12:1L:67:HIS:HE1	12:1L:75:GLU:HB3	1.69	0.58
12:1L:356:ILE:HA	12:1L:359:MET:HE1	1.86	0.58
40:1o:46:ASN:HA	40:1o:55:ARG:HH21	1.69	0.58
3:1C:192:GLN:OE1	9:1I:115:LYS:NZ	2.36	0.58
5:1E:48:LEU:O	5:1E:90:TYR:OH	2.21	0.58
10:1J:25:SER:OG	10:1J:81:GLU:O	2.18	0.58
12:1L:154:LEU:HB3	12:1L:243:VAL:HG11	1.86	0.58
14:1N:272:LYS:HB3	33:1h:108:LEU:HD11	1.85	0.58
15:1O:61:SER:HA	15:1O:66:GLY:HA2	1.86	0.58
21:1V:67:LEU:HA	21:1V:70:GLN:HG2	1.86	0.58
4:1D:305:ARG:NH2	25:1Z:23:ARG:HG2	2.19	0.58
12:1L:49:VAL:HG22	41:1p:32:LEU:HD22	1.86	0.58
12:1L:52:LEU:HA	12:1L:55:MET:HB2	1.84	0.58
12:1L:294:THR:O	12:1L:524:ASN:ND2	2.37	0.58
14:1N:174:GLN:NE2	14:1N:225:THR:O	2.36	0.58
38:1m:40:SER:OG	39:1n:148:PRO:O	2.21	0.58
3:1C:74:SER:HB2	3:1C:97:LEU:HB3	1.85	0.58
4:1D:149:ASN:O	4:1D:153:ALA:N	2.37	0.58
5:1E:111:ARG:HB3	5:1E:152:PRO:HD3	1.85	0.58
17:1Q:13:VAL:N	22:1W:15:THR:O	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:123:SER:OG	17:1Q:126:LYS:O	2.21	0.58
24:1Y:50:GLU:OE1	24:1Y:50:GLU:N	2.27	0.58
4:1D:156:THR:O	4:1D:160:ASP:N	2.33	0.57
13:1M:282:LEU:HD23	13:1M:342:MET:HG3	1.86	0.57
3:1C:71:GLN:HB2	3:1C:73:LYS:NZ	2.19	0.57
6:1F:385:ARG:HG3	6:1F:387:ALA:H	1.69	0.57
7:1G:194:GLU:OE2	7:1G:194:GLU:N	2.26	0.57
12:1L:313:MET:HE2	12:1L:329:ILE:HD13	1.85	0.57
13:1M:14:MET:HG3	31:1f:12:VAL:HG22	1.85	0.57
13:1M:430:PHE:HB3	32:1g:46:GLY:HA3	1.85	0.57
15:1O:161:CYS:SG	15:1O:162:GLU:N	2.77	0.57
40:1o:57:TYR:O	40:1o:60:HIS:ND1	2.31	0.57
2:1B:44:SER:HA	2:1B:73:GLY:HA3	1.85	0.57
6:1F:261:HIS:ND1	6:1F:261:HIS:O	2.38	0.57
7:1G:145:LEU:HB2	7:1G:269:PHE:CE2	2.40	0.57
10:1J:55:MET:HB3	10:1J:59:ILE:HD11	1.87	0.57
10:1J:124:ASP:OD1	10:1J:124:ASP:N	2.37	0.57
16:1P:113:ILE:O	16:1P:117:ILE:HG12	2.05	0.57
24:1Y:61:THR:O	24:1Y:65:ILE:HG12	2.04	0.57
44:1s:60:LYS:O	44:1s:60:LYS:NZ	2.37	0.57
6:1F:150:GLN:HA	6:1F:153:ILE:HG22	1.87	0.57
7:1G:12:PHE:HA	7:1G:17:SER:HA	1.87	0.57
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	1.86	0.57
9:1I:116:CYS:SG	9:1I:117:ILE:N	2.77	0.57
11:1K:47:ILE:HG12	14:1N:79:LEU:HD13	1.84	0.57
23:1X:144:ARG:O	23:1X:146:ARG:NH1	2.36	0.57
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.37	0.57
2:1B:162:GLN:OE1	42:1q:116:ASN:ND2	2.37	0.57
3:1C:90:PHE:CE1	3:1C:113:GLU:HG3	2.39	0.57
5:1E:99:HIS:H	5:1E:157:ASN:HA	1.70	0.57
12:1L:142:ILE:HD13	13:1M:370:PRO:HB2	1.86	0.57
13:1M:428:ALA:N	39:1n:105:ASP:OD2	2.36	0.57
14:1N:139:LEU:HD23	14:1N:205:LEU:HD22	1.86	0.57
4:1D:283:PHE:O	9:1I:1:THR:OG1	2.22	0.57
6:1F:68:ARG:HE	6:1F:226:GLU:HB3	1.69	0.57
6:1F:402:HIS:O	7:1G:53:ARG:NE	2.32	0.57
8:1H:168:THR:OG1	25:1Z:57:ARG:NH1	2.38	0.57
8:1H:181:LEU:HA	8:1H:184:MET:HB2	1.85	0.57
30:1e:68:ARG:HD3	30:1e:71:THR:HG21	1.87	0.57
33:1h:49:GLU:O	41:1p:59:ARG:NH2	2.36	0.57
13:1M:317:ILE:HB	13:1M:454:ILE:HD11	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:108:ASP:HA	16:1P:112:LYS:HB2	1.86	0.57
34:1i:112:THR:HG23	34:1i:114:GLU:H	1.67	0.57
40:1o:66:LEU:HD12	40:1o:66:LEU:H	1.70	0.57
5:1E:83:VAL:HG12	5:1E:90:TYR:HE2	1.69	0.57
14:1N:234:TRP:CD2	14:1N:304:MET:HB3	2.40	0.57
15:1O:317:ILE:HA	15:1O:320:LYS:HG2	1.87	0.57
16:1P:167:LYS:HZ1	16:1P:227:THR:HG22	1.68	0.57
16:1P:176:ASP:O	16:1P:177:ARG:HG2	2.05	0.57
18:1R:73:ILE:HD11	18:1R:84:CYS:HA	1.86	0.57
36:1k:48:GLU:OE2	39:1n:33:ARG:NH2	2.36	0.57
39:1n:135:GLU:HB2	39:1n:164:PRO:HA	1.86	0.57
4:1D:369:ALA:N	4:1D:372:GLY:O	2.37	0.57
7:1G:195:LEU:HA	7:1G:264:SER:HA	1.87	0.57
8:1H:215:TYR:OH	8:1H:219:PRO:HB2	2.05	0.57
13:1M:48:ASN:HD22	33:1h:90:THR:HG21	1.68	0.57
13:1M:130:LEU:O	13:1M:134:THR:OG1	2.19	0.57
21:1V:8:THR:OG1	21:1V:13:LEU:O	2.22	0.57
40:1o:36:ARG:NH2	40:1o:93:ASP:OD2	2.38	0.57
3:1C:58:ILE:H	3:1C:58:ILE:HD12	1.69	0.57
7:1G:159:CYS:HA	7:1G:202:ILE:HD11	1.85	0.57
7:1G:577:GLU:OE2	7:1G:579:ARG:NE	2.29	0.57
9:1I:48:ILE:HG23	9:1I:53:GLU:HB3	1.87	0.57
10:1J:1:FME:SD	10:1J:2:THR:N	2.78	0.57
13:1M:70:THR:HA	13:1M:103:GLN:HE22	1.70	0.57
50:1N:401:3PE:N	15:1O:304:TYR:OH	2.38	0.57
15:1O:208:LYS:HD2	15:1O:208:LYS:H	1.70	0.57
20:1U:28:GLU:HG2	20:1U:29:LYS:HD2	1.85	0.57
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.22	0.57
35:1j:67:LEU:O	40:1o:110:ARG:NH1	2.38	0.57
37:1l:137:ASP:O	37:1l:142:ARG:NH2	2.38	0.57
44:1s:58:LEU:HD23	44:1s:62:ARG:HH11	1.70	0.57
1:1A:17:LEU:HD12	1:1A:20:ILE:HG21	1.85	0.56
1:1A:77:TRP:HZ3	10:1J:51:PHE:HD2	1.53	0.56
6:1F:272:MET:HE2	6:1F:317:MET:HE1	1.86	0.56
7:1G:112:GLY:HA3	7:1G:219:PRO:HG2	1.88	0.56
11:1K:38:LEU:O	11:1K:42:ILE:HD12	2.05	0.56
13:1M:22:MET:HA	13:1M:22:MET:HE3	1.86	0.56
21:1V:43:TYR:CZ	21:1V:93:MET:HE1	2.40	0.56
39:1n:48:ASP:N	39:1n:48:ASP:OD1	2.38	0.56
7:1G:147:LYS:HB2	7:1G:211:LYS:HG2	1.87	0.56
8:1H:96:ILE:HG23	25:1Z:144:THR:HG21	1.85	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:158:ALA:O	14:1N:161:SER:OG	2.22	0.56
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	1.87	0.56
39:1n:83:GLU:CD	39:1n:83:GLU:H	2.12	0.56
1:1A:60:ILE:HD11	11:1K:72:ALA:HA	1.87	0.56
1:1A:81:THR:O	27:1b:45:ASN:ND2	2.38	0.56
3:1C:167:PRO:HA	17:1Q:82:LEU:HD21	1.86	0.56
5:1E:159:ASN:ND2	5:1E:159:ASN:C	2.62	0.56
6:1F:91:LYS:HG3	6:1F:219:PRO:HB2	1.86	0.56
6:1F:365:CYS:HB2	46:1F:502:SF4:S2	2.44	0.56
7:1G:215:PHE:HB3	9:1I:104:ARG:HG2	1.88	0.56
9:1I:61:PHE:HE1	9:1I:137:PHE:HD2	1.53	0.56
12:1L:432:LEU:HD21	36:1k:65:ALA:HB2	1.88	0.56
14:1N:73:ALA:HB2	14:1N:97:MET:HG3	1.87	0.56
20:1U:51:ILE:O	20:1U:55:GLU:N	2.35	0.56
29:1d:72:GLY:O	29:1d:76:LEU:HD22	2.05	0.56
30:1e:94:PRO:HD2	30:1e:97:HIS:CD2	2.40	0.56
34:1i:108:THR:HB	34:1i:115:VAL:HG12	1.86	0.56
3:1C:210:ARG:HH12	7:1G:35:MET:HA	1.69	0.56
6:1F:230:VAL:O	6:1F:234:ILE:HG13	2.05	0.56
6:1F:355:LYS:HD3	6:1F:373:ASN:HD22	1.70	0.56
7:1G:229:ASP:OD1	7:1G:230:VAL:N	2.39	0.56
13:1M:116:ILE:O	13:1M:120:ILE:HD12	2.06	0.56
14:1N:309:ASN:HD22	15:1O:95:ARG:HG3	1.71	0.56
14:1N:320:THR:O	14:1N:322:GLN:NE2	2.38	0.56
17:1Q:123:SER:HB2	17:1Q:126:LYS:HE2	1.86	0.56
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.38	0.56
3:1C:67:HIS:HB3	3:1C:70:ALA:HB3	1.87	0.56
4:1D:146:ARG:HG3	4:1D:150:HIS:HE1	1.70	0.56
6:1F:17:ASP:HA	6:1F:20:ARG:HG3	1.87	0.56
7:1G:601:ARG:HE	7:1G:614:ASP:HA	1.69	0.56
12:1L:224:SER:HB3	12:1L:226:GLN:HE22	1.70	0.56
13:1M:1:FME:HG2	13:1M:111:THR:HG21	1.86	0.56
15:1O:176:VAL:HG21	15:1O:200:GLN:HA	1.87	0.56
16:1P:195:SER:O	16:1P:195:SER:OG	2.22	0.56
3:1C:139:GLY:HA3	3:1C:160:HIS:CD2	2.41	0.56
3:1C:168:LEU:HD12	4:1D:89:LYS:HG3	1.88	0.56
5:1E:159:ASN:HD21	5:1E:161:TYR:HE1	1.54	0.56
9:1I:32:ARG:NH2	25:1Z:26:PRO:O	2.37	0.56
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.41	0.56
12:1L:491:LEU:O	12:1L:495:ILE:HG12	2.04	0.56
14:1N:270:MET:HE1	14:1N:282:MET:SD	2.46	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:2:GLN:HG2	15:1O:4:GLY:H	1.70	0.56
29:1d:106:LYS:HE3	41:1p:77:GLU:HG3	1.88	0.56
39:1n:60:THR:HA	39:1n:63:LEU:HD12	1.87	0.56
40:1o:62:LEU:HD13	40:1o:86:TRP:CE2	2.40	0.56
6:1F:242:PHE:CE1	6:1F:252:GLY:HA3	2.40	0.56
7:1G:257:ASP:OD2	7:1G:579:ARG:NH2	2.38	0.56
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.22	0.56
12:1L:496:MET:O	12:1L:500:LEU:HD23	2.05	0.56
13:1M:25:ILE:HG23	32:1g:60:VAL:HG11	1.88	0.56
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.41	0.56
22:1W:99:GLN:H	22:1W:102:HIS:HD2	1.53	0.56
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.88	0.56
1:1A:69:ILE:HG12	8:1H:148:ILE:HD11	1.88	0.56
2:1B:144:ILE:HA	9:1I:142:GLU:HA	1.87	0.56
3:1C:92:ILE:HG12	3:1C:142:PHE:HZ	1.70	0.56
5:1E:26:GLU:HA	5:1E:29:LYS:HE3	1.88	0.56
5:1E:165:THR:HG22	5:1E:167:LYS:H	1.70	0.56
8:1H:70:MET:HE2	8:1H:70:MET:HA	1.88	0.56
15:1O:197:ALA:O	15:1O:201:ASP:N	2.37	0.56
19:1S:20:ILE:O	19:1S:21:HIS:ND1	2.39	0.56
38:1m:1:SER:OG	38:1m:2:PHE:N	2.35	0.56
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.39	0.56
4:1D:151:ILE:O	4:1D:155:THR:OG1	2.16	0.56
7:1G:644:GLN:HB3	19:1S:40:TYR:CE2	2.40	0.56
8:1H:85:MET:HG2	8:1H:233:MET:SD	2.46	0.56
12:1L:339:LEU:HD22	12:1L:373:LEU:HD22	1.88	0.56
14:1N:37:LEU:HD21	14:1N:60:PHE:HD1	1.71	0.56
21:1V:23:LEU:HD22	21:1V:58:VAL:HG21	1.86	0.56
2:1B:38:ASN:ND2	2:1B:170:GLU:OE1	2.36	0.56
7:1G:372:GLU:N	7:1G:372:GLU:OE1	2.38	0.56
7:1G:673:MET:HE2	7:1G:673:MET:HA	1.88	0.56
16:1P:128:LYS:NZ	16:1P:217:ALA:O	2.39	0.56
17:1Q:27:GLU:H	17:1Q:27:GLU:CD	2.14	0.56
24:1Y:89:TYR:CD2	24:1Y:125:LYS:HB2	2.41	0.56
44:1s:52:LEU:HA	44:1s:55:ASN:HB3	1.87	0.56
4:1D:176:LYS:NZ	43:1r:24:GLN:O	2.36	0.55
5:1E:131:THR:HG23	5:1E:138:THR:HB	1.87	0.55
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.39	0.55
13:1M:124:ALA:HB1	14:1N:256:PRO:HD3	1.88	0.55
14:1N:116:PRO:HG3	14:1N:181:TYR:HE1	1.70	0.55
37:1l:30:ARG:HH12	38:1m:35:ARG:CG	2.19	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:87:TYR:HD2	6:1F:181:ALA:HB3	1.71	0.55
7:1G:276:ARG:HH22	7:1G:682:GLN:HB2	1.71	0.55
7:1G:316:ALA:HB3	7:1G:519:PRO:HG3	1.88	0.55
7:1G:410:GLY:HA3	7:1G:661:LEU:HB2	1.87	0.55
14:1N:292:PHE:HA	14:1N:295:ARG:HB3	1.88	0.55
23:1X:51:ASP:HB3	23:1X:54:ARG:HG2	1.86	0.55
36:1k:48:GLU:HG2	39:1n:33:ARG:HB3	1.87	0.55
3:1C:135:TRP:HB3	3:1C:148:LEU:HD11	1.87	0.55
6:1F:303:SER:OG	6:1F:354:TYR:OH	2.21	0.55
7:1G:333:ASP:OD2	7:1G:622:ARG:NH2	2.37	0.55
7:1G:453:LEU:H	7:1G:492:ILE:HA	1.71	0.55
13:1M:76:MET:HG2	13:1M:226:ALA:O	2.07	0.55
20:1U:43:ASP:OD1	20:1U:46:ASP:N	2.37	0.55
2:1B:98:PRO:HG3	22:1W:101:THR:HG21	1.89	0.55
4:1D:202:ASP:HB2	4:1D:323:ILE:HD13	1.89	0.55
11:1K:42:ILE:HD12	11:1K:42:ILE:H	1.72	0.55
12:1L:350:LEU:O	12:1L:350:LEU:HD23	2.06	0.55
13:1M:452:LYS:HG3	13:1M:459:TYR:HE2	1.72	0.55
15:1O:175:PRO:HG2	15:1O:178:GLU:HB2	1.87	0.55
15:1O:204:ASN:HB2	15:1O:208:LYS:HZ3	1.71	0.55
16:1P:162:GLU:N	16:1P:162:GLU:OE1	2.40	0.55
27:1b:39:ASN:HA	27:1b:42:ILE:HD12	1.89	0.55
2:1B:51:GLY:HA2	2:1B:89:ALA:HB3	1.89	0.55
2:1B:162:GLN:NE2	9:1I:140:SER:OG	2.40	0.55
5:1E:184:PRO:HG2	44:1s:44:HIS:HA	1.89	0.55
7:1G:344:CYS:HA	7:1G:508:LYS:HB3	1.88	0.55
9:1I:69:ARG:NH1	9:1I:73:GLY:O	2.39	0.55
11:1K:25:HIS:NE2	11:1K:88:ASP:OD1	2.39	0.55
12:1L:79:SER:H	12:1L:139:GLN:NE2	2.04	0.55
12:1L:485:TYR:HB2	58:1l:201:MYR:H132	1.88	0.55
16:1P:59:LEU:HA	16:1P:62:MET:HE3	1.88	0.55
10:1J:169:MET:HA	10:1J:172:THR:HG22	1.87	0.55
12:1L:62:ILE:HD13	12:1L:81:LYS:HA	1.88	0.55
13:1M:148:TYR:O	13:1M:152:TYR:HB2	2.07	0.55
14:1N:95:MET:HE2	14:1N:149:ILE:HD12	1.87	0.55
29:1d:17:GLU:H	29:1d:17:GLU:CD	2.13	0.55
1:1A:67:LEU:HD12	11:1K:65:VAL:HA	1.89	0.55
3:1C:79:THR:HG22	4:1D:390:LYS:HG2	1.87	0.55
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.07	0.55
4:1D:339:LYS:HB3	18:1R:69:PRO:HA	1.89	0.55
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	1.88	0.55
12:1L:216:LEU:HD22	12:1L:259:LEU:HD21	1.87	0.55
12:1L:502:LEU:O	12:1L:506:ASN:ND2	2.39	0.55
16:1P:90:VAL:HG13	16:1P:128:LYS:HB2	1.88	0.55
20:1U:9:GLU:HA	20:1U:12:LYS:NZ	2.21	0.55
33:1h:114:MET:HG3	33:1h:122:TRP:HE1	1.71	0.55
17:1Q:59:PHE:HD1	17:1Q:79:LEU:HB3	1.72	0.55
21:1V:54:LYS:HA	21:1V:57:MET:SD	2.47	0.55
37:1l:102:CYS:O	37:1l:106:SER:OG	2.18	0.55
6:1F:9:LYS:HE2	6:1F:245:PHE:HA	1.89	0.55
6:1F:246:GLY:HA3	6:1F:251:SER:HA	1.87	0.55
6:1F:361:GLN:HG2	7:1G:51:ASN:OD1	2.06	0.55
7:1G:171:ASP:OD1	7:1G:172:LEU:N	2.39	0.55
12:1L:316:THR:OG1	12:1L:325:ALA:HB2	2.07	0.55
12:1L:478:PRO:HD2	40:1o:86:TRP:HH2	1.72	0.55
37:1l:58:ARG:NH1	37:1l:70:ARG:O	2.39	0.55
41:1p:55:HIS:O	41:1p:59:ARG:NH1	2.36	0.55
1:1A:72:LEU:HD23	1:1A:72:LEU:H	1.71	0.55
2:1B:121:ASN:HD22	2:1B:145:TYR:HD2	1.53	0.55
6:1F:57:LEU:HA	6:1F:60:VAL:HG22	1.89	0.55
6:1F:200:GLN:OE1	6:1F:200:GLN:N	2.39	0.55
7:1G:231:MET:HB3	7:1G:266:LYS:HD2	1.89	0.55
10:1J:52:LEU:N	10:1J:139:GLU:OE2	2.23	0.55
12:1L:159:HIS:CE1	39:1n:95:CYS:HG	2.24	0.55
12:1L:313:MET:HB2	12:1L:325:ALA:HB1	1.88	0.55
16:1P:319:ARG:HA	16:1P:322:ARG:HG3	1.88	0.55
37:1l:128:VAL:HG21	40:1o:94:TYR:HE1	1.72	0.55
39:1n:167:TRP:O	39:1n:171:THR:OG1	2.20	0.55
7:1G:319:ALA:HA	7:1G:525:LEU:HD23	1.87	0.54
10:1J:105:TYR:O	10:1J:109:LYS:HG2	2.07	0.54
3:1C:58:ILE:O	3:1C:62:THR:OG1	2.16	0.54
6:1F:36:ALA:HA	6:1F:39:ARG:HB2	1.88	0.54
7:1G:231:MET:O	7:1G:266:LYS:NZ	2.40	0.54
17:1Q:95:PHE:HA	17:1Q:98:LYS:HE3	1.88	0.54
20:1U:45:LEU:N	57:1n:201:EHZ:O9	2.30	0.54
28:1c:6:GLU:HG3	28:1c:7:PRO:HD3	1.89	0.54
31:1f:46:ARG:NH1	31:1f:52:GLU:OE2	2.40	0.54
33:1h:7:ARG:HG2	34:1i:27:LEU:HD21	1.89	0.54
4:1D:136:TRP:HE3	4:1D:319:PRO:HG3	1.73	0.54
8:1H:55:LEU:HA	8:1H:217:ALA:HB1	1.90	0.54
8:1H:116:ILE:HD13	8:1H:211:PHE:HB3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:96:VAL:O	12:1L:100:ILE:HG22	2.08	0.54
13:1M:418:LYS:HB3	37:1l:68:ASP:HB3	1.90	0.54
35:1j:10:ARG:NH1	35:1j:14:PHE:O	2.40	0.54
39:1n:178:MET:HE2	39:1n:178:MET:N	2.20	0.54
5:1E:100:ILE:HD12	5:1E:156:ILE:HG13	1.89	0.54
5:1E:164:LEU:HD13	5:1E:169:ILE:HD13	1.88	0.54
6:1F:118:LEU:HD11	6:1F:225:VAL:HG13	1.87	0.54
6:1F:281:GLU:HA	6:1F:286:GLY:HA2	1.88	0.54
7:1G:276:ARG:HH12	7:1G:682:GLN:HB2	1.73	0.54
7:1G:599:ILE:HA	22:1W:122:PHE:HE1	1.72	0.54
14:1N:319:HIS:HB3	29:1d:49:ARG:HH22	1.73	0.54
35:1j:10:ARG:HG3	35:1j:15:PRO:HA	1.89	0.54
36:1k:27:PRO:HD2	36:1k:52:TYR:HB3	1.89	0.54
3:1C:129:TRP:HH2	4:1D:80:ILE:HG12	1.72	0.54
4:1D:146:ARG:O	4:1D:150:HIS:ND1	2.41	0.54
8:1H:3:MET:H	8:1H:3:MET:CE	2.19	0.54
13:1M:176:PHE:HE2	13:1M:245:ARG:HB3	1.73	0.54
13:1M:225:ILE:HG12	13:1M:331:ASN:HB2	1.90	0.54
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	1.89	0.54
18:1R:4:THR:HA	18:1R:10:LYS:HA	1.88	0.54
35:1j:37:LEU:HB2	36:1k:77:PHE:CE1	2.43	0.54
1:1A:106:TRP:CH2	27:1b:18:LEU:HD21	2.42	0.54
4:1D:328:ALA:H	7:1G:126:ASP:HB2	1.72	0.54
6:1F:205:LEU:N	17:1Q:118:TYR:OH	2.36	0.54
7:1G:142:ILE:HD12	7:1G:142:ILE:O	2.06	0.54
32:1g:111:ASN:HD22	32:1g:115:PRO:HG3	1.73	0.54
34:1i:22:LEU:HA	34:1i:25:GLN:HG2	1.89	0.54
2:1B:77:ARG:NH1	8:1H:24:GLU:OE1	2.37	0.54
4:1D:253:TYR:OH	4:1D:404:LYS:NZ	2.28	0.54
5:1E:124:LEU:HD11	5:1E:137:PHE:CD2	2.35	0.54
5:1E:128:VAL:HA	5:1E:139:LEU:HG	1.88	0.54
6:1F:112:ARG:N	6:1F:145:GLU:OE1	2.41	0.54
7:1G:191:PHE:HA	7:1G:192:MET:HE3	1.90	0.54
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.43	0.54
22:1W:32:VAL:HG13	22:1W:67:PHE:HE1	1.73	0.54
23:1X:123:GLU:HA	23:1X:126:LYS:HG3	1.90	0.54
5:1E:105:THR:HB	5:1E:143:GLU:HG3	1.90	0.54
9:1I:44:GLU:OE1	9:1I:44:GLU:N	2.41	0.54
9:1I:81:LYS:HG2	9:1I:94:ILE:HD13	1.90	0.54
15:1O:58:TYR:OH	15:1O:110:ASP:OD2	2.23	0.54
21:1V:107:PRO:HD2	21:1V:110:GLN:HG2	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:68:ILE:HG23	32:1g:69:VAL:HG23	1.90	0.54
2:1B:41:ARG:HD3	2:1B:110:PRO:HG3	1.88	0.54
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.90	0.54
8:1H:190:LEU:HD11	8:1H:273:ILE:HD13	1.89	0.54
39:1n:75:HIS:HD2	39:1n:77:GLN:H	1.55	0.54
40:1o:75:ASN:HB3	41:1p:23:THR:HG21	1.90	0.54
6:1F:68:ARG:O	6:1F:331:THR:HA	2.07	0.54
7:1G:46:LEU:HD22	7:1G:47:SER:H	1.73	0.54
7:1G:54:MET:HE1	7:1G:94:MET:HB2	1.90	0.54
7:1G:229:ASP:OD1	7:1G:231:MET:N	2.40	0.54
12:1L:400:ASN:O	37:1l:126:GLN:NE2	2.40	0.54
22:1W:34:GLU:OE1	22:1W:34:GLU:N	2.36	0.54
24:1Y:11:ILE:HB	24:1Y:20:LYS:HD3	1.89	0.54
27:1b:6:SER:O	27:1b:10:ASN:ND2	2.41	0.54
29:1d:53:VAL:HG23	29:1d:54:VAL:N	2.20	0.54
34:1i:120:LYS:NZ	40:1o:39:VAL:HG23	2.23	0.54
1:1A:87:MET:HA	10:1J:147:TYR:HB3	1.89	0.53
2:1B:62:MET:HE3	2:1B:69:MET:HB3	1.89	0.53
7:1G:122:MET:N	7:1G:122:MET:SD	2.81	0.53
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	1.88	0.53
20:1T:56:ASP:N	20:1T:56:ASP:OD1	2.41	0.53
4:1D:175:GLU:OE1	4:1D:175:GLU:N	2.41	0.53
12:1L:361:GLY:N	12:1L:433:GLY:O	2.41	0.53
16:1P:119:GLN:HA	16:1P:122:LYS:HD3	1.90	0.53
16:1P:198:LYS:HA	16:1P:237:LEU:HD11	1.89	0.53
16:1P:319:ARG:NH2	22:1W:51:GLN:OE1	2.42	0.53
20:1U:21:LEU:HA	36:1k:18:TYR:OH	2.08	0.53
23:1X:12:LEU:HD11	25:1Z:84:LEU:HD12	1.90	0.53
37:1l:12:PRO:HA	38:1m:78:ASN:OD1	2.08	0.53
3:1C:136:ASP:CG	3:1C:150:ARG:HA	2.33	0.53
5:1E:78:MET:HE3	5:1E:81:TYR:HB2	1.91	0.53
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.90	0.53
7:1G:26:VAL:HB	7:1G:68:ALA:HB1	1.89	0.53
8:1H:154:LEU:HA	8:1H:157:ASN:HB3	1.91	0.53
10:1J:163:ILE:HA	10:1J:166:VAL:HG12	1.90	0.53
12:1L:13:ILE:O	12:1L:16:THR:OG1	2.27	0.53
23:1X:63:ASN:O	23:1X:67:LEU:HD22	2.09	0.53
41:1p:28:PRO:O	41:1p:32:LEU:HD12	2.08	0.53
43:1r:63:MET:HE3	43:1r:64:PRO:CD	2.34	0.53
5:1E:45:ALA:HA	6:1F:198:GLY:HA3	1.89	0.53
6:1F:70:GLY:HA2	6:1F:330:GLY:HA2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:105:CYS:H	6:1F:257:ASN:ND2	2.06	0.53
6:1F:107:ASP:O	6:1F:111:ILE:HG12	2.08	0.53
6:1F:305:PRO:HD2	6:1F:328:GLY:H	1.73	0.53
7:1G:118:ASP:OD1	17:1Q:46:GLN:NE2	2.41	0.53
14:1N:1:FME:HB3	14:1N:6:TYR:HB2	1.89	0.53
14:1N:190:MET:HB3	14:1N:204:ASN:HB3	1.91	0.53
14:1N:194:LEU:HD23	14:1N:201:THR:HG21	1.89	0.53
15:1O:137:ALA:HA	15:1O:201:ASP:OD2	2.08	0.53
20:1T:52:MET:SD	22:1W:41:ARG:HG2	2.48	0.53
20:1T:65:ILE:HG13	22:1W:30:ARG:HH22	1.72	0.53
20:1T:75:GLU:OE1	20:1T:75:GLU:N	2.41	0.53
20:1U:72:CYS:HB2	20:1U:75:GLU:HG3	1.89	0.53
35:1j:10:ARG:HB3	35:1j:13:GLN:HG2	1.91	0.53
4:1D:165:THR:HG21	8:1H:275:ALA:HB1	1.90	0.53
4:1D:286:PRO:HA	9:1I:3:LYS:O	2.08	0.53
6:1F:26:TYR:OH	6:1F:266:CYS:SG	2.57	0.53
6:1F:342:ASP:HB3	6:1F:429:ARG:HH12	1.73	0.53
7:1G:211:LYS:HD3	7:1G:700:GLU:HB3	1.90	0.53
7:1G:234:VAL:HG21	7:1G:390:LEU:HB2	1.91	0.53
7:1G:396:ARG:HD2	7:1G:399:TRP:HD1	1.74	0.53
10:1J:35:VAL:O	10:1J:39:VAL:HG12	2.09	0.53
12:1L:577:VAL:HA	50:1Y:201:3PE:H331	1.90	0.53
14:1N:309:ASN:N	14:1N:309:ASN:OD1	2.41	0.53
15:1O:79:LEU:H	15:1O:79:LEU:HD23	1.74	0.53
37:1l:30:ARG:NE	37:1l:33:ASP:OD2	2.39	0.53
4:1D:146:ARG:HG3	4:1D:150:HIS:CE1	2.43	0.53
15:1O:50:HIS:NE2	15:1O:125:GLU:OE1	2.41	0.53
20:1T:31:SER:N	20:1T:34:SER:OG	2.41	0.53
26:1a:55:SER:HA	26:1a:64:LYS:HD2	1.90	0.53
5:1E:55:GLN:HE22	5:1E:90:TYR:HA	1.73	0.53
8:1H:28:LEU:HG	8:1H:275:ALA:HB2	1.91	0.53
9:1I:135:PRO:HG3	9:1I:164:GLU:HG2	1.91	0.53
12:1L:101:MET:HG3	12:1L:118:PHE:HE2	1.74	0.53
12:1L:596:MET:O	12:1L:600:THR:OG1	2.25	0.53
33:1h:62:GLU:OE1	33:1h:63:HIS:ND1	2.42	0.53
35:1j:56:PRO:HA	35:1j:59:TRP:CZ3	2.43	0.53
2:1B:42:ARG:O	2:1B:164:GLN:NE2	2.29	0.53
3:1C:109:THR:OG1	3:1C:110:TYR:N	2.40	0.53
5:1E:85:THR:HG21	7:1G:175:THR:HA	1.90	0.53
5:1E:159:ASN:C	5:1E:159:ASN:HD22	2.17	0.53
5:1E:196:ALA:H	6:1F:264:HIS:HB3	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:102:PRO:HG3	7:1G:151:THR:HG23	1.91	0.53
8:1H:29:GLY:O	8:1H:34:ARG:N	2.41	0.53
15:1O:94:TYR:CG	15:1O:148:CYS:HB3	2.44	0.53
15:1O:219:GLU:OE1	15:1O:219:GLU:N	2.36	0.53
16:1P:221:PRO:O	16:1P:224:LYS:NZ	2.29	0.53
23:1X:48:GLU:HB2	23:1X:134:ARG:HH22	1.74	0.53
31:1f:42:LEU:HD11	41:1p:70:VAL:HG22	1.90	0.53
5:1E:38:TYR:OH	5:1E:49:PRO:HG2	2.09	0.53
6:1F:154:ARG:HD2	44:1s:57:GLU:HG3	1.90	0.53
8:1H:294:LEU:HD13	8:1H:298:LEU:HD13	1.91	0.53
12:1L:535:ARG:NH2	37:1l:92:SER:OG	2.41	0.53
16:1P:98:GLU:HG2	16:1P:99:TRP:HE3	1.73	0.53
33:1h:7:ARG:NH2	34:1i:27:LEU:O	2.36	0.53
38:1m:51:ASN:OD1	39:1n:168:HIS:ND1	2.34	0.53
39:1n:83:GLU:OE1	39:1n:83:GLU:N	2.42	0.53
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.90	0.53
6:1F:50:LEU:HA	6:1F:127:ARG:HH12	1.74	0.53
6:1F:398:GLN:O	6:1F:402:HIS:ND1	2.42	0.53
7:1G:154:ILE:HD11	7:1G:204:PRO:HG2	1.91	0.53
9:1I:3:LYS:HZ3	43:1r:111:TYR:HA	1.73	0.53
12:1L:293:ILE:HG21	12:1L:418:LEU:HD12	1.91	0.53
13:1M:14:MET:HE3	13:1M:26:ASN:HB3	1.90	0.53
13:1M:46:GLY:HA2	32:1g:84:ARG:HD3	1.89	0.53
40:1o:95:VAL:O	40:1o:99:LYS:HG3	2.08	0.53
2:1B:75:VAL:HG13	2:1B:77:ARG:H	1.74	0.52
5:1E:150:ASN:HD21	5:1E:163:ASP:H	1.56	0.52
6:1F:287:VAL:HG11	6:1F:294:LEU:HB2	1.91	0.52
7:1G:177:ARG:HH12	7:1G:178:GLY:HA3	1.74	0.52
8:1H:269:THR:HA	8:1H:272:TRP:HB3	1.90	0.52
12:1L:237:MET:SD	12:1L:303:ALA:HB2	2.49	0.52
14:1N:237:MET:HB2	14:1N:240:ILE:HD13	1.90	0.52
15:1O:24:VAL:HB	15:1O:166:PRO:HB3	1.91	0.52
16:1P:193:LEU:HD13	16:1P:242:VAL:HG21	1.89	0.52
21:1V:40:ASN:OD1	21:1V:40:ASN:N	2.41	0.52
25:1Z:10:MET:HE3	25:1Z:10:MET:HA	1.91	0.52
25:1Z:127:LEU:HD13	30:1e:97:HIS:CE1	2.45	0.52
35:1j:18:THR:HG23	35:1j:21:GLN:H	1.74	0.52
40:1o:20:ARG:NH1	40:1o:20:ARG:O	2.41	0.52
2:1B:68:ASP:OD2	2:1B:71:ARG:N	2.42	0.52
3:1C:77:ASP:HA	3:1C:130:TYR:CE1	2.35	0.52
6:1F:127:ARG:HD2	6:1F:127:ARG:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.49	0.52
7:1G:592:LEU:HA	7:1G:594:ARG:HH21	1.74	0.52
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.09	0.52
13:1M:68:LEU:HD22	13:1M:317:ILE:HG23	1.90	0.52
14:1N:24:SER:HB2	30:1e:1:PRO:HG3	1.90	0.52
29:1d:2:MET:O	29:1d:4:GLY:N	2.42	0.52
33:1h:134:ASP:OD1	33:1h:136:SER:OG	2.28	0.52
4:1D:72:MET:HE1	4:1D:408:GLY:HA2	1.91	0.52
7:1G:248:MET:HA	7:1G:248:MET:HE3	1.92	0.52
12:1L:55:MET:CE	12:1L:471:ASN:HB3	2.39	0.52
12:1L:102:GLU:HB2	12:1L:453:SER:HB3	1.90	0.52
13:1M:360:LEU:O	13:1M:363:SER:OG	2.24	0.52
15:1O:165:PRO:HB3	15:1O:214:MET:HE1	1.90	0.52
17:1Q:37:ILE:HD11	17:1Q:105:VAL:HA	1.91	0.52
33:1h:34:ILE:O	33:1h:37:ALA:N	2.42	0.52
34:1i:89:VAL:O	34:1i:95:THR:OG1	2.20	0.52
34:1i:106:GLY:H	34:1i:116:ILE:HG23	1.73	0.52
4:1D:322:GLU:CD	43:1r:44:PRO:HD3	2.34	0.52
5:1E:36:LYS:HB3	44:1s:62:ARG:HH21	1.74	0.52
5:1E:156:ILE:HG21	5:1E:176:LEU:HD13	1.90	0.52
8:1H:212:ASN:HA	8:1H:215:TYR:HB3	1.92	0.52
16:1P:38:LEU:HB3	16:1P:45:VAL:HG11	1.91	0.52
34:1i:105:PRO:O	40:1o:67:LYS:NZ	2.41	0.52
38:1m:94:ILE:HA	38:1m:97:LEU:HD12	1.91	0.52
4:1D:269:LEU:HB2	4:1D:368:GLU:HB3	1.92	0.52
6:1F:343:ILE:HG21	6:1F:418:LEU:HD11	1.91	0.52
7:1G:41:CYS:CB	7:1G:52:CYS:SG	2.84	0.52
7:1G:522:LEU:HB3	7:1G:543:ILE:HD13	1.91	0.52
8:1H:90:PRO:HA	8:1H:94:PRO:HB3	1.92	0.52
16:1P:133:SER:O	16:1P:168:PRO:HD2	2.10	0.52
20:1U:85:ASP:HB2	34:1i:22:LEU:HD11	1.92	0.52
21:1V:43:TYR:OH	21:1V:86:GLU:OE2	2.21	0.52
34:1i:3:TYR:HB3	34:1i:8:LYS:HB2	1.91	0.52
39:1n:153:LEU:HD11	39:1n:165:LEU:HD12	1.92	0.52
4:1D:276:ASP:CG	4:1D:277:VAL:N	2.65	0.52
4:1D:298:LEU:HB3	9:1I:5:VAL:HG21	1.92	0.52
5:1E:144:CYS:HB3	47:1E:301:FES:S2	2.50	0.52
6:1F:121:GLY:HA3	6:1F:228:VAL:O	2.10	0.52
7:1G:80:LEU:HB3	7:1G:83:SER:HB3	1.92	0.52
12:1L:124:PHE:CZ	12:1L:252:MET:HB2	2.44	0.52
13:1M:44:GLN:HB2	32:1g:83:TYR:HE1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:347:ASN:O	29:1d:8:ARG:NH2	2.43	0.52
17:1Q:40:PRO:HD3	17:1Q:56:LYS:HE2	1.90	0.52
5:1E:48:LEU:HB3	5:1E:49:PRO:HD3	1.92	0.52
7:1G:340:SER:O	7:1G:340:SER:OG	2.26	0.52
12:1L:341:MET:O	12:1L:345:SER:N	2.40	0.52
12:1L:533:MET:O	12:1L:537:PRO:HD2	2.09	0.52
14:1N:11:MET:HA	14:1N:14:MET:HB2	1.90	0.52
16:1P:37:HIS:CD2	16:1P:40:ARG:HH12	2.27	0.52
16:1P:262:ALA:HA	16:1P:265:TRP:HE3	1.75	0.52
23:1X:29:HIS:HB2	23:1X:118:ARG:HH21	1.75	0.52
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.91	0.52
38:1m:2:PHE:HZ	39:1n:69:GLU:HA	1.75	0.52
40:1o:100:GLU:HA	40:1o:103:ARG:HB3	1.91	0.52
3:1C:64:LEU:HB3	3:1C:72:PHE:HB2	1.92	0.52
5:1E:163:ASP:OD2	5:1E:186:PRO:HB3	2.10	0.52
6:1F:343:ILE:CG2	6:1F:418:LEU:HD11	2.40	0.52
14:1N:64:ALA:O	14:1N:68:MET:HG2	2.10	0.52
1:1A:6:THR:O	1:1A:10:ASN:ND2	2.42	0.52
1:1A:102:LEU:HD13	8:1H:294:LEU:HD12	1.92	0.52
5:1E:81:TYR:HE2	7:1G:187:ILE:HG12	1.75	0.52
7:1G:45:ARG:NH2	7:1G:254:MET:SD	2.82	0.52
7:1G:199:ILE:HA	7:1G:202:ILE:HG12	1.92	0.52
7:1G:243:ARG:HG2	7:1G:248:MET:SD	2.49	0.52
7:1G:562:PRO:HB2	7:1G:593:ALA:HB2	1.92	0.52
8:1H:9:LEU:HD11	8:1H:86:TRP:HB3	1.91	0.52
8:1H:75:PRO:HB2	8:1H:222:MET:HB2	1.92	0.52
12:1L:319:ILE:HG21	12:1L:404:THR:HG22	1.92	0.52
21:1V:36:GLN:OE1	21:1V:36:GLN:N	2.40	0.52
2:1B:57:VAL:HG12	2:1B:61:HIS:HE1	1.75	0.52
2:1B:64:ALA:HB2	4:1D:171:PHE:HD2	1.75	0.52
3:1C:114:LEU:O	22:1W:20:ILE:HD11	2.10	0.52
5:1E:100:ILE:HB	5:1E:139:LEU:HA	1.92	0.52
5:1E:156:ILE:N	5:1E:159:ASN:O	2.38	0.52
7:1G:194:GLU:H	7:1G:194:GLU:CD	2.16	0.52
13:1M:198:ALA:HB2	51:1M:501:PGT:H381	1.92	0.52
16:1P:91:VAL:HG23	16:1P:126:VAL:HG21	1.92	0.52
19:1S:74:LYS:HE2	19:1S:74:LYS:HA	1.92	0.52
32:1g:93:ALA:HB1	41:1p:101:ILE:HD13	1.92	0.52
34:1i:102:ARG:HG3	40:1o:49:GLN:HB2	1.92	0.52
3:1C:182:ARG:HD3	22:1W:101:THR:HA	1.92	0.51
8:1H:306:SER:O	8:1H:310:MET:N	2.42	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:82:VAL:O	10:1J:85:SER:OG	2.22	0.51
13:1M:143:LEU:HD11	14:1N:303:THR:HG21	1.92	0.51
13:1M:403:THR:O	13:1M:407:SER:OG	2.23	0.51
16:1P:191:VAL:HG12	16:1P:193:LEU:HD22	1.92	0.51
23:1X:76:HIS:CD2	23:1X:114:LEU:HG	2.45	0.51
3:1C:35:LYS:O	21:1V:102:LEU:HA	2.10	0.51
5:1E:108:CYS:SG	5:1E:153:MET:HG2	2.49	0.51
13:1M:430:PHE:HB2	13:1M:433:GLU:HG3	1.93	0.51
14:1N:119:THR:HG21	14:1N:180:ALA:HB2	1.91	0.51
14:1N:320:THR:HG21	15:1O:265:ASN:HA	1.92	0.51
19:1S:14:GLY:HA2	19:1S:97:LYS:HB2	1.92	0.51
19:1S:82:SER:H	19:1S:85:GLN:NE2	2.08	0.51
21:1V:36:GLN:O	21:1V:37:ILE:HD13	2.08	0.51
37:1l:156:TYR:HB2	40:1o:33:ARG:CZ	2.40	0.51
41:1p:93:ARG:O	41:1p:97:VAL:HG12	2.10	0.51
6:1F:59:GLU:OE1	6:1F:239:GLY:N	2.37	0.51
6:1F:90:PRO:HB3	44:1s:66:PRO:HG2	1.92	0.51
6:1F:202:LYS:HB3	6:1F:361:GLN:CD	2.34	0.51
6:1F:258:ILE:HD11	6:1F:262:VAL:HG21	1.93	0.51
7:1G:343:LEU:O	7:1G:508:LYS:N	2.40	0.51
9:1I:68:ARG:NH2	9:1I:129:ASP:OD2	2.43	0.51
10:1J:160:SER:O	10:1J:164:GLY:N	2.41	0.51
12:1L:286:LEU:HD22	12:1L:411:MET:SD	2.51	0.51
14:1N:120:GLN:HE21	14:1N:177:LYS:HG2	1.75	0.51
14:1N:150:ASN:HB3	14:1N:153:LEU:HB2	1.92	0.51
16:1P:98:GLU:HG2	16:1P:99:TRP:CE3	2.45	0.51
29:1d:25:LYS:HG2	29:1d:27:THR:H	1.76	0.51
42:1q:69:ASN:HB2	42:1q:115:PHE:HE1	1.75	0.51
6:1F:272:MET:SD	6:1F:273:SER:N	2.84	0.51
12:1L:345:SER:O	12:1L:349:SER:OG	2.21	0.51
12:1L:534:HIS:HB3	50:1L:701:3PE:H31	1.93	0.51
13:1M:347:GLY:HA3	13:1M:419:TYR:HA	1.92	0.51
29:1d:-2:ACE:H1	29:1d:3:SER:HB3	1.92	0.51
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.92	0.51
37:1l:34:TYR:HE1	37:1l:48:PRO:HG3	1.75	0.51
3:1C:175:ARG:NH1	3:1C:176:TYR:O	2.44	0.51
3:1C:199:LEU:HD22	4:1D:354:GLU:HA	1.91	0.51
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.39	0.51
5:1E:55:GLN:OE1	5:1E:91:ASN:ND2	2.43	0.51
6:1F:273:SER:HA	6:1F:318:ASP:HB3	1.92	0.51
16:1P:23:VAL:HG12	16:1P:92:ILE:HB	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:20:ILE:HG22	19:1S:54:ILE:HA	1.92	0.51
22:1W:48:HIS:O	22:1W:51:GLN:NE2	2.43	0.51
37:1l:158:ILE:HG21	40:1o:100:GLU:HB3	1.92	0.51
5:1E:15:ASN:HD21	5:1E:60:TRP:HE1	1.58	0.51
7:1G:409:ILE:HD13	7:1G:429:LEU:HD21	1.92	0.51
9:1I:39:SER:HB3	43:1r:14:ALA:HB3	1.93	0.51
11:1K:91:GLN:HA	12:1L:583:LEU:HD11	1.93	0.51
22:1W:34:GLU:HA	22:1W:37:ARG:HG3	1.92	0.51
24:1Y:61:THR:HG22	24:1Y:103:ARG:HD3	1.92	0.51
33:1h:62:GLU:OE1	33:1h:63:HIS:N	2.42	0.51
35:1j:51:PHE:HB2	40:1o:91:HIS:CE1	2.45	0.51
39:1n:50:HIS:ND1	39:1n:50:HIS:O	2.44	0.51
42:1q:141:SER:O	42:1q:143:PRO:HD3	2.11	0.51
1:1A:66:ASP:OD1	10:1J:59:ILE:HG22	2.11	0.51
3:1C:51:PHE:HD2	21:1V:111:TRP:CE2	2.27	0.51
4:1D:87:THR:HG21	4:1D:106:LEU:HD21	1.91	0.51
4:1D:156:THR:HA	4:1D:159:LEU:HB3	1.91	0.51
6:1F:256:PHE:CZ	6:1F:317:MET:HE3	2.45	0.51
7:1G:363:LEU:N	7:1G:492:ILE:HD11	2.26	0.51
7:1G:455:SER:N	7:1G:493:LEU:O	2.42	0.51
8:1H:121:TRP:CD1	10:1J:27:ILE:HG21	2.46	0.51
11:1K:66:PHE:CD2	14:1N:31:ILE:HD12	2.46	0.51
16:1P:91:VAL:C	16:1P:92:ILE:HD13	2.35	0.51
16:1P:175:GLU:OE1	16:1P:175:GLU:N	2.43	0.51
20:1U:35:HIS:CE1	20:1U:71:MET:HE2	2.46	0.51
22:1W:90:LEU:O	22:1W:94:ILE:HG23	2.10	0.51
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.44	0.51
43:1r:19:LEU:H	43:1r:19:LEU:HD12	1.76	0.51
3:1C:133:GLU:O	3:1C:137:MET:N	2.41	0.51
5:1E:143:GLU:HG2	6:1F:353:PHE:CD1	2.43	0.51
7:1G:303:VAL:HG12	7:1G:307:LEU:HD23	1.92	0.51
7:1G:695:ILE:HG23	7:1G:696:GLN:H	1.76	0.51
10:1J:55:MET:HE2	10:1J:55:MET:HA	1.92	0.51
22:1W:114:ARG:HA	22:1W:114:ARG:NE	2.25	0.51
39:1n:30:CYS:O	39:1n:32:HIS:N	2.42	0.51
4:1D:328:ALA:HB3	4:1D:347:HIS:HD2	1.76	0.51
5:1E:98:TYR:HB2	5:1E:137:PHE:HD1	1.75	0.51
5:1E:190:ARG:HG2	5:1E:194:GLU:HG2	1.93	0.51
7:1G:237:ASN:HB3	7:1G:253:ARG:CZ	2.41	0.51
7:1G:582:GLN:HB2	7:1G:633:TYR:CE1	2.46	0.51
8:1H:183:MET:HB3	45:1I:203:PC1:H2F2	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1H:401:PC1:H11	25:1Z:28:ARG:O	2.11	0.51
9:1I:74:GLU:OE2	9:1I:99:ARG:NH2	2.37	0.51
9:1I:95:GLU:OE2	9:1I:108:ARG:NH1	2.44	0.51
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.46	0.51
13:1M:365:THR:HG21	13:1M:444:LEU:HD21	1.93	0.51
15:1O:37:ARG:NH2	15:1O:41:GLU:OE2	2.44	0.51
34:1i:119:MET:HE3	40:1o:40:ALA:HB2	1.93	0.51
1:1A:1:FME:HE1	10:1J:5:ILE:HD13	1.93	0.51
4:1D:238:ARG:HD2	8:1H:281:ARG:HB2	1.92	0.51
4:1D:300:ARG:NH2	4:1D:420:THR:O	2.38	0.51
7:1G:524:LEU:N	7:1G:544:ILE:O	2.43	0.51
12:1L:73:THR:HG22	38:1m:127:SER:HB3	1.92	0.51
12:1L:482:MET:SD	12:1L:487:LYS:HB2	2.51	0.51
20:1T:66:ASP:O	20:1T:69:LYS:HG3	2.11	0.51
28:1c:32:ILE:O	28:1c:36:LYS:HG2	2.11	0.51
35:1j:60:THR:HG22	35:1j:62:GLU:H	1.76	0.51
35:1j:60:THR:HB	35:1j:63:GLU:HG2	1.92	0.51
36:1k:18:TYR:O	36:1k:20:GLN:N	2.41	0.51
37:1l:157:GLU:O	40:1o:33:ARG:NE	2.44	0.51
1:1A:72:LEU:O	1:1A:75:LEU:HB2	2.12	0.50
2:1B:57:VAL:O	2:1B:61:HIS:ND1	2.44	0.50
5:1E:160:TYR:HE1	44:1s:43:HIS:CE1	2.29	0.50
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.76	0.50
7:1G:617:ASP:OD1	7:1G:617:ASP:N	2.44	0.50
12:1L:107:TYR:HD2	12:1L:108:MET:HG3	1.76	0.50
14:1N:11:MET:HA	14:1N:14:MET:HG2	1.92	0.50
14:1N:112:HIS:HB2	14:1N:184:ILE:HD13	1.93	0.50
14:1N:159:MET:HA	14:1N:162:ILE:HG12	1.93	0.50
24:1Y:58:TYR:OH	50:1Y:201:3PE:O14	2.20	0.50
40:1o:41:THR:N	40:1o:44:GLU:OE2	2.44	0.50
4:1D:141:PHE:CE2	4:1D:184:VAL:HG21	2.45	0.50
5:1E:42:HIS:CE1	17:1Q:129:ARG:HE	2.29	0.50
5:1E:84:ALA:HA	5:1E:90:TYR:CD2	2.46	0.50
5:1E:211:PHE:HB3	6:1F:237:ARG:HD2	1.93	0.50
6:1F:33:LEU:HA	6:1F:36:ALA:HB3	1.92	0.50
7:1G:383:ASN:HD22	7:1G:666:LEU:HA	1.76	0.50
10:1J:120:ASN:OD1	10:1J:122:LEU:HD23	2.11	0.50
15:1O:112:LEU:HD11	15:1O:248:TRP:CZ2	2.41	0.50
20:1T:54:MET:HE3	20:1T:76:ILE:HG21	1.92	0.50
26:1a:59:ARG:HB2	26:1a:62:VAL:HG12	1.93	0.50
4:1D:112:MET:HE1	4:1D:193:TYR:HB3	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:68:ARG:HH12	6:1F:331:THR:HB	1.77	0.50
6:1F:278:GLU:HA	6:1F:281:GLU:HB2	1.93	0.50
7:1G:488:LYS:NZ	7:1G:639:ALA:O	2.36	0.50
9:1I:74:GLU:OE2	9:1I:105:ARG:NH2	2.44	0.50
10:1J:103:MET:O	10:1J:107:ALA:N	2.42	0.50
12:1L:51:LEU:O	12:1L:55:MET:HG3	2.11	0.50
14:1N:44:LEU:HB3	14:1N:122:ILE:HG21	1.92	0.50
16:1P:2:HIS:CE1	16:1P:4:ALA:H	2.29	0.50
17:1Q:112:LYS:H	17:1Q:114:LYS:HZ1	1.59	0.50
19:1S:36:ILE:HG21	19:1S:54:ILE:HD11	1.92	0.50
20:1U:9:GLU:HA	20:1U:12:LYS:HZ3	1.75	0.50
20:1U:54:MET:HA	20:1U:54:MET:HE3	1.94	0.50
20:1U:70:LEU:HD13	20:1U:76:ILE:HA	1.93	0.50
21:1V:93:MET:HA	21:1V:96:TRP:HB2	1.92	0.50
22:1W:80:ASP:HA	22:1W:83:VAL:HB	1.91	0.50
28:1c:43:LYS:HD2	28:1c:48:LEU:HB2	1.93	0.50
30:1e:21:SER:N	30:1e:36:GLU:OE2	2.43	0.50
40:1o:44:GLU:HA	40:1o:47:ASP:HB3	1.93	0.50
40:1o:87:ASP:HA	40:1o:90:GLU:HG2	1.92	0.50
3:1C:71:GLN:HB2	3:1C:73:LYS:HZ1	1.75	0.50
7:1G:647:GLU:HA	7:1G:650:LYS:HE3	1.92	0.50
11:1K:10:MET:O	11:1K:14:ILE:HD12	2.11	0.50
12:1L:129:MET:N	12:1L:129:MET:SD	2.84	0.50
12:1L:155:ILE:HD11	12:1L:248:HIS:NE2	2.27	0.50
45:1M:502:PC1:H3D1	33:1h:71:ILE:HD11	1.93	0.50
14:1N:112:HIS:CE1	14:1N:164:ILE:HG21	2.47	0.50
16:1P:167:LYS:NZ	16:1P:227:THR:HG22	2.26	0.50
28:1c:17:VAL:O	28:1c:21:LEU:HD12	2.12	0.50
37:1l:145:ASP:OD2	37:1l:147:THR:OG1	2.28	0.50
38:1m:109:ASP:OD1	38:1m:110:LYS:N	2.44	0.50
41:1p:98:ASP:OD2	41:1p:141:ARG:NH2	2.45	0.50
3:1C:35:LYS:HG2	3:1C:36:TYR:CE2	2.46	0.50
4:1D:285:VAL:H	9:1I:2:TYR:HA	1.75	0.50
6:1F:26:TYR:HB3	6:1F:28:ARG:HH11	1.77	0.50
6:1F:50:LEU:HA	6:1F:127:ARG:NH1	2.26	0.50
9:1I:70:TYR:HE2	18:1R:87:CYS:HA	1.77	0.50
9:1I:168:ASN:HA	42:1q:88:ARG:HH22	1.77	0.50
12:1L:65:ASN:ND2	12:1L:78:LEU:O	2.44	0.50
16:1P:240:ASP:HA	16:1P:243:GLN:NE2	2.27	0.50
36:1k:49:ALA:O	36:1k:53:SER:OG	2.20	0.50
2:1B:125:TYR:HD2	9:1I:117:ILE:HG21	1.74	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:53:LEU:HD23	44:1s:52:LEU:HD21	1.93	0.50
7:1G:599:ILE:HA	22:1W:122:PHE:CE1	2.46	0.50
14:1N:97:MET:HA	14:1N:97:MET:HE2	1.94	0.50
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.47	0.50
14:1N:339:MET:HE2	14:1N:339:MET:HA	1.94	0.50
20:1T:33:ASN:O	20:1T:73:PRO:HD2	2.11	0.50
31:1f:15:LEU:H	31:1f:15:LEU:HD12	1.76	0.50
33:1h:32:THR:C	33:1h:35:PRO:HD2	2.37	0.50
6:1F:185:ILE:HD11	6:1F:203:PRO:HD3	1.93	0.50
8:1H:134:ARG:HB2	8:1H:282:TYR:CE2	2.47	0.50
12:1L:48:LEU:O	12:1L:52:LEU:HD12	2.12	0.50
15:1O:258:ARG:HH22	15:1O:259:LEU:HD13	1.76	0.50
18:1R:56:VAL:C	18:1R:57:ILE:HD12	2.37	0.50
21:1V:91:ARG:O	21:1V:95:ARG:NH2	2.33	0.50
27:1b:27:LEU:O	27:1b:31:LEU:HD12	2.12	0.50
32:1g:117:LYS:HD2	32:1g:117:LYS:C	2.37	0.50
2:1B:92:LEU:HD21	2:1B:139:ILE:HD12	1.94	0.50
3:1C:155:TYR:HB2	22:1W:102:HIS:CE1	2.46	0.50
6:1F:15:LEU:HB2	6:1F:271:GLU:HB2	1.93	0.50
6:1F:262:VAL:HG23	6:1F:287:VAL:HA	1.94	0.50
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.45	0.50
7:1G:518:PRO:HG2	7:1G:537:LEU:HA	1.94	0.50
13:1M:215:TRP:CD1	13:1M:215:TRP:H	2.30	0.50
14:1N:132:THR:HG21	14:1N:213:LEU:HD22	1.94	0.50
15:1O:223:TYR:HB3	15:1O:227:GLU:HB2	1.94	0.50
16:1P:133:SER:N	16:1P:166:ILE:O	2.41	0.50
20:1T:64:ASP:HB3	22:1W:30:ARG:CZ	2.41	0.50
20:1U:16:LEU:HD12	20:1U:30:LEU:HB3	1.94	0.50
24:1Y:91:ILE:HD12	24:1Y:92:GLY:N	2.27	0.50
29:1d:-1:MET:SD	33:1h:111:ARG:NH1	2.85	0.50
30:1e:63:VAL:O	30:1e:67:LEU:N	2.37	0.50
4:1D:150:HIS:HA	4:1D:153:ALA:HB3	1.94	0.50
4:1D:396:PHE:HE1	4:1D:430:ARG:HH22	1.59	0.50
5:1E:66:MET:HE1	7:1G:186:TYR:CE2	2.47	0.50
6:1F:122:CYS:O	6:1F:126:GLY:N	2.40	0.50
7:1G:30:CYS:HB3	7:1G:35:MET:HB3	1.93	0.50
7:1G:255:HIS:CG	7:1G:255:HIS:O	2.65	0.50
8:1H:26:LYS:HA	8:1H:36:GLY:HA3	1.94	0.50
8:1H:287:HIS:HA	8:1H:291:LYS:NZ	2.27	0.50
12:1L:60:GLU:HG2	12:1L:83:ASP:HA	1.94	0.50
13:1M:252:PRO:HB3	29:1d:117:HIS:CD2	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:322:THR:O	13:1M:326:LEU:HD12	2.12	0.50
14:1N:124:LEU:HD21	14:1N:219:LEU:HB3	1.92	0.50
17:1Q:8:THR:H	17:1Q:10:LEU:HD13	1.76	0.50
19:1S:67:ARG:HD2	19:1S:73:GLU:OE2	2.11	0.50
29:1d:2:MET:HE2	29:1d:2:MET:N	2.27	0.50
33:1h:30:LEU:HA	33:1h:33:GLY:HA3	1.93	0.50
37:1l:132:GLN:HB3	37:1l:155:HIS:CD2	2.47	0.50
2:1B:118:SER:N	46:1B:201:SF4:S1	2.85	0.49
4:1D:36:VAL:HA	14:1N:49:ASN:OD1	2.12	0.49
7:1G:54:MET:HA	7:1G:93:VAL:HG21	1.94	0.49
7:1G:155:GLN:HG2	7:1G:181:MET:SD	2.51	0.49
7:1G:276:ARG:HE	42:1q:135:GLN:NE2	2.10	0.49
9:1I:94:ILE:HA	9:1I:108:ARG:O	2.12	0.49
13:1M:196:TRP:HH2	13:1M:302:MET:HE1	1.75	0.49
13:1M:205:VAL:HG23	13:1M:212:LEU:HD13	1.94	0.49
14:1N:207:ILE:HG22	14:1N:211:MET:SD	2.52	0.49
14:1N:267:ILE:O	14:1N:271:THR:OG1	2.24	0.49
15:1O:133:VAL:HG21	15:1O:206:TYR:CE2	2.47	0.49
16:1P:280:THR:H	16:1P:283:LYS:HD3	1.77	0.49
22:1W:75:ASP:OD1	22:1W:76:PRO:HD2	2.12	0.49
30:1e:83:ASP:HA	30:1e:86:ILE:HG12	1.94	0.49
38:1m:2:PHE:CZ	39:1n:69:GLU:HA	2.47	0.49
44:1s:72:SER:OG	44:1s:75:HIS:ND1	2.28	0.49
2:1B:57:VAL:HG12	2:1B:61:HIS:CE1	2.47	0.49
3:1C:168:LEU:HB2	4:1D:93:TYR:HE2	1.77	0.49
4:1D:294:TYR:O	4:1D:298:LEU:HD12	2.12	0.49
5:1E:150:ASN:CG	5:1E:162:GLU:HB3	2.37	0.49
6:1F:433:PHE:O	6:1F:437:HIS:HB2	2.12	0.49
12:1L:561:ILE:HG23	12:1L:562:LEU:H	1.77	0.49
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.95	0.49
19:1S:64:LEU:HD12	19:1S:76:VAL:HG22	1.94	0.49
23:1X:77:CYS:HB2	23:1X:80:PRO:HD2	1.93	0.49
26:1a:28:LYS:HG3	26:1a:33:GLY:HA2	1.94	0.49
30:1e:40:ILE:HD13	33:1h:128:ILE:HG21	1.94	0.49
42:1q:53:LYS:H	42:1q:53:LYS:HD3	1.76	0.49
1:1A:58:VAL:HG12	1:1A:113:TRP:CE2	2.48	0.49
4:1D:19:MET:HG2	14:1N:295:ARG:NE	2.28	0.49
6:1F:161:LEU:HA	6:1F:167:CYS:HA	1.94	0.49
7:1G:243:ARG:HG3	7:1G:244:THR:H	1.76	0.49
7:1G:376:VAL:HG12	7:1G:405:LYS:HB2	1.93	0.49
8:1H:114:TYR:HE2	10:1J:61:LEU:HD23	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:297:ASP:OD2	12:1L:300:LYS:N	2.45	0.49
13:1M:325:MET:HE1	13:1M:441:ILE:HB	1.94	0.49
13:1M:392:THR:O	13:1M:396:MET:N	2.38	0.49
30:1e:86:ILE:HG22	30:1e:91:TYR:HD1	1.77	0.49
3:1C:55:ASP:OD1	3:1C:55:ASP:N	2.38	0.49
3:1C:135:TRP:CB	3:1C:148:LEU:HD11	2.42	0.49
6:1F:40:GLY:O	6:1F:236:ARG:NH1	2.46	0.49
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.47	0.49
12:1L:306:THR:O	12:1L:310:LEU:HD22	2.11	0.49
21:1V:47:THR:HA	21:1V:50:ILE:HG13	1.93	0.49
27:1b:42:ILE:HG22	27:1b:46:ARG:HE	1.77	0.49
34:1i:91:ALA:O	41:1p:3:SER:OG	2.30	0.49
34:1i:93:PRO:HB3	41:1p:4:TRP:CD2	2.47	0.49
35:1j:12:ARG:HB3	36:1k:50:TRP:CD2	2.47	0.49
40:1o:102:GLU:OE2	40:1o:105:ARG:HD2	2.11	0.49
44:1s:63:MET:HE3	44:1s:63:MET:HA	1.95	0.49
1:1A:25:PRO:HB2	8:1H:60:PRO:HD3	1.95	0.49
2:1B:51:GLY:HA3	2:1B:56:ALA:HB2	1.94	0.49
3:1C:69:ASN:ND2	43:1r:94:VAL:O	2.29	0.49
3:1C:196:LYS:NZ	7:1G:223:ARG:HH21	2.07	0.49
5:1E:68:LYS:O	5:1E:72:ILE:HG22	2.12	0.49
6:1F:190:THR:HB	6:1F:204:ARG:N	2.27	0.49
7:1G:237:ASN:N	7:1G:259:ASN:OD1	2.43	0.49
12:1L:190:LEU:HD21	13:1M:307:TRP:CH2	2.48	0.49
12:1L:292:ALA:HB2	12:1L:304:PHE:HB3	1.95	0.49
13:1M:209:LEU:HB3	13:1M:212:LEU:HB2	1.94	0.49
23:1X:144:ARG:HH12	30:1e:57:ILE:HD13	1.77	0.49
34:1i:43:GLU:HG2	34:1i:47:ASN:HD22	1.77	0.49
43:1r:57:ASP:O	43:1r:60:ARG:N	2.42	0.49
3:1C:88:ASN:ND2	21:1V:107:PRO:HG2	2.27	0.49
4:1D:202:ASP:HA	4:1D:323:ILE:HG21	1.94	0.49
7:1G:177:ARG:NH1	7:1G:178:GLY:HA3	2.27	0.49
7:1G:495:ARG:HH21	7:1G:496:ILE:HB	1.77	0.49
8:1H:31:MET:HE1	8:1H:272:TRP:HA	1.93	0.49
12:1L:486:MET:N	12:1L:486:MET:HE3	2.26	0.49
12:1L:573:MET:HB3	14:1N:167:TRP:CD1	2.47	0.49
29:1d:97:HIS:NE2	33:1h:119:ASP:OD2	2.39	0.49
34:1i:122:PHE:HD1	34:1i:123:PRO:HD2	1.76	0.49
40:1o:51:MET:SD	40:1o:53:GLN:NE2	2.85	0.49
1:1A:90:MET:O	1:1A:93:PHE:HB3	2.12	0.49
3:1C:132:ARG:HD3	3:1C:149:ARG:HB3	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:109:VAL:HG22	4:1D:152:MET:HG2	1.94	0.49
4:1D:338:MET:HE1	4:1D:348:HIS:CD2	2.46	0.49
6:1F:352:GLU:HG2	6:1F:373:ASN:HD21	1.78	0.49
12:1L:76:LEU:HD11	12:1L:196:TRP:HZ3	1.78	0.49
12:1L:288:THR:HG21	12:1L:307:SER:HB2	1.95	0.49
12:1L:299:LYS:HD3	12:1L:354:GLN:HG2	1.92	0.49
13:1M:48:ASN:ND2	33:1h:90:THR:HG21	2.28	0.49
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.44	0.49
32:1g:94:GLU:OE2	41:1p:9:TYR:OH	2.27	0.49
6:1F:123:LEU:HD12	6:1F:124:VAL:HG13	1.95	0.49
12:1L:228:GLY:O	12:1L:529:TYR:OH	2.24	0.49
16:1P:168:PRO:HG2	55:1P:501:NDP:H5N	1.94	0.49
31:1f:43:LEU:HD12	33:1h:87:TYR:CE2	2.48	0.49
32:1g:45:HIS:CG	32:1g:58:MET:HE3	2.48	0.49
37:1l:157:GLU:OE1	37:1l:157:GLU:N	2.45	0.49
38:1m:25:SER:O	38:1m:28:THR:OG1	2.30	0.49
41:1p:73:ILE:HD12	41:1p:87:ALA:HB1	1.94	0.49
2:1B:47:PRO:HA	2:1B:85:VAL:O	2.12	0.49
2:1B:55:CYS:HB3	2:1B:116:MET:HG2	1.95	0.49
7:1G:125:SER:OG	7:1G:126:ASP:N	2.45	0.49
8:1H:70:MET:HB3	8:1H:122:ALA:HB2	1.95	0.49
9:1I:54:LYS:HD3	42:1q:91:HIS:NE2	2.27	0.49
9:1I:62:ARG:HH21	9:1I:119:CYS:HA	1.78	0.49
13:1M:151:PHE:CD1	14:1N:287:LEU:HD12	2.48	0.49
14:1N:238:PRO:HB2	50:1N:401:3PE:O32	2.12	0.49
14:1N:338:PRO:HA	23:1X:169:TRP:HZ2	1.77	0.49
15:1O:216:GLU:OE1	15:1O:216:GLU:N	2.46	0.49
16:1P:180:ASN:N	16:1P:180:ASN:OD1	2.45	0.49
20:1T:73:PRO:O	20:1T:77:VAL:N	2.36	0.49
23:1X:46:ARG:NH1	25:1Z:80:ASP:OD1	2.46	0.49
27:1b:7:PHE:HA	27:1b:10:ASN:HD21	1.78	0.49
28:1c:44:ARG:HH21	28:1c:45:ARG:HB2	1.78	0.49
3:1C:31:GLU:OE1	21:1V:46:TYR:OH	2.29	0.49
3:1C:196:LYS:NZ	17:1Q:81:ASN:HA	2.28	0.49
4:1D:238:ARG:HH12	4:1D:412:ALA:HB1	1.77	0.49
6:1F:66:ARG:HA	6:1F:74:PRO:HA	1.95	0.49
6:1F:143:TYR:HB3	6:1F:179:ARG:HH12	1.78	0.49
7:1G:462:ASP:HB3	7:1G:657:LEU:HD23	1.95	0.49
8:1H:133:LEU:HD21	10:1J:73:ALA:HB1	1.95	0.49
8:1H:183:MET:HB2	9:1I:27:TRP:CH2	2.48	0.49
14:1N:147:GLN:HB3	33:1h:125:TYR:CZ	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:237:LEU:HB3	16:1P:240:ASP:OD2	2.12	0.49
17:1Q:104:ASP:OD1	17:1Q:104:ASP:N	2.44	0.49
39:1n:9:LEU:O	39:1n:14:LYS:NZ	2.35	0.49
3:1C:118:GLU:H	3:1C:118:GLU:CD	2.19	0.48
3:1C:136:ASP:OD1	3:1C:150:ARG:HA	2.12	0.48
3:1C:160:HIS:HD2	3:1C:163:ARG:NE	2.11	0.48
6:1F:82:MET:HE3	6:1F:221:THR:HG22	1.94	0.48
6:1F:163:GLY:N	6:1F:173:PHE:O	2.44	0.48
6:1F:305:PRO:HD3	6:1F:413:TRP:HB3	1.95	0.48
7:1G:212:PRO:HB2	7:1G:271:TYR:OH	2.13	0.48
13:1M:47:GLU:OE2	41:1p:93:ARG:HG2	2.12	0.48
14:1N:329:MET:HA	14:1N:329:MET:HE3	1.94	0.48
33:1h:114:MET:HE1	33:1h:121:PRO:HD2	1.95	0.48
7:1G:87:LYS:HB3	43:1r:54:CYS:SG	2.53	0.48
8:1H:61:LEU:HD22	8:1H:216:ALA:HB3	1.94	0.48
10:1J:152:TRP:CE3	10:1J:155:ILE:HG21	2.48	0.48
12:1L:548:SER:HA	12:1L:552:LEU:HB3	1.95	0.48
20:1T:72:CYS:HB2	20:1T:75:GLU:OE1	2.12	0.48
21:1V:46:TYR:CE1	43:1r:91:LYS:HD2	2.48	0.48
29:1d:34:MET:HE2	29:1d:34:MET:HA	1.95	0.48
34:1i:15:ARG:O	34:1i:19:ARG:HG2	2.14	0.48
42:1q:135:GLN:OE1	42:1q:135:GLN:N	2.43	0.48
2:1B:25:ARG:NE	2:1B:27:GLU:HB2	2.29	0.48
4:1D:88:GLU:HA	4:1D:91:ILE:HB	1.95	0.48
6:1F:134:ALA:C	6:1F:175:VAL:HG23	2.37	0.48
7:1G:9:ILE:HG23	7:1G:75:LYS:HD2	1.96	0.48
7:1G:49:ALA:HB2	7:1G:161:ARG:NH1	2.27	0.48
7:1G:201:ASP:O	17:1Q:45:MET:HA	2.13	0.48
7:1G:285:ARG:HG3	7:1G:558:ASP:HA	1.94	0.48
8:1H:9:LEU:HD22	26:1a:19:PRO:HB3	1.95	0.48
8:1H:86:TRP:CD1	8:1H:233:MET:HE3	2.49	0.48
8:1H:175:ILE:HB	8:1H:242:PHE:HB3	1.95	0.48
9:1I:8:ARG:NH1	43:1r:111:TYR:HB3	2.26	0.48
10:1J:51:PHE:HE1	10:1J:55:MET:SD	2.36	0.48
12:1L:10:THR:HA	12:1L:13:ILE:HG22	1.96	0.48
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.47	0.48
13:1M:452:LYS:HD2	32:1g:86:GLN:NE2	2.26	0.48
14:1N:335:LEU:HB2	29:1d:37:LEU:HD21	1.94	0.48
15:1O:25:ILE:HG12	15:1O:168:VAL:HG12	1.94	0.48
21:1V:47:THR:O	21:1V:51:THR:N	2.29	0.48
22:1W:61:ASP:HA	22:1W:64:ARG:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:88:MET:HA	22:1W:91:GLU:HG2	1.95	0.48
23:1X:109:CYS:O	23:1X:113:LYS:N	2.44	0.48
33:1h:46:PHE:HA	41:1p:54:GLN:HE22	1.78	0.48
5:1E:14:GLU:O	5:1E:19:THR:OG1	2.20	0.48
12:1L:555:LEU:HD11	38:1m:75:ILE:HD13	1.94	0.48
45:1M:502:PC1:H361	32:1g:76:PHE:CE2	2.48	0.48
28:1c:48:LEU:H	28:1c:48:LEU:HD12	1.78	0.48
34:1i:79:TRP:HE1	41:1p:40:VAL:HA	1.79	0.48
42:1q:107:LYS:N	42:1q:107:LYS:HD2	2.29	0.48
4:1D:184:VAL:HG23	4:1D:185:SER:H	1.78	0.48
4:1D:246:THR:HA	21:1V:11:VAL:HG13	1.96	0.48
5:1E:162:GLU:C	5:1E:186:PRO:HA	2.38	0.48
6:1F:136:ILE:HG23	6:1F:177:VAL:HA	1.95	0.48
7:1G:418:ARG:NH2	7:1G:419:TYR:O	2.47	0.48
12:1L:237:MET:O	12:1L:299:LYS:NZ	2.40	0.48
12:1L:428:PHE:HB2	36:1k:62:PHE:HE2	1.79	0.48
15:1O:192:MET:N	15:1O:192:MET:SD	2.86	0.48
15:1O:201:ASP:HA	15:1O:204:ASN:OD1	2.11	0.48
32:1g:37:LEU:HD13	32:1g:46:GLY:HA2	1.95	0.48
35:1j:70:ASP:OD1	35:1j:70:ASP:N	2.44	0.48
2:1B:116:MET:SD	2:1B:156:LEU:HD13	2.54	0.48
5:1E:175:GLU:HG2	5:1E:180:LYS:HB2	1.96	0.48
6:1F:258:ILE:HG23	6:1F:266:CYS:H	1.79	0.48
45:1H:401:PC1:H131	9:1I:19:ASP:HB3	1.96	0.48
12:1L:483:PRO:HB2	12:1L:486:MET:HE1	1.96	0.48
13:1M:40:SER:O	33:1h:80:TYR:OH	2.30	0.48
13:1M:66:LEU:HD21	13:1M:107:ILE:HA	1.95	0.48
13:1M:269:MET:HA	13:1M:272:THR:HG22	1.93	0.48
15:1O:19:THR:OG1	15:1O:20:GLU:N	2.46	0.48
15:1O:74:SER:O	15:1O:74:SER:OG	2.27	0.48
15:1O:211:LEU:O	15:1O:215:SER:N	2.46	0.48
19:1S:15:LEU:O	19:1S:16:ARG:NH1	2.47	0.48
20:1U:47:GLN:NE2	20:1U:70:LEU:O	2.47	0.48
34:1i:71:VAL:HG13	34:1i:75:LEU:HD12	1.94	0.48
37:1l:69:LEU:HB2	37:1l:71:LEU:CD2	2.44	0.48
41:1p:99:GLN:O	41:1p:103:ASN:ND2	2.47	0.48
2:1B:87:ILE:HD13	2:1B:156:LEU:HD21	1.96	0.48
2:1B:144:ILE:HD11	2:1B:162:GLN:HG2	1.95	0.48
4:1D:347:HIS:CD2	7:1G:126:ASP:HA	2.49	0.48
9:1I:70:TYR:CE2	18:1R:87:CYS:HA	2.49	0.48
16:1P:98:GLU:HG3	16:1P:177:ARG:HD2	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.44	0.48
16:1P:202:LYS:O	16:1P:236:TYR:N	2.47	0.48
20:1T:24:LYS:O	20:1T:24:LYS:NZ	2.38	0.48
26:1a:50:ARG:O	26:1a:54:ILE:HG22	2.14	0.48
33:1h:17:TYR:HE1	39:1n:107:HIS:HB2	1.78	0.48
2:1B:44:SER:O	8:1H:54:LYS:HE2	2.13	0.48
6:1F:60:VAL:HG21	6:1F:79:TRP:CD1	2.44	0.48
6:1F:291:TRP:CD1	6:1F:294:LEU:HD23	2.49	0.48
7:1G:178:GLY:O	7:1G:181:MET:HG3	2.14	0.48
7:1G:243:ARG:HG3	7:1G:244:THR:N	2.29	0.48
12:1L:261:ILE:HG12	12:1L:326:PHE:HB2	1.96	0.48
13:1M:139:GLN:O	13:1M:142:ARG:NH1	2.47	0.48
15:1O:232:GLU:C	15:1O:233:LYS:HE2	2.38	0.48
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD11	1.96	0.48
19:1S:19:ARG:HH22	19:1S:65:TRP:CD1	2.31	0.48
19:1S:32:VAL:O	19:1S:36:ILE:HG13	2.13	0.48
22:1W:54:ILE:HG21	22:1W:107:PHE:CE2	2.49	0.48
37:1l:46:ASP:OD1	37:1l:46:ASP:N	2.45	0.48
2:1B:25:ARG:HE	2:1B:27:GLU:HB2	1.79	0.48
3:1C:177:ASP:OD2	3:1C:179:GLU:HG2	2.13	0.48
4:1D:76:CYS:HB2	4:1D:403:ASP:HA	1.95	0.48
6:1F:393:TRP:HB2	6:1F:419:ILE:HD13	1.96	0.48
7:1G:66:VAL:HG23	7:1G:71:MET:HG3	1.96	0.48
8:1H:149:ILE:HD13	8:1H:185:TRP:HA	1.95	0.48
12:1L:71:LEU:N	12:1L:74:VAL:O	2.47	0.48
12:1L:85:PHE:HA	12:1L:326:PHE:CZ	2.48	0.48
14:1N:66:ALA:HB2	14:1N:104:MET:HB3	1.96	0.48
22:1W:58:GLN:HA	22:1W:61:ASP:OD2	2.13	0.48
29:1d:34:MET:HG3	29:1d:72:GLY:HA3	1.95	0.48
32:1g:84:ARG:HD2	41:1p:96:LYS:NZ	2.28	0.48
35:1j:45:ASP:OD2	35:1j:50:HIS:ND1	2.46	0.48
1:1A:17:LEU:HA	1:1A:20:ILE:HG22	1.96	0.48
1:1A:73:LEU:HB3	10:1J:51:PHE:HZ	1.79	0.48
3:1C:10:THR:HG21	43:1r:56:ARG:HD2	1.96	0.48
3:1C:15:ASN:HB3	3:1C:46:ASN:HD21	1.78	0.48
5:1E:86:PHE:C	5:1E:86:PHE:CD1	2.91	0.48
6:1F:248:GLU:O	6:1F:250:ASN:N	2.47	0.48
6:1F:354:TYR:CE2	6:1F:411:ALA:HA	2.49	0.48
6:1F:381:LYS:HE3	6:1F:383:ASP:HB2	1.96	0.48
7:1G:475:GLN:HB2	7:1G:646:ASN:ND2	2.28	0.48
9:1I:142:GLU:OE1	9:1I:142:GLU:N	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:84:VAL:HG13	10:1J:85:SER:H	1.79	0.48
12:1L:478:PRO:HD2	40:1o:86:TRP:CH2	2.49	0.48
12:1L:489:THR:HA	12:1L:492:ILE:HB	1.94	0.48
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	1.96	0.48
6:1F:136:ILE:HG22	6:1F:175:VAL:HG22	1.95	0.47
6:1F:200:GLN:HE22	17:1Q:132:THR:HG22	1.79	0.47
6:1F:263:ASN:HB3	6:1F:264:HIS:CE1	2.48	0.47
7:1G:106:PRO:HB3	9:1I:80:CYS:CB	2.44	0.47
7:1G:254:MET:HA	7:1G:260:GLU:O	2.14	0.47
7:1G:382:THR:O	7:1G:408:LEU:HD21	2.14	0.47
9:1I:123:GLN:HE22	9:1I:133:GLU:CG	2.27	0.47
12:1L:73:THR:HG21	12:1L:194:ASN:HD21	1.79	0.47
12:1L:257:VAL:HG11	12:1L:313:MET:HG3	1.97	0.47
15:1O:211:LEU:HD12	15:1O:211:LEU:H	1.79	0.47
15:1O:262:LEU:HD12	15:1O:268:GLU:HG3	1.96	0.47
17:1Q:124:TRP:O	44:1s:68:SER:OG	2.31	0.47
21:1V:6:LYS:HB2	21:1V:6:LYS:HE2	1.64	0.47
33:1h:24:LEU:O	33:1h:28:TYR:HB3	2.14	0.47
33:1h:40:ILE:O	33:1h:44:ASN:ND2	2.47	0.47
34:1i:26:GLU:OE1	34:1i:26:GLU:N	2.43	0.47
4:1D:34:ASN:HD22	15:1O:158:VAL:HA	1.79	0.47
4:1D:151:ILE:CG2	4:1D:174:ARG:HD2	2.44	0.47
6:1F:120:GLU:O	6:1F:124:VAL:HG22	2.14	0.47
7:1G:418:ARG:HB2	44:1s:74:ARG:NH1	2.29	0.47
7:1G:448:LYS:HE2	7:1G:487:TRP:CE3	2.49	0.47
8:1H:26:LYS:HG2	26:1a:5:ILE:HG22	1.95	0.47
10:1J:67:VAL:HA	10:1J:70:TYR:HB3	1.95	0.47
10:1J:133:SER:HB2	10:1J:138:GLU:OE1	2.14	0.47
13:1M:377:GLY:O	13:1M:381:ILE:HG12	2.14	0.47
14:1N:319:HIS:HB3	29:1d:49:ARG:HH12	1.79	0.47
16:1P:2:HIS:HB3	16:1P:5:LEU:HB2	1.97	0.47
16:1P:234:ASN:ND2	16:1P:339:THR:OG1	2.27	0.47
23:1X:67:LEU:HB3	23:1X:71:ARG:NH1	2.28	0.47
25:1Z:69:ILE:HD11	27:1b:49:PRO:HB2	1.96	0.47
28:1c:17:VAL:O	28:1c:20:THR:OG1	2.26	0.47
6:1F:255:LEU:HA	6:1F:269:GLU:HA	1.96	0.47
7:1G:345:THR:N	7:1G:510:GLY:O	2.42	0.47
11:1K:89:TYR:HB3	11:1K:91:GLN:HG3	1.95	0.47
51:1M:501:PGT:H121	51:1M:501:PGT:H32	1.61	0.47
14:1N:150:ASN:OD1	14:1N:153:LEU:HB2	2.14	0.47
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:261:PHE:CG	16:1P:262:ALA:N	2.81	0.47
18:1R:84:CYS:SG	18:1R:86:TYR:HB2	2.54	0.47
19:1S:44:LYS:HZ3	19:1S:52:ILE:H	1.62	0.47
20:1U:61:GLU:OE1	39:1n:81:PHE:HB2	2.14	0.47
23:1X:126:LYS:HD2	27:1b:66:PRO:HG3	1.97	0.47
2:1B:79:SER:O	2:1B:81:ARG:N	2.46	0.47
3:1C:149:ARG:CB	22:1W:88:MET:HE1	2.45	0.47
7:1G:41:CYS:N	7:1G:52:CYS:SG	2.87	0.47
7:1G:460:ARG:NH2	7:1G:462:ASP:OD2	2.42	0.47
10:1J:175:ASN:HB2	14:1N:48:PHE:HD2	1.80	0.47
12:1L:473:PRO:O	12:1L:475:MET:HG3	2.13	0.47
16:1P:41:MET:SD	16:1P:41:MET:N	2.81	0.47
25:1Z:20:ASP:OD1	25:1Z:20:ASP:N	2.47	0.47
43:1r:63:MET:CE	43:1r:64:PRO:HD2	2.39	0.47
5:1E:35:VAL:O	5:1E:43:LYS:NZ	2.42	0.47
6:1F:42:TRP:NE1	6:1F:116:HIS:HB2	2.26	0.47
6:1F:68:ARG:HA	6:1F:319:PHE:HZ	1.79	0.47
6:1F:299:PRO:HD2	6:1F:300:GLY:N	2.29	0.47
6:1F:406:ALA:O	6:1F:410:GLY:N	2.37	0.47
7:1G:32:LYS:O	7:1G:32:LYS:NZ	2.36	0.47
7:1G:36:GLN:OE1	7:1G:39:ARG:NH2	2.48	0.47
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.96	0.47
9:1I:75:GLU:HG3	9:1I:105:ARG:HD2	1.96	0.47
11:1K:34:GLU:HA	11:1K:34:GLU:OE2	2.14	0.47
12:1L:100:ILE:O	12:1L:104:SER:N	2.40	0.47
14:1N:222:SER:HB2	14:1N:233:THR:HG21	1.95	0.47
15:1O:90:ASP:HA	32:1g:24:ILE:HG12	1.95	0.47
16:1P:23:VAL:O	16:1P:48:PRO:HD2	2.14	0.47
22:1W:64:ARG:HD3	22:1W:68:MET:HE1	1.96	0.47
25:1Z:104:TRP:CZ2	30:1e:74:ARG:HG3	2.50	0.47
25:1Z:127:LEU:HD22	30:1e:97:HIS:HE1	1.78	0.47
29:1d:108:THR:OG1	29:1d:111:GLU:OE1	2.22	0.47
36:1k:59:ASN:HD22	36:1k:60:VAL:N	2.12	0.47
37:1l:97:SER:OG	37:1l:100:THR:OG1	2.21	0.47
6:1F:263:ASN:HB2	6:1F:284:ALA:O	2.15	0.47
6:1F:320:ASP:O	6:1F:324:GLN:HG2	2.15	0.47
7:1G:359:ARG:CZ	7:1G:363:LEU:HD11	2.45	0.47
7:1G:556:MET:HE3	7:1G:556:MET:HB3	1.79	0.47
11:1K:73:LEU:HD11	14:1N:38:LEU:HA	1.96	0.47
13:1M:208:PRO:HD3	13:1M:216:LEU:HD11	1.96	0.47
51:1M:501:PGT:H181	51:1M:501:PGT:H152	1.65	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:162:ILE:HG13	14:1N:163:LEU:HD12	1.96	0.47
16:1P:315:ILE:HD13	16:1P:330:GLU:HA	1.96	0.47
16:1P:339:THR:HG23	16:1P:339:THR:O	2.14	0.47
19:1S:15:LEU:O	19:1S:50:LEU:HD22	2.14	0.47
34:1i:47:ASN:OD1	34:1i:48:LYS:N	2.48	0.47
1:1A:93:PHE:C	1:1A:93:PHE:CD1	2.92	0.47
3:1C:18:VAL:HG23	3:1C:21:GLN:HE21	1.80	0.47
4:1D:169:TRP:HH2	9:1I:37:THR:HG22	1.80	0.47
4:1D:222:ILE:O	4:1D:226:GLU:HG3	2.15	0.47
6:1F:82:MET:HE1	6:1F:210:PRO:C	2.40	0.47
6:1F:184:TYR:CZ	48:1F:501:FMN:H6	2.50	0.47
6:1F:294:LEU:HD21	6:1F:297:VAL:HG23	1.96	0.47
7:1G:127:ARG:NH2	43:1r:45:SER:O	2.47	0.47
7:1G:362:TYR:C	7:1G:492:ILE:HD11	2.40	0.47
7:1G:525:LEU:HD12	7:1G:546:GLN:NE2	2.30	0.47
7:1G:670:ASP:OD1	7:1G:670:ASP:N	2.47	0.47
8:1H:88:PRO:HG3	8:1H:104:PHE:HD2	1.79	0.47
8:1H:185:TRP:O	8:1H:189:THR:HG23	2.14	0.47
9:1I:61:PHE:HE1	9:1I:137:PHE:CD2	2.30	0.47
9:1I:156:ASN:ND2	18:1R:34:GLU:HB3	2.29	0.47
11:1K:66:PHE:CE2	14:1N:31:ILE:HG23	2.50	0.47
12:1L:3:PRO:HB2	12:1L:7:LEU:HD11	1.96	0.47
13:1M:341:THR:HG21	38:1m:64:LEU:HD11	1.97	0.47
14:1N:147:GLN:HB3	33:1h:125:TYR:CE1	2.50	0.47
15:1O:185:LYS:O	15:1O:185:LYS:NZ	2.32	0.47
16:1P:24:PHE:CZ	16:1P:81:ILE:HG23	2.50	0.47
16:1P:258:LEU:HD23	16:1P:263:TYR:HB2	1.96	0.47
17:1Q:39:VAL:HG21	17:1Q:108:ARG:NE	2.30	0.47
20:1T:55:GLU:OE2	20:1T:62:ILE:HG23	2.15	0.47
20:1U:14:ARG:HH21	20:1U:58:PHE:HD1	1.63	0.47
25:1Z:28:ARG:HH21	43:1r:13:TRP:HE1	1.61	0.47
27:1b:79:TRP:CD1	27:1b:79:TRP:H	2.32	0.47
32:1g:91:ARG:NH2	32:1g:92:GLU:OE1	2.41	0.47
33:1h:21:PHE:CZ	33:1h:25:MET:HE2	2.50	0.47
34:1i:120:LYS:HG2	34:1i:121:GLU:H	1.80	0.47
42:1q:47:LYS:C	42:1q:48:TYR:HD1	2.22	0.47
1:1A:68:GLU:OE1	1:1A:98:LEU:HD22	2.15	0.47
2:1B:59:MET:O	2:1B:62:MET:HB2	2.15	0.47
3:1C:53:HIS:CG	3:1C:54:PRO:HD2	2.50	0.47
4:1D:205:LEU:HD21	25:1Z:7:LYS:O	2.14	0.47
5:1E:82:GLU:CD	7:1G:174:THR:H	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:272:TRP:CZ2	9:1I:34:LEU:HB3	2.50	0.47
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.97	0.47
9:1I:36:MET:O	9:1I:36:MET:HE3	2.15	0.47
12:1L:375:ILE:HD11	35:1j:32:MET:HG2	1.95	0.47
12:1L:487:LYS:NZ	35:1j:49:GLY:HA2	2.29	0.47
13:1M:185:PRO:HB3	29:1d:117:HIS:HE1	1.78	0.47
13:1M:329:LEU:HD13	13:1M:359:TRP:CD1	2.50	0.47
15:1O:307:GLY:O	15:1O:320:LYS:NZ	2.43	0.47
17:1Q:28:GLU:H	17:1Q:28:GLU:CD	2.17	0.47
23:1X:131:LYS:HE2	23:1X:131:LYS:HB2	1.77	0.47
32:1g:84:ARG:HD2	41:1p:96:LYS:HZ1	1.80	0.47
35:1j:17:LEU:HD13	35:1j:22:LEU:HD21	1.96	0.47
1:1A:1:FME:O1	1:1A:2:ASN:N	2.48	0.47
7:1G:138:GLU:CD	18:1R:74:ASN:HD21	2.22	0.47
7:1G:268:ARG:HD2	7:1G:269:PHE:CE1	2.41	0.47
11:1K:48:ILE:HD13	11:1K:56:ALA:HB1	1.96	0.47
12:1L:310:LEU:HA	12:1L:313:MET:SD	2.55	0.47
15:1O:197:ALA:HA	15:1O:200:GLN:HB3	1.97	0.47
21:1V:43:TYR:O	21:1V:47:THR:OG1	2.17	0.47
33:1h:129:ASP:OD1	33:1h:129:ASP:N	2.48	0.47
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.14	0.47
41:1p:72:ASP:OD1	41:1p:74:THR:HG22	2.14	0.47
1:1A:8:LEU:O	1:1A:12:THR:HG23	2.15	0.47
3:1C:40:VAL:HG22	43:1r:69:MET:HB3	1.97	0.47
3:1C:203:TRP:CZ3	7:1G:38:PRO:HA	2.49	0.47
6:1F:141:GLU:OE1	6:1F:141:GLU:N	2.47	0.47
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.80	0.47
9:1I:52:PHE:CZ	42:1q:30:ALA:HA	2.50	0.47
12:1L:231:PRO:C	12:1L:234:PRO:HD2	2.40	0.47
12:1L:488:MET:HA	12:1L:488:MET:HE3	1.97	0.47
13:1M:230:VAL:HG12	13:1M:235:LEU:HD11	1.96	0.47
13:1M:278:ARG:NH2	37:1l:82:ASP:OD1	2.48	0.47
16:1P:335:LYS:HD2	16:1P:335:LYS:O	2.15	0.47
17:1Q:10:LEU:O	22:1W:23:ARG:NH2	2.48	0.47
20:1T:26:ASP:OD2	20:1T:29:LYS:HD3	2.15	0.47
33:1h:34:ILE:CG1	33:1h:35:PRO:HD3	2.45	0.47
33:1h:64:TRP:CD1	33:1h:77:ARG:HA	2.49	0.47
42:1q:98:PRO:HA	42:1q:101:LYS:O	2.14	0.47
4:1D:294:TYR:CZ	4:1D:298:LEU:HD11	2.50	0.46
5:1E:122:LYS:HA	5:1E:122:LYS:HE2	1.97	0.46
7:1G:378:LEU:HD23	7:1G:439:PHE:CE2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:3:LYS:HE3	9:1I:4:PHE:O	2.16	0.46
13:1M:333:ASN:O	13:1M:337:VAL:HG12	2.15	0.46
14:1N:40:MET:HA	14:1N:40:MET:HE3	1.97	0.46
15:1O:62:THR:O	28:1c:5:ARG:NH2	2.26	0.46
17:1Q:133:LYS:HE2	17:1Q:133:LYS:HB2	1.79	0.46
20:1T:51:ILE:O	20:1T:54:MET:HB2	2.15	0.46
22:1W:83:VAL:O	22:1W:87:LYS:N	2.44	0.46
27:1b:42:ILE:O	27:1b:46:ARG:HG2	2.14	0.46
37:1l:25:LYS:HE2	37:1l:25:LYS:HA	1.96	0.46
39:1n:49:GLU:OE2	39:1n:49:GLU:N	2.44	0.46
5:1E:116:ILE:HG23	5:1E:169:ILE:HG21	1.97	0.46
5:1E:191:PHE:H	5:1E:194:GLU:CD	2.23	0.46
6:1F:47:GLU:OE1	6:1F:47:GLU:N	2.45	0.46
7:1G:471:SER:O	7:1G:646:ASN:ND2	2.38	0.46
7:1G:508:LYS:HE2	7:1G:513:ALA:H	1.78	0.46
11:1K:27:MET:HE3	11:1K:27:MET:HA	1.98	0.46
12:1L:71:LEU:O	12:1L:74:VAL:N	2.38	0.46
12:1L:81:LYS:C	12:1L:82:MET:HE2	2.40	0.46
21:1V:23:LEU:O	21:1V:27:TYR:HB2	2.16	0.46
22:1W:22:SER:OG	22:1W:24:ASP:O	2.33	0.46
29:1d:120:ARG:HB2	38:1m:108:ARG:HH22	1.80	0.46
37:1l:6:LYS:HE2	37:1l:6:LYS:HA	1.97	0.46
1:1A:111:LEU:HD22	1:1A:111:LEU:H	1.80	0.46
3:1C:206:PHE:CZ	4:1D:357:GLN:HB3	2.50	0.46
4:1D:103:PHE:HE2	4:1D:376:VAL:HG11	1.80	0.46
5:1E:114:ASP:N	5:1E:114:ASP:OD1	2.47	0.46
6:1F:226:GLU:OE2	6:1F:227:THR:OG1	2.30	0.46
7:1G:348:VAL:N	7:1G:459:GLN:OE1	2.48	0.46
7:1G:516:LYS:HE3	7:1G:516:LYS:HB3	1.56	0.46
10:1J:104:VAL:O	10:1J:108:LEU:HG	2.16	0.46
12:1L:69:MET:HE3	12:1L:70:THR:N	2.20	0.46
12:1L:100:ILE:HD13	12:1L:246:LEU:HB2	1.96	0.46
13:1M:329:LEU:HD22	13:1M:359:TRP:CG	2.50	0.46
50:1N:401:3PE:H291	29:1d:43:LEU:HD11	1.95	0.46
17:1Q:93:VAL:O	17:1Q:97:GLU:HG3	2.16	0.46
21:1V:37:ILE:O	21:1V:44:ARG:HD2	2.16	0.46
23:1X:58:GLU:OE1	23:1X:58:GLU:N	2.41	0.46
40:1o:26:PRO:HB3	40:1o:33:ARG:NH1	2.28	0.46
42:1q:107:LYS:HD2	42:1q:107:LYS:H	1.80	0.46
6:1F:147:SER:OG	44:1s:42:GLN:NE2	2.48	0.46
6:1F:165:ASN:OD1	6:1F:170:GLY:N	2.46	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:46:LEU:HD21	7:1G:161:ARG:HB3	1.96	0.46
8:1H:134:ARG:NH1	8:1H:200:LEU:HD21	2.30	0.46
12:1L:233:LEU:HD11	12:1L:248:HIS:HB3	1.96	0.46
12:1L:481:THR:HG1	40:1o:91:HIS:CG	2.33	0.46
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.15	0.46
20:1T:51:ILE:HD11	20:1T:70:LEU:HD13	1.96	0.46
3:1C:155:TYR:HE1	22:1W:97:TRP:HB3	1.80	0.46
5:1E:169:ILE:HD12	5:1E:172:ILE:HD11	1.97	0.46
6:1F:46:LYS:HB2	6:1F:169:SER:HB3	1.97	0.46
6:1F:298:ILE:HG13	6:1F:301:GLY:H	1.80	0.46
7:1G:56:LEU:HD12	7:1G:65:VAL:HG12	1.96	0.46
7:1G:269:PHE:N	7:1G:269:PHE:CD1	2.84	0.46
7:1G:409:ILE:HD12	7:1G:661:LEU:HG	1.97	0.46
10:1J:141:MET:HA	10:1J:141:MET:HE2	1.98	0.46
13:1M:227:GLY:O	13:1M:231:LEU:HD22	2.15	0.46
52:1N:402:CDL:H332	15:1O:9:VAL:HG21	1.97	0.46
52:1N:402:CDL:H751	52:1N:402:CDL:H611	1.96	0.46
15:1O:199:LEU:HA	15:1O:202:ILE:HG12	1.98	0.46
16:1P:172:PHE:CZ	16:1P:206:TYR:HB2	2.51	0.46
16:1P:270:PHE:HB3	16:1P:279:THR:H	1.80	0.46
23:1X:14:VAL:HG21	23:1X:60:LYS:HG2	1.97	0.46
25:1Z:127:LEU:HD12	25:1Z:128:ARG:N	2.31	0.46
27:1b:31:LEU:N	27:1b:32:PRO:HD2	2.30	0.46
33:1h:115:ARG:NH1	33:1h:123:TYR:OH	2.49	0.46
42:1q:52:ASN:N	42:1q:52:ASN:OD1	2.48	0.46
4:1D:205:LEU:HA	4:1D:205:LEU:HD23	1.78	0.46
4:1D:306:GLN:OE1	4:1D:309:ARG:NE	2.48	0.46
6:1F:217:GLY:HA3	17:1Q:123:SER:C	2.40	0.46
6:1F:277:LYS:NZ	6:1F:314:THR:HA	2.27	0.46
7:1G:10:GLU:HA	7:1G:19:MET:HA	1.98	0.46
8:1H:228:TYR:HA	8:1H:231:ILE:HD12	1.97	0.46
12:1L:69:MET:HB2	12:1L:76:LEU:HB2	1.97	0.46
12:1L:176:ARG:HA	12:1L:179:ASP:OD2	2.15	0.46
12:1L:546:GLN:HB2	13:1M:278:ARG:NH1	2.31	0.46
13:1M:119:TYR:CZ	13:1M:161:LEU:HB2	2.50	0.46
16:1P:210:VAL:HG13	16:1P:230:PHE:HD2	1.81	0.46
22:1W:93:THR:HG22	22:1W:103:ILE:HD11	1.98	0.46
23:1X:120:ASP:N	23:1X:123:GLU:OE2	2.47	0.46
34:1i:86:LYS:HD2	34:1i:86:LYS:HA	1.63	0.46
36:1k:35:LEU:HB3	36:1k:40:LEU:O	2.14	0.46
41:1p:89:MET:O	41:1p:93:ARG:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:128:TYR:OH	3:1C:192:GLN:OE1	2.34	0.46
5:1E:12:THR:O	5:1E:16:ASN:HB3	2.15	0.46
6:1F:25:LEU:HD22	6:1F:255:LEU:HD21	1.98	0.46
6:1F:102:PRO:HD3	6:1F:353:PHE:CZ	2.51	0.46
6:1F:157:TYR:OH	6:1F:174:ASP:HB2	2.15	0.46
7:1G:329:VAL:HG21	7:1G:623:LEU:HB2	1.98	0.46
7:1G:478:ARG:O	7:1G:478:ARG:NE	2.35	0.46
10:1J:75:ALA:O	10:1J:76:THR:OG1	2.30	0.46
12:1L:176:ARG:HB3	13:1M:401:MET:SD	2.56	0.46
12:1L:488:MET:O	12:1L:492:ILE:HG13	2.16	0.46
13:1M:73:LEU:HA	13:1M:76:MET:HE3	1.97	0.46
13:1M:324:SER:OG	13:1M:440:HIS:NE2	2.33	0.46
16:1P:20:VAL:HB	16:1P:89:ASN:H	1.80	0.46
16:1P:48:PRO:HB3	16:1P:84:VAL:HG11	1.97	0.46
16:1P:242:VAL:HG12	16:1P:253:PHE:HE1	1.79	0.46
23:1X:101:LYS:HB2	23:1X:101:LYS:HE2	1.73	0.46
25:1Z:50:MET:HE2	25:1Z:50:MET:HB2	1.79	0.46
30:1e:44:HIS:ND1	33:1h:130:LYS:HG2	2.31	0.46
2:1B:65:PRO:HG2	4:1D:172:GLU:HB2	1.98	0.46
7:1G:117:GLN:NE2	46:1G:801:SF4:S3	2.88	0.46
8:1H:138:GLN:HA	8:1H:286:MET:HE1	1.97	0.46
12:1L:496:MET:O	12:1L:499:MET:N	2.49	0.46
13:1M:168:GLN:HA	13:1M:172:GLY:O	2.15	0.46
14:1N:261:MET:HB3	14:1N:262:PRO:HD3	1.98	0.46
15:1O:49:ARG:HD2	15:1O:114:HIS:CD2	2.50	0.46
16:1P:143:SER:O	16:1P:147:ARG:N	2.36	0.46
23:1X:44:LEU:HD21	27:1b:57:ARG:HE	1.81	0.46
23:1X:79:GLU:HB2	23:1X:80:PRO:HD3	1.98	0.46
50:1Y:201:3PE:H221	50:1Y:201:3PE:H2	1.61	0.46
34:1i:77:PRO:O	34:1i:81:ILE:HG12	2.15	0.46
38:1m:108:ARG:O	38:1m:112:GLU:HG3	2.15	0.46
39:1n:25:HIS:CE1	39:1n:78:PRO:HB3	2.50	0.46
1:1A:92:LEU:O	1:1A:96:ILE:HG23	2.16	0.46
2:1B:157:LEU:O	2:1B:161:LEU:HG	2.16	0.46
3:1C:32:ILE:HD13	3:1C:63:PHE:HZ	1.80	0.46
3:1C:79:THR:OG1	3:1C:93:VAL:HB	2.15	0.46
3:1C:89:ARG:HG3	3:1C:90:PHE:CD1	2.51	0.46
3:1C:182:ARG:CZ	22:1W:104:MET:HG3	2.46	0.46
4:1D:371:LYS:HE2	4:1D:371:LYS:HB2	1.78	0.46
9:1I:3:LYS:HD2	9:1I:4:PHE:H	1.78	0.46
14:1N:269:GLU:HA	14:1N:272:LYS:HD3	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:29:PRO:HB2	33:1h:143:ASN:HD22	1.81	0.46
41:1p:77:GLU:OE1	41:1p:77:GLU:N	2.49	0.46
3:1C:150:ARG:HH12	3:1C:155:TYR:HA	1.81	0.46
6:1F:99:GLU:HG3	6:1F:104:THR:O	2.16	0.46
7:1G:349:PHE:HD2	7:1G:350:PRO:HD2	1.80	0.46
12:1L:279:CYS:O	12:1L:283:ILE:HG22	2.16	0.46
13:1M:22:MET:HB3	13:1M:26:ASN:ND2	2.31	0.46
13:1M:282:LEU:HD12	13:1M:330:ALA:HB2	1.98	0.46
16:1P:78:LYS:NZ	16:1P:116:ALA:HB1	2.31	0.46
16:1P:259:PRO:HG2	16:1P:261:PHE:CE1	2.51	0.46
21:1V:35:GLY:HA2	21:1V:44:ARG:HH12	1.81	0.46
24:1Y:80:ARG:HB3	24:1Y:82:LYS:HG3	1.98	0.46
30:1e:72:MET:HA	30:1e:75:LEU:HB2	1.96	0.46
35:1j:54:PRO:HB2	35:1j:59:TRP:NE1	2.21	0.46
37:1l:132:GLN:H	40:1o:97:ARG:HH12	1.63	0.46
38:1m:48:LEU:HD21	39:1n:139:LEU:HD13	1.98	0.46
42:1q:32:ASP:OD1	42:1q:33:VAL:N	2.49	0.46
3:1C:33:LEU:O	3:1C:37:VAL:HG22	2.16	0.45
5:1E:150:ASN:ND2	5:1E:163:ASP:H	2.13	0.45
6:1F:15:LEU:HD13	6:1F:253:THR:HB	1.99	0.45
7:1G:211:LYS:NZ	7:1G:700:GLU:O	2.35	0.45
7:1G:366:THR:OG1	7:1G:491:ASN:ND2	2.49	0.45
7:1G:549:HIS:CE1	7:1G:677:ILE:HA	2.51	0.45
12:1L:305:SER:O	12:1L:309:GLN:HG2	2.16	0.45
51:1M:501:PGT:H321	51:1M:501:PGT:H352	1.63	0.45
16:1P:134:HIS:HB2	16:1P:149:LYS:HE3	1.97	0.45
16:1P:263:TYR:O	16:1P:266:VAL:HG12	2.17	0.45
20:1T:36:PHE:HB3	20:1T:42:LEU:HD23	1.98	0.45
1:1A:84:LEU:HD23	1:1A:84:LEU:H	1.81	0.45
3:1C:75:LEU:HD23	3:1C:126:ALA:HB3	1.96	0.45
3:1C:117:ILE:HB	3:1C:142:PHE:CD2	2.50	0.45
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.51	0.45
5:1E:114:ASP:O	5:1E:118:GLU:HG2	2.16	0.45
6:1F:12:PHE:HB3	6:1F:274:VAL:HG22	1.98	0.45
6:1F:298:ILE:HD12	6:1F:299:PRO:HD3	1.98	0.45
7:1G:523:PHE:HD1	7:1G:544:ILE:HB	1.82	0.45
7:1G:628:PRO:HD3	19:1S:21:HIS:CE1	2.50	0.45
8:1H:91:MET:O	8:1H:93:TYR:N	2.49	0.45
13:1M:272:THR:HG21	13:1M:291:VAL:HG12	1.98	0.45
14:1N:49:ASN:ND2	14:1N:51:ARG:HB2	2.31	0.45
14:1N:115:VAL:O	14:1N:119:THR:HG22	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:29:PHE:HB2	16:1P:177:ARG:HH22	1.81	0.45
18:1R:2:VAL:HG22	18:1R:10:LYS:HD2	1.97	0.45
22:1W:54:ILE:HG13	22:1W:107:PHE:CE2	2.51	0.45
24:1Y:130:GLU:OE1	24:1Y:132:TRP:NE1	2.49	0.45
28:1c:4:ILE:H	28:1c:4:ILE:HD12	1.80	0.45
3:1C:80:ALA:HB3	3:1C:138:PHE:CD2	2.51	0.45
3:1C:153:THR:OG1	3:1C:154:GLY:N	2.48	0.45
6:1F:308:PRO:HD3	6:1F:421:HIS:CG	2.51	0.45
7:1G:415:LEU:HB3	7:1G:417:TYR:CE1	2.52	0.45
7:1G:647:GLU:HA	7:1G:650:LYS:HB2	1.97	0.45
8:1H:134:ARG:HH12	8:1H:207:LEU:HD11	1.80	0.45
9:1I:106:THR:O	9:1I:151:LYS:NZ	2.49	0.45
10:1J:28:TYR:HB3	10:1J:83:TRP:CZ3	2.52	0.45
12:1L:483:PRO:HG3	35:1j:53:TYR:CE2	2.50	0.45
13:1M:61:LEU:HD22	13:1M:241:TYR:HD1	1.81	0.45
13:1M:209:LEU:O	13:1M:213:HIS:N	2.49	0.45
13:1M:422:HIS:HA	38:1m:50:TYR:CE1	2.51	0.45
13:1M:455:LEU:HD12	13:1M:455:LEU:HA	1.75	0.45
15:1O:86:PRO:HG2	15:1O:87:LYS:HD3	1.98	0.45
15:1O:165:PRO:HG3	15:1O:217:LYS:HD3	1.97	0.45
18:1R:46:GLU:OE1	18:1R:46:GLU:N	2.46	0.45
20:1T:25:ILE:HD11	20:1T:42:LEU:HD21	1.98	0.45
31:1f:42:LEU:HD21	41:1p:71:PRO:HD2	1.98	0.45
33:1h:95:GLN:O	33:1h:99:GLU:HG2	2.16	0.45
37:1l:34:TYR:CE1	37:1l:48:PRO:HG3	2.52	0.45
39:1n:100:GLU:OE1	39:1n:100:GLU:N	2.47	0.45
41:1p:27:ASN:C	41:1p:27:ASN:OD1	2.60	0.45
41:1p:69:ARG:NH1	41:1p:90:GLN:OE1	2.49	0.45
3:1C:53:HIS:NE2	21:1V:104:GLU:OE1	2.50	0.45
4:1D:61:VAL:HG21	4:1D:83:LEU:HB2	1.98	0.45
4:1D:84:HIS:N	4:1D:429:ASP:OD2	2.49	0.45
7:1G:405:LYS:NZ	17:1Q:127:ARG:HH22	2.14	0.45
7:1G:449:PRO:HD2	7:1G:483:VAL:HG23	1.99	0.45
9:1I:3:LYS:HZ1	43:1r:111:TYR:HA	1.81	0.45
12:1L:8:THR:O	12:1L:11:THR:OG1	2.31	0.45
14:1N:1:FME:HG2	14:1N:46:LYS:HG2	1.99	0.45
14:1N:95:MET:HE3	14:1N:95:MET:O	2.17	0.45
19:1S:15:LEU:C	19:1S:16:ARG:HD2	2.41	0.45
20:1U:22:TYR:HB3	20:1U:25:ILE:HB	1.98	0.45
22:1W:90:LEU:O	22:1W:93:THR:OG1	2.32	0.45
25:1Z:5:LYS:N	25:1Z:5:LYS:HE2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:62:TYR:OH	37:1l:72:ASN:ND2	2.43	0.45
37:1l:85:ILE:HG22	37:1l:88:ARG:HB2	1.98	0.45
1:1A:56:PHE:CZ	11:1K:75:LEU:HB3	2.44	0.45
3:1C:57:VAL:O	3:1C:61:LEU:HG	2.16	0.45
4:1D:182:GLU:HG3	9:1I:58:SER:HB3	1.97	0.45
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.97	0.45
5:1E:156:ILE:HD13	5:1E:161:TYR:CD1	2.51	0.45
6:1F:259:SER:HA	6:1F:265:PRO:HB3	1.98	0.45
8:1H:43:TYR:CZ	52:1r:201:CDL:H141	2.51	0.45
9:1I:67:LEU:HD12	9:1I:154:LEU:HD12	1.99	0.45
12:1L:3:PRO:HB3	41:1p:36:PHE:CE1	2.51	0.45
12:1L:79:SER:H	12:1L:139:GLN:HE22	1.63	0.45
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.42	0.45
14:1N:321:LYS:HG3	14:1N:323:MET:H	1.81	0.45
15:1O:243:CYS:O	15:1O:249:PRO:HG2	2.17	0.45
16:1P:140:LYS:HD2	16:1P:140:LYS:HA	1.79	0.45
17:1Q:56:LYS:HB2	17:1Q:58:GLU:OE1	2.17	0.45
31:1f:16:VAL:HB	31:1f:17:PRO:HD3	1.99	0.45
32:1g:66:PHE:HB2	33:1h:28:TYR:CE2	2.52	0.45
34:1i:94:TYR:CE2	41:1p:9:TYR:HB3	2.52	0.45
35:1j:32:MET:SD	35:1j:33:TRP:N	2.90	0.45
36:1k:43:PRO:HG2	36:1k:44:TRP:HD1	1.82	0.45
40:1o:58:CYS:HB3	40:1o:90:GLU:OE2	2.15	0.45
42:1q:51:ASP:OD1	42:1q:54:GLN:N	2.47	0.45
42:1q:101:LYS:HD2	42:1q:101:LYS:C	2.42	0.45
1:1A:84:LEU:HA	1:1A:87:MET:HB3	1.99	0.45
3:1C:89:ARG:HH12	3:1C:163:ARG:HD3	1.82	0.45
3:1C:114:LEU:HB2	22:1W:77:ARG:NH2	2.27	0.45
4:1D:294:TYR:CE2	4:1D:298:LEU:HD11	2.52	0.45
5:1E:190:ARG:NE	5:1E:194:GLU:O	2.44	0.45
7:1G:141:ASN:HB2	7:1G:699:GLU:OE1	2.16	0.45
8:1H:54:LYS:O	8:1H:58:LYS:N	2.39	0.45
11:1K:63:LEU:HD21	14:1N:71:MET:HG2	1.98	0.45
12:1L:166:THR:HG22	37:1l:87:ASN:HA	1.99	0.45
13:1M:216:LEU:HD22	13:1M:220:HIS:NE2	2.32	0.45
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	1.98	0.45
14:1N:72:MET:HE2	14:1N:72:MET:HB2	1.88	0.45
15:1O:49:ARG:HD2	15:1O:114:HIS:CG	2.52	0.45
16:1P:204:PRO:HG2	16:1P:310:LEU:HD12	1.98	0.45
31:1f:47:GLU:OE1	31:1f:48:LEU:N	2.49	0.45
39:1n:75:HIS:CD2	39:1n:77:GLN:H	2.35	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:145:LEU:HD11	41:1p:154:CYS:HB2	1.98	0.45
42:1q:42:ASP:OD1	42:1q:42:ASP:N	2.49	0.45
1:1A:104:TYR:OH	14:1N:5:ILE:HG12	2.17	0.45
4:1D:151:ILE:HG21	4:1D:174:ARG:HD2	1.98	0.45
6:1F:305:PRO:HA	6:1F:414:PRO:HA	1.99	0.45
7:1G:59:ILE:HD11	7:1G:77:TRP:HB3	1.97	0.45
7:1G:376:VAL:HA	7:1G:405:LYS:O	2.17	0.45
8:1H:19:PHE:HE2	8:1H:45:LEU:HD23	1.81	0.45
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.98	0.45
10:1J:23:LYS:NZ	11:1K:32:CYS:SG	2.90	0.45
12:1L:435:PRO:HG2	36:1k:56:PHE:HB3	1.99	0.45
13:1M:17:MET:HA	13:1M:17:MET:HE3	1.97	0.45
13:1M:116:ILE:HG21	23:1X:167:PHE:CD1	2.52	0.45
13:1M:431:THR:HG21	32:1g:58:MET:HE2	1.97	0.45
14:1N:210:THR:HG22	14:1N:329:MET:HE1	1.98	0.45
15:1O:245:LYS:HG2	15:1O:245:LYS:O	2.17	0.45
16:1P:315:ILE:HB	16:1P:319:ARG:HG3	1.99	0.45
17:1Q:10:LEU:HB3	22:1W:16:SER:OG	2.17	0.45
18:1R:70:ARG:HD3	18:1R:72:TYR:CE1	2.52	0.45
19:1S:23:CYS:HB3	19:1S:26:SER:HB3	1.99	0.45
20:1T:43:ASP:HB2	57:1W:201:EHZ:O7	2.15	0.45
20:1U:21:LEU:HD13	36:1k:18:TYR:OH	2.16	0.45
22:1W:84:ILE:HG13	22:1W:85:LYS:N	2.32	0.45
37:1l:40:ASP:OD2	38:1m:84:LYS:HD2	2.17	0.45
41:1p:58:ASN:N	41:1p:58:ASN:OD1	2.48	0.45
2:1B:71:ARG:HA	8:1H:36:GLY:O	2.17	0.45
4:1D:338:MET:HE1	4:1D:348:HIS:CG	2.52	0.45
5:1E:82:GLU:OE2	7:1G:174:THR:OG1	2.25	0.45
6:1F:53:PRO:HG3	6:1F:127:ARG:HE	1.80	0.45
7:1G:60:GLU:HB3	7:1G:78:ASN:HB3	1.99	0.45
7:1G:285:ARG:NH1	7:1G:555:PRO:O	2.44	0.45
7:1G:302:ARG:O	7:1G:306:MET:HG2	2.17	0.45
7:1G:632:ARG:HB3	7:1G:635:ASP:HB2	1.98	0.45
8:1H:30:TYR:CE1	8:1H:35:LYS:HD2	2.52	0.45
9:1I:78:ILE:HD12	9:1I:78:ILE:O	2.16	0.45
12:1L:298:ILE:HD12	12:1L:354:GLN:HA	1.98	0.45
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.52	0.45
13:1M:406:TYR:HA	13:1M:409:TYR:HB3	1.99	0.45
15:1O:233:LYS:HE2	15:1O:233:LYS:N	2.32	0.45
16:1P:38:LEU:O	16:1P:43:SER:OG	2.31	0.45
18:1R:57:ILE:HD13	18:1R:75:LEU:HD12	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:106:PRO:HA	21:1V:107:PRO:HD3	1.81	0.45
23:1X:61:LEU:HA	23:1X:64:GLN:HB3	1.99	0.45
23:1X:100:ARG:HD3	23:1X:100:ARG:HA	1.78	0.45
37:1l:112:MET:HA	37:1l:112:MET:HE3	1.98	0.45
40:1o:38:MET:SD	40:1o:57:TYR:HA	2.57	0.45
4:1D:22:THR:HG22	4:1D:24:GLU:H	1.82	0.45
6:1F:233:THR:O	6:1F:237:ARG:HB3	2.17	0.45
6:1F:275:PRO:HB3	6:1F:277:LYS:HE3	1.99	0.45
6:1F:375:VAL:HG23	6:1F:392:LEU:HD12	1.98	0.45
7:1G:378:LEU:HD23	7:1G:439:PHE:HE2	1.82	0.45
8:1H:179:TRP:NE1	25:1Z:43:LEU:HG	2.32	0.45
10:1J:86:ASN:HB3	10:1J:89:VAL:HG23	1.98	0.45
12:1L:209:PRO:HG2	12:1L:213:LEU:HG	1.97	0.45
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.99	0.45
12:1L:293:ILE:HG22	12:1L:422:TYR:HB3	1.97	0.45
13:1M:4:ILE:C	13:1M:7:PRO:HD2	2.42	0.45
13:1M:44:GLN:HB2	32:1g:83:TYR:CE1	2.52	0.45
13:1M:51:ASN:HA	13:1M:57:PHE:HB2	1.98	0.45
13:1M:278:ARG:NH2	38:1m:71:ARG:HH21	2.14	0.45
13:1M:410:MET:HE3	13:1M:410:MET:HB3	1.77	0.45
14:1N:260:PHE:HD2	14:1N:337:LEU:HD11	1.81	0.45
19:1S:44:LYS:HE2	19:1S:52:ILE:HG22	1.97	0.45
21:1V:21:GLU:O	21:1V:25:ILE:HG12	2.17	0.45
22:1W:34:GLU:HA	22:1W:37:ARG:HB2	1.99	0.45
24:1Y:139:LYS:HE3	33:1h:112:ARG:HD3	1.99	0.45
31:1f:14:ILE:C	31:1f:17:PRO:HD2	2.42	0.45
34:1i:43:GLU:HG2	34:1i:47:ASN:ND2	2.32	0.45
34:1i:75:LEU:HD23	34:1i:75:LEU:HA	1.82	0.45
37:1l:71:LEU:HD13	37:1l:77:ILE:HG21	1.99	0.45
39:1n:58:LYS:HD2	39:1n:58:LYS:HA	1.79	0.45
2:1B:61:HIS:NE2	4:1D:178:PHE:HE2	2.15	0.45
3:1C:127:ALA:O	3:1C:131:GLU:N	2.42	0.45
4:1D:169:TRP:NE1	9:1I:40:TYR:CG	2.85	0.45
4:1D:371:LYS:NZ	4:1D:422:ASP:OD2	2.49	0.45
5:1E:9:HIS:CD2	5:1E:63:ILE:HG21	2.52	0.45
5:1E:193:CYS:SG	6:1F:267:THR:HG22	2.57	0.45
6:1F:349:ARG:HD2	6:1F:349:ARG:HA	1.84	0.45
7:1G:134:LYS:HE3	7:1G:134:LYS:HB3	1.79	0.45
7:1G:142:ILE:HG22	7:1G:189:LYS:O	2.16	0.45
8:1H:99:ASN:N	8:1H:99:ASN:OD1	2.50	0.45
8:1H:154:LEU:HD12	8:1H:157:ASN:HD22	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:287:PHE:CE1	12:1L:527:GLY:HA3	2.52	0.45
13:1M:12:LEU:HB3	13:1M:13:PRO:HD3	1.99	0.45
13:1M:30:HIS:HE1	31:1f:13:HIS:HA	1.82	0.45
13:1M:70:THR:HA	13:1M:103:GLN:NE2	2.31	0.45
13:1M:395:LEU:HD23	13:1M:395:LEU:HA	1.74	0.45
15:1O:78:SER:OG	15:1O:80:GLU:OE1	2.29	0.45
15:1O:79:LEU:HA	15:1O:96:LEU:HD22	1.98	0.45
15:1O:227:GLU:HA	15:1O:230:ASP:HB3	1.99	0.45
15:1O:262:LEU:HG	15:1O:269:VAL:HG12	1.99	0.45
19:1S:20:ILE:HD11	19:1S:78:LEU:HD22	1.99	0.45
21:1V:18:THR:HB	21:1V:21:GLU:OE1	2.17	0.45
22:1W:96:VAL:O	22:1W:96:VAL:HG22	2.17	0.45
22:1W:107:PHE:O	22:1W:109:GLU:HG2	2.16	0.45
34:1i:50:LEU:HD11	34:1i:61:TYR:CZ	2.52	0.45
40:1o:117:ARG:HH21	40:1o:118:GLU:HB3	1.82	0.45
3:1C:202:PRO:O	17:1Q:50:ASN:N	2.34	0.44
7:1G:141:ASN:OD1	7:1G:141:ASN:O	2.36	0.44
7:1G:261:GLU:N	7:1G:261:GLU:OE2	2.50	0.44
7:1G:347:GLU:OE1	7:1G:455:SER:OG	2.28	0.44
9:1I:148:LEU:HD22	17:1Q:72:TRP:HH2	1.82	0.44
12:1L:2:ASN:HB2	12:1L:3:PRO:HD2	1.98	0.44
12:1L:359:MET:N	12:1L:359:MET:SD	2.90	0.44
13:1M:177:LEU:HB3	33:1h:94:LEU:HD21	1.99	0.44
13:1M:282:LEU:O	13:1M:286:ILE:HG13	2.17	0.44
15:1O:295:LYS:HE3	15:1O:295:LYS:HB2	1.69	0.44
16:1P:314:ALA:H	16:1P:331:MET:HE3	1.82	0.44
17:1Q:30:ILE:HD11	17:1Q:100:GLY:O	2.18	0.44
20:1T:52:MET:HE3	20:1T:52:MET:HB2	1.80	0.44
23:1X:38:PRO:HG3	23:1X:65:CYS:SG	2.57	0.44
23:1X:111:LEU:HA	23:1X:116:TRP:O	2.17	0.44
23:1X:130:VAL:HG22	23:1X:132:THR:HG22	1.98	0.44
30:1e:50:ARG:NH2	30:1e:54:GLU:OE1	2.50	0.44
31:1f:3:VAL:HA	31:1f:6:ILE:HB	1.99	0.44
34:1i:102:ARG:NH1	40:1o:49:GLN:O	2.50	0.44
37:1l:141:GLU:HA	41:1p:122:GLN:HB3	1.99	0.44
43:1r:25:LEU:HB2	43:1r:27:TYR:HE1	1.82	0.44
43:1r:92:LYS:HE2	43:1r:92:LYS:HB2	1.79	0.44
4:1D:198:GLY:HA3	4:1D:324:LYS:HA	1.99	0.44
6:1F:317:MET:HE2	6:1F:317:MET:O	2.17	0.44
7:1G:252:PRO:O	17:1Q:44:ASN:ND2	2.49	0.44
12:1L:305:SER:OG	12:1L:380:LEU:HD11	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:440:LEU:HB2	20:1U:14:ARG:NH1	2.31	0.44
15:1O:266:LYS:O	15:1O:269:VAL:HG22	2.17	0.44
21:1V:22:ARG:HD2	21:1V:26:LEU:HD23	1.99	0.44
22:1W:85:LYS:HE3	22:1W:85:LYS:HB2	1.87	0.44
23:1X:46:ARG:NH1	25:1Z:76:GLN:OE1	2.50	0.44
23:1X:76:HIS:O	23:1X:78:ALA:N	2.51	0.44
23:1X:165:ARG:NH1	33:1h:103:LEU:HD23	2.32	0.44
39:1n:91:GLU:HB3	39:1n:94:GLU:HB2	1.98	0.44
40:1o:14:LYS:HE3	40:1o:109:GLN:HG3	1.99	0.44
42:1q:43:LYS:NZ	42:1q:111:THR:O	2.50	0.44
5:1E:60:TRP:CG	5:1E:94:PRO:HA	2.52	0.44
7:1G:240:VAL:HG13	7:1G:247:VAL:HG23	1.98	0.44
10:1J:161:LEU:O	10:1J:165:VAL:HG23	2.17	0.44
11:1K:5:TYR:HE1	11:1K:46:LEU:HD12	1.81	0.44
12:1L:174:TYR:CD2	12:1L:232:TRP:HB3	2.52	0.44
13:1M:16:TRP:CH2	50:1N:401:3PE:H241	2.52	0.44
13:1M:437:MET:O	13:1M:441:ILE:HG22	2.17	0.44
14:1N:128:LEU:HD12	14:1N:129:LEU:N	2.32	0.44
16:1P:96:GLY:HA3	55:1P:501:NDP:O3D	2.18	0.44
16:1P:110:PHE:HB2	16:1P:148:SER:HB3	1.99	0.44
20:1U:18:VAL:O	20:1U:21:LEU:HB2	2.17	0.44
25:1Z:121:MET:SD	25:1Z:122:GLY:N	2.90	0.44
39:1n:92:ARG:HG3	39:1n:93:TYR:CD1	2.51	0.44
39:1n:122:GLU:OE1	39:1n:123:GLN:NE2	2.50	0.44
1:1A:17:LEU:HB3	8:1H:222:MET:CE	2.48	0.44
4:1D:292:ASP:OD1	4:1D:295:ASP:HB2	2.17	0.44
5:1E:209:PRO:HA	6:1F:40:GLY:HA2	1.99	0.44
7:1G:210:SER:OG	7:1G:213:TYR:HB3	2.18	0.44
7:1G:340:SER:O	7:1G:342:SER:N	2.48	0.44
9:1I:68:ARG:HB2	9:1I:76:ARG:HD2	2.00	0.44
10:1J:122:LEU:HB3	10:1J:126:VAL:HG21	2.00	0.44
10:1J:152:TRP:HE1	14:1N:19:LEU:HD11	1.82	0.44
11:1K:24:SER:HG	11:1K:89:TYR:HE2	1.66	0.44
12:1L:297:ASP:CG	12:1L:300:LYS:H	2.25	0.44
12:1L:420:ALA:O	12:1L:424:THR:HG23	2.17	0.44
12:1L:545:SER:HB2	13:1M:278:ARG:HG3	1.99	0.44
14:1N:133:TRP:CE3	14:1N:136:LEU:HD13	2.52	0.44
15:1O:242:LYS:HB3	15:1O:242:LYS:HE3	1.72	0.44
16:1P:135:LEU:HD13	16:1P:169:SER:HB3	1.99	0.44
16:1P:286:ARG:HA	16:1P:286:ARG:HD2	1.85	0.44
18:1R:28:PHE:CE1	18:1R:33:LYS:HB2	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:12:LYS:HZ1	20:1T:32:VAL:HA	1.82	0.44
20:1T:46:ASP:O	20:1T:50:ILE:HD12	2.17	0.44
22:1W:117:ASP:OD1	22:1W:120:SER:N	2.51	0.44
23:1X:110:VAL:HA	23:1X:114:LEU:HB2	2.00	0.44
36:1k:71:LYS:HA	36:1k:71:LYS:HD3	1.82	0.44
44:1s:49:TYR:HB3	44:1s:52:LEU:HD11	1.99	0.44
5:1E:89:MET:SD	5:1E:89:MET:N	2.90	0.44
6:1F:41:ASP:HB2	6:1F:120:GLU:OE1	2.17	0.44
7:1G:226:GLU:HB2	7:1G:253:ARG:HD3	2.00	0.44
7:1G:524:LEU:HB2	7:1G:545:TYR:HA	1.99	0.44
8:1H:54:LYS:HA	8:1H:57:THR:OG1	2.18	0.44
8:1H:233:MET:O	8:1H:237:PHE:N	2.43	0.44
12:1L:9:LEU:HD23	34:1i:81:ILE:HG23	2.00	0.44
12:1L:539:TYR:HB2	38:1m:10:LEU:HD21	1.99	0.44
14:1N:13:VAL:HB	14:1N:39:ALA:HB3	1.98	0.44
14:1N:175:LEU:HD21	14:1N:227:THR:HA	1.99	0.44
20:1T:60:PHE:CD1	20:1T:60:PHE:C	2.95	0.44
30:1e:6:GLN:CD	30:1e:15:ARG:HE	2.26	0.44
40:1o:111:LYS:HE3	40:1o:111:LYS:HB3	1.72	0.44
1:1A:83:ASN:ND2	45:1A:201:PC1:H122	2.33	0.44
3:1C:77:ASP:N	3:1C:77:ASP:OD1	2.51	0.44
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.52	0.44
4:1D:86:GLY:O	4:1D:90:LEU:HD12	2.17	0.44
6:1F:63:SER:HB2	6:1F:242:PHE:CD2	2.53	0.44
7:1G:666:LEU:N	7:1G:670:ASP:OD2	2.48	0.44
8:1H:165:LEU:HD11	8:1H:241:LEU:HD23	2.00	0.44
8:1H:169:GLN:CD	8:1H:244:GLY:H	2.25	0.44
8:1H:249:PRO:HG2	23:1X:98:HIS:CD2	2.52	0.44
10:1J:30:GLY:O	10:1J:34:ILE:HG12	2.17	0.44
12:1L:341:MET:SD	12:1L:341:MET:N	2.90	0.44
13:1M:151:PHE:HZ	14:1N:291:TYR:HA	1.83	0.44
14:1N:174:GLN:O	14:1N:178:ILE:HD12	2.17	0.44
16:1P:32:ARG:NE	16:1P:175:GLU:OE2	2.51	0.44
16:1P:45:VAL:HG23	16:1P:45:VAL:O	2.18	0.44
16:1P:119:GLN:OE1	16:1P:119:GLN:N	2.50	0.44
22:1W:92:GLU:HG2	22:1W:98:LYS:HG3	2.00	0.44
31:1f:55:THR:OG1	31:1f:56:TRP:N	2.49	0.44
39:1n:24:ARG:HA	39:1n:24:ARG:HD3	1.81	0.44
42:1q:29:ARG:HH22	42:1q:64:TYR:C	2.26	0.44
2:1B:55:CYS:SG	2:1B:117:GLY:HA3	2.57	0.44
2:1B:96:MET:SD	4:1D:82:LEU:HD12	2.57	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:199:LEU:HB3	4:1D:354:GLU:HB2	1.99	0.44
5:1E:126:ILE:HG21	5:1E:132:THR:HA	2.00	0.44
6:1F:101:GLU:HG2	6:1F:302:SER:HB3	2.00	0.44
6:1F:273:SER:N	6:1F:317:MET:SD	2.90	0.44
7:1G:38:PRO:HG3	7:1G:123:PHE:CE2	2.52	0.44
7:1G:194:GLU:OE1	7:1G:385:ARG:NH1	2.51	0.44
7:1G:195:LEU:HD12	7:1G:195:LEU:O	2.17	0.44
10:1J:115:ILE:O	10:1J:117:PHE:N	2.51	0.44
11:1K:97:GLN:NE2	12:1L:580:GLN:O	2.51	0.44
12:1L:7:LEU:HD13	12:1L:49:VAL:CG1	2.47	0.44
12:1L:103:PHE:CD1	12:1L:341:MET:HB2	2.52	0.44
13:1M:114:GLU:HG2	23:1X:168:PHE:HB3	1.98	0.44
13:1M:115:LEU:HD21	13:1M:246:ILE:HD13	2.00	0.44
15:1O:67:LYS:HA	15:1O:67:LYS:HD2	1.78	0.44
16:1P:214:ILE:O	16:1P:218:ILE:HG12	2.18	0.44
16:1P:248:VAL:HA	16:1P:334:VAL:HG21	2.00	0.44
23:1X:103:GLN:OE1	23:1X:118:ARG:NH1	2.51	0.44
28:1c:19:LEU:O	28:1c:23:THR:HG23	2.18	0.44
5:1E:23:PHE:HB2	5:1E:28:TYR:CZ	2.53	0.44
7:1G:257:ASP:OD1	7:1G:369:ALA:N	2.50	0.44
7:1G:647:GLU:CD	7:1G:647:GLU:H	2.25	0.44
8:1H:125:SER:HB2	8:1H:128:ALA:HB3	1.99	0.44
8:1H:141:SER:C	8:1H:289:LEU:HD11	2.43	0.44
8:1H:190:LEU:HD11	8:1H:273:ILE:HG21	1.99	0.44
8:1H:241:LEU:HD23	8:1H:241:LEU:HA	1.85	0.44
8:1H:310:MET:HG3	8:1H:311:THR:HG23	1.99	0.44
9:1I:12:MET:HE2	9:1I:12:MET:HA	1.99	0.44
9:1I:143:THR:OG1	9:1I:146:GLU:HG2	2.18	0.44
10:1J:108:LEU:C	10:1J:109:LYS:HD3	2.43	0.44
10:1J:139:GLU:HA	11:1K:57:ASN:ND2	2.33	0.44
12:1L:56:HIS:ND1	41:1p:29:VAL:HG11	2.33	0.44
12:1L:387:THR:OG1	12:1L:461:SER:O	2.21	0.44
12:1L:576:MET:SD	50:1Y:201:3PE:H112	2.58	0.44
13:1M:204:MET:HE3	13:1M:204:MET:HB3	1.79	0.44
14:1N:2:ASN:O	14:1N:5:ILE:HG22	2.17	0.44
16:1P:33:TYR:O	16:1P:37:HIS:ND1	2.41	0.44
19:1S:15:LEU:HD22	19:1S:16:ARG:H	1.83	0.44
20:1U:36:PHE:HB2	20:1U:71:MET:HE1	2.00	0.44
20:1U:49:GLU:HA	20:1U:52:MET:SD	2.57	0.44
22:1W:91:GLU:O	22:1W:94:ILE:HG12	2.17	0.44
24:1Y:94:CYS:HA	24:1Y:114:CYS:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:123:LEU:HA	24:1Y:126:MET:HB2	1.99	0.44
28:1c:1:LYS:O	28:1c:3:TYR:N	2.51	0.44
29:1d:30:ARG:HE	29:1d:30:ARG:HB2	1.63	0.44
35:1j:7:ILE:HA	35:1j:16:GLN:HE21	1.82	0.44
42:1q:59:HIS:NE2	42:1q:92:CYS:SG	2.87	0.44
1:1A:65:PHE:HD2	8:1H:290:TRP:HZ3	1.66	0.44
3:1C:209:TYR:OH	43:1r:62:ALA:HB1	2.18	0.44
5:1E:86:PHE:O	5:1E:88:THR:N	2.49	0.44
5:1E:104:THR:HG21	5:1E:117:LEU:HD12	1.99	0.44
6:1F:245:PHE:O	6:1F:252:GLY:N	2.40	0.44
6:1F:249:ARG:HD2	6:1F:249:ARG:HA	1.86	0.44
7:1G:254:MET:HE3	7:1G:254:MET:HB3	1.89	0.44
7:1G:303:VAL:HA	7:1G:542:PHE:HE2	1.83	0.44
8:1H:41:GLY:HA3	8:1H:46:LEU:HB2	2.00	0.44
8:1H:162:LEU:HA	8:1H:165:LEU:HD23	2.00	0.44
9:1I:123:GLN:H	9:1I:123:GLN:CD	2.21	0.44
12:1L:51:LEU:C	12:1L:55:MET:HG3	2.43	0.44
12:1L:204:LEU:HD23	12:1L:204:LEU:HA	1.79	0.44
12:1L:487:LYS:HZ1	35:1j:49:GLY:HA2	1.83	0.44
13:1M:329:LEU:O	13:1M:332:THR:OG1	2.36	0.44
13:1M:333:ASN:OD1	13:1M:333:ASN:N	2.50	0.44
13:1M:346:ARG:NE	37:1l:68:ASP:OD2	2.51	0.44
15:1O:24:VAL:HG23	15:1O:167:HIS:ND1	2.33	0.44
16:1P:323:THR:HG22	16:1P:324:TYR:H	1.83	0.44
19:1S:47:ASN:HB3	19:1S:49:ASP:OD1	2.18	0.44
21:1V:18:THR:O	21:1V:18:THR:OG1	2.21	0.44
32:1g:63:PHE:HA	33:1h:28:TYR:CE1	2.52	0.44
32:1g:68:ILE:HD12	32:1g:68:ILE:HA	1.86	0.44
34:1i:80:ILE:HG13	34:1i:81:ILE:HD13	2.00	0.44
37:1l:25:LYS:O	37:1l:25:LYS:HD3	2.17	0.44
39:1n:50:HIS:NE2	57:1n:201:EHZ:O1	2.51	0.44
39:1n:65:GLN:HA	39:1n:68:GLU:HB3	2.00	0.44
40:1o:14:LYS:HA	40:1o:108:LEU:HD22	1.99	0.44
40:1o:21:MET:HA	40:1o:23:THR:HG23	2.00	0.44
42:1q:46:ASN:OD1	42:1q:46:ASN:O	2.36	0.44
2:1B:179:ARG:HD3	16:1P:97:ARG:NH2	2.33	0.43
3:1C:30:ALA:HA	3:1C:37:VAL:HG21	2.00	0.43
3:1C:36:TYR:CE1	3:1C:56:GLY:HA2	2.53	0.43
4:1D:2:ARG:HG2	32:1g:31:ASP:OD2	2.18	0.43
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.33	0.43
6:1F:66:ARG:HB3	6:1F:249:ARG:HH21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:101:GLU:OE1	6:1F:104:THR:HG23	2.18	0.43
7:1G:546:GLN:HA	7:1G:561:LEU:HB2	2.00	0.43
11:1K:79:VAL:O	11:1K:83:ASN:N	2.48	0.43
12:1L:189:PHE:O	12:1L:194:ASN:N	2.51	0.43
12:1L:225:ALA:HB2	12:1L:232:TRP:CZ2	2.53	0.43
12:1L:319:ILE:O	12:1L:321:GLN:HG2	2.18	0.43
12:1L:364:LYS:HZ3	12:1L:364:LYS:HG2	1.72	0.43
13:1M:390:ASN:O	13:1M:393:ILE:HG22	2.18	0.43
14:1N:243:LEU:HD21	29:1d:44:ILE:HD12	1.99	0.43
16:1P:208:VAL:HA	16:1P:211:SER:OG	2.18	0.43
17:1Q:54:LYS:HD3	17:1Q:54:LYS:HA	1.67	0.43
21:1V:4:LEU:HD23	21:1V:4:LEU:HA	1.82	0.43
21:1V:47:THR:O	21:1V:50:ILE:HG13	2.18	0.43
23:1X:114:LEU:HD23	23:1X:114:LEU:HA	1.88	0.43
29:1d:43:LEU:HD23	29:1d:43:LEU:HA	1.83	0.43
40:1o:14:LYS:HE3	40:1o:14:LYS:HB3	1.66	0.43
1:1A:108:GLN:HB2	10:1J:169:MET:HE1	2.00	0.43
4:1D:134:ALA:O	4:1D:138:ARG:HG3	2.17	0.43
5:1E:129:GLY:N	5:1E:139:LEU:O	2.39	0.43
6:1F:92:TYR:CE2	6:1F:133:ALA:HB3	2.53	0.43
6:1F:99:GLU:CD	6:1F:104:THR:HB	2.43	0.43
7:1G:255:HIS:HB2	17:1Q:109:LYS:NZ	2.33	0.43
7:1G:306:MET:HE2	7:1G:306:MET:N	2.32	0.43
8:1H:283:ASP:OD1	8:1H:283:ASP:N	2.51	0.43
11:1K:89:TYR:HB2	11:1K:92:ASN:ND2	2.33	0.43
12:1L:136:ASN:OD1	12:1L:139:GLN:N	2.40	0.43
12:1L:267:MET:HE1	12:1L:273:VAL:HG22	2.00	0.43
13:1M:30:HIS:HA	13:1M:33:LEU:HB2	1.99	0.43
16:1P:237:LEU:HD22	16:1P:238:LEU:H	1.84	0.43
17:1Q:42:ARG:NH1	17:1Q:44:ASN:HA	2.32	0.43
19:1S:19:ARG:HG2	19:1S:53:LEU:HD22	1.99	0.43
30:1e:87:LYS:HE2	30:1e:87:LYS:HB3	1.78	0.43
2:1B:125:TYR:CE2	9:1I:88:PRO:HB2	2.53	0.43
3:1C:130:TYR:HH	4:1D:392:LYS:HZ3	1.60	0.43
4:1D:88:GLU:HG3	4:1D:388:ARG:NH1	2.33	0.43
6:1F:142:PHE:N	6:1F:142:PHE:CD1	2.85	0.43
7:1G:228:ILE:HG21	7:1G:581:GLN:HB3	2.01	0.43
8:1H:121:TRP:HD1	10:1J:27:ILE:HG21	1.82	0.43
9:1I:50:TYR:OH	9:1I:138:GLU:OE1	2.31	0.43
10:1J:120:ASN:OD1	10:1J:121:GLY:N	2.51	0.43
10:1J:157:THR:O	10:1J:161:LEU:HD23	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:190:LEU:HD13	12:1L:196:TRP:CE2	2.53	0.43
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.32	0.43
12:1L:556:ILE:HD13	12:1L:556:ILE:HA	1.82	0.43
13:1M:116:ILE:HD12	13:1M:116:ILE:HA	1.80	0.43
13:1M:196:TRP:HE1	13:1M:254:THR:HB	1.84	0.43
14:1N:89:MET:HG3	14:1N:95:MET:SD	2.59	0.43
14:1N:232:HIS:O	14:1N:311:MET:HE1	2.19	0.43
16:1P:154:LYS:HA	16:1P:157:ARG:HB3	2.00	0.43
20:1T:64:ASP:HB3	22:1W:30:ARG:NH2	2.34	0.43
33:1h:42:LEU:O	33:1h:46:PHE:N	2.51	0.43
35:1j:42:HIS:NE2	36:1k:84:GLU:OE1	2.51	0.43
39:1n:137:LYS:HE3	39:1n:137:LYS:HB3	1.84	0.43
40:1o:3:HIS:HA	40:1o:6:ARG:HE	1.83	0.43
41:1p:126:LYS:HB3	41:1p:126:LYS:HE3	1.80	0.43
3:1C:32:ILE:HA	21:1V:42:ALA:HB3	1.99	0.43
4:1D:322:GLU:CD	4:1D:322:GLU:H	2.26	0.43
5:1E:10:ARG:HH12	18:1R:77:LYS:HA	1.83	0.43
5:1E:51:LEU:HD12	5:1E:51:LEU:HA	1.88	0.43
6:1F:89:ARG:NH2	6:1F:218:CYS:HA	2.33	0.43
6:1F:131:ALA:HB3	6:1F:173:PHE:CZ	2.54	0.43
6:1F:144:ASN:OD1	44:1s:42:GLN:NE2	2.50	0.43
6:1F:206:LYS:NZ	6:1F:208:PRO:O	2.36	0.43
6:1F:295:LEU:HB2	6:1F:338:ASP:C	2.44	0.43
6:1F:348:ALA:HA	6:1F:376:MET:CE	2.48	0.43
7:1G:285:ARG:HG2	7:1G:291:LEU:CD2	2.47	0.43
7:1G:348:VAL:HA	7:1G:510:GLY:HA2	2.00	0.43
9:1I:53:GLU:HG2	42:1q:58:ARG:HA	2.00	0.43
9:1I:56:PRO:C	9:1I:57:LEU:HD22	2.44	0.43
10:1J:65:LEU:HA	10:1J:68:PHE:HB2	1.99	0.43
11:1K:26:LEU:HB2	11:1K:78:LEU:HD12	2.00	0.43
11:1K:51:THR:O	30:1e:31:ARG:HB2	2.18	0.43
12:1L:7:LEU:HD13	12:1L:49:VAL:HG12	2.00	0.43
12:1L:455:LYS:O	12:1L:459:ILE:HG23	2.18	0.43
13:1M:75:LEU:HB3	13:1M:440:HIS:HE1	1.84	0.43
13:1M:249:ILE:HD12	13:1M:249:ILE:HA	1.84	0.43
17:1Q:11:ILE:HB	22:1W:23:ARG:NH1	2.33	0.43
19:1S:18:ILE:CD1	19:1S:64:LEU:HD21	2.44	0.43
5:1E:86:PHE:HD2	6:1F:200:GLN:HB2	1.82	0.43
7:1G:71:MET:HE2	7:1G:71:MET:HA	1.99	0.43
8:1H:88:PRO:HG3	8:1H:104:PHE:CD2	2.53	0.43
9:1I:68:ARG:HH21	9:1I:76:ARG:CZ	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:67:HIS:CE1	12:1L:75:GLU:HB3	2.52	0.43
12:1L:362:LEU:HA	12:1L:365:ALA:HB3	2.01	0.43
13:1M:60:SER:HB3	13:1M:457:PRO:HA	2.00	0.43
13:1M:181:TYR:HE1	41:1p:88:GLU:HG2	1.83	0.43
13:1M:186:LEU:HD22	13:1M:250:LEU:HA	1.99	0.43
14:1N:109:SER:HB2	14:1N:110:PRO:HD2	1.99	0.43
15:1O:64:GLY:O	28:1c:3:TYR:HA	2.18	0.43
16:1P:185:MET:N	16:1P:185:MET:SD	2.91	0.43
16:1P:196:LEU:HD23	16:1P:196:LEU:HA	1.81	0.43
18:1R:39:PHE:O	18:1R:43:LEU:HD12	2.19	0.43
19:1S:23:CYS:SG	19:1S:24:GLN:N	2.90	0.43
21:1V:54:LYS:HB3	21:1V:71:LEU:HD23	2.01	0.43
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.51	0.43
29:1d:46:ASN:HA	29:1d:51:ARG:HG3	1.99	0.43
29:1d:76:LEU:HA	29:1d:79:GLN:HB3	2.00	0.43
30:1e:1:PRO:HB2	30:1e:4:ASP:HA	2.00	0.43
35:1j:56:PRO:HA	35:1j:59:TRP:CH2	2.53	0.43
37:1l:129:GLY:HA3	40:1o:100:GLU:OE2	2.18	0.43
39:1n:107:HIS:O	39:1n:111:LYS:HG3	2.19	0.43
39:1n:120:LYS:HA	39:1n:123:GLN:HG2	2.00	0.43
2:1B:48:MET:SD	2:1B:49:THR:N	2.91	0.43
3:1C:20:LYS:HD2	3:1C:20:LYS:HA	1.80	0.43
4:1D:98:GLN:HB3	9:1I:88:PRO:HB3	1.99	0.43
4:1D:338:MET:HE1	4:1D:348:HIS:CE1	2.53	0.43
6:1F:91:LYS:HE2	6:1F:91:LYS:HB2	1.76	0.43
6:1F:94:VAL:N	6:1F:221:THR:O	2.49	0.43
6:1F:300:GLY:HA2	6:1F:329:LEU:O	2.18	0.43
6:1F:305:PRO:HB3	6:1F:417:GLY:HA3	2.01	0.43
6:1F:343:ILE:H	6:1F:343:ILE:HD12	1.82	0.43
6:1F:371:TRP:O	6:1F:375:VAL:HG22	2.18	0.43
7:1G:327:ALA:HB2	7:1G:596:ASP:HB3	1.99	0.43
8:1H:202:GLU:HB2	8:1H:211:PHE:CZ	2.54	0.43
9:1I:147:LEU:HD23	9:1I:147:LEU:HA	1.87	0.43
10:1J:120:ASN:OD1	10:1J:120:ASN:C	2.61	0.43
10:1J:132:ASP:OD1	10:1J:132:ASP:N	2.38	0.43
12:1L:521:LYS:HB2	12:1L:521:LYS:HE3	1.77	0.43
13:1M:420:THR:HB	13:1M:423:ILE:HG12	2.01	0.43
14:1N:118:VAL:O	14:1N:122:ILE:HG13	2.18	0.43
15:1O:87:LYS:HE2	15:1O:87:LYS:HB2	1.87	0.43
15:1O:183:ILE:HA	15:1O:186:LYS:HG2	1.99	0.43
17:1Q:114:LYS:HD3	17:1Q:114:LYS:N	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:143:TYR:CZ	26:1a:48:MET:HE1	2.54	0.43
32:1g:121:PRO:O	32:1g:122:GLU:HG3	2.18	0.43
39:1n:67:GLU:HA	39:1n:70:PHE:HB3	2.00	0.43
2:1B:92:LEU:HD22	2:1B:136:CYS:SG	2.59	0.43
2:1B:125:TYR:CE1	4:1D:102:TYR:CZ	3.07	0.43
3:1C:168:LEU:HB2	4:1D:93:TYR:CE2	2.54	0.43
4:1D:51:PHE:HD2	4:1D:58:ALA:HB2	1.82	0.43
5:1E:107:PRO:HB2	5:1E:148:CYS:HB3	2.00	0.43
6:1F:36:ALA:HB2	6:1F:39:ARG:HH21	1.84	0.43
6:1F:120:GLU:O	6:1F:123:LEU:HG	2.19	0.43
6:1F:369:VAL:HA	6:1F:372:MET:HG2	2.00	0.43
7:1G:402:ASN:OD1	7:1G:402:ASN:N	2.51	0.43
12:1L:226:GLN:NE2	12:1L:314:MET:SD	2.91	0.43
12:1L:240:PRO:HB2	12:1L:243:VAL:HG23	2.00	0.43
13:1M:121:LEU:H	13:1M:121:LEU:HD12	1.84	0.43
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.01	0.43
20:1T:25:ILE:HD13	20:1T:40:LEU:HG	2.00	0.43
20:1T:71:MET:N	20:1T:71:MET:SD	2.92	0.43
33:1h:42:LEU:HA	33:1h:45:VAL:HG22	2.01	0.43
36:1k:12:LYS:HA	36:1k:12:LYS:HE2	2.00	0.43
38:1m:31:ALA:O	38:1m:35:ARG:HG3	2.19	0.43
3:1C:182:ARG:HD2	3:1C:183:VAL:O	2.19	0.43
5:1E:132:THR:HG23	5:1E:137:PHE:O	2.18	0.43
7:1G:227:SER:OG	7:1G:583:THR:HG23	2.19	0.43
12:1L:81:LYS:HD3	12:1L:262:ARG:NH1	2.33	0.43
12:1L:88:MET:O	12:1L:91:PRO:HD2	2.18	0.43
12:1L:124:PHE:CE2	12:1L:247:LEU:HG	2.54	0.43
12:1L:463:PHE:O	12:1L:465:GLY:N	2.52	0.43
13:1M:263:MET:HE1	38:1m:104:PHE:CD2	2.53	0.43
13:1M:315:LEU:HD21	13:1M:378:GLU:HG2	2.01	0.43
14:1N:116:PRO:CG	14:1N:181:TYR:HE1	2.31	0.43
14:1N:275:SER:OG	14:1N:278:MET:HB2	2.19	0.43
15:1O:35:LYS:HB3	15:1O:35:LYS:HE3	1.87	0.43
15:1O:65:ASP:HB3	28:1c:2:PHE:CD1	2.54	0.43
15:1O:134:PHE:O	15:1O:138:MET:N	2.43	0.43
15:1O:179:ILE:O	15:1O:183:ILE:HG23	2.18	0.43
17:1Q:62:ARG:HA	17:1Q:62:ARG:HD3	1.84	0.43
18:1R:75:LEU:HD23	18:1R:75:LEU:HA	1.82	0.43
19:1S:20:ILE:CD1	19:1S:64:LEU:HD23	2.48	0.43
20:1U:11:ILE:HD13	20:1U:11:ILE:HA	1.86	0.43
23:1X:167:PHE:H	33:1h:104:ARG:HH12	1.66	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1b:12:TRP:HD1	27:1b:19:VAL:HG11	1.83	0.43
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.18	0.43
36:1k:17:ASP:OD1	36:1k:19:LYS:N	2.52	0.43
41:1p:158:GLN:HG3	41:1p:161:ARG:NH2	2.31	0.43
3:1C:64:LEU:HD12	3:1C:72:PHE:CD1	2.53	0.43
3:1C:111:THR:HG22	3:1C:112:ASP:O	2.18	0.43
4:1D:22:THR:O	4:1D:26:ALA:N	2.52	0.43
6:1F:250:ASN:ND2	6:1F:320:ASP:H	2.17	0.43
7:1G:38:PRO:HB2	7:1G:54:MET:SD	2.59	0.43
7:1G:171:ASP:C	7:1G:172:LEU:HD23	2.44	0.43
8:1H:24:GLU:HA	8:1H:271:LEU:HD21	2.01	0.43
45:1H:401:PC1:H2B2	45:1I:203:PC1:H2F1	2.01	0.43
10:1J:95:SER:O	10:1J:98:MET:HG3	2.19	0.43
14:1N:49:ASN:ND2	14:1N:51:ARG:H	2.17	0.43
17:1Q:12:ALA:HA	22:1W:16:SER:HA	2.00	0.43
19:1S:23:CYS:O	19:1S:33:ARG:NH1	2.50	0.43
25:1Z:137:THR:OG1	25:1Z:138:TYR:N	2.52	0.43
29:1d:101:PHE:CZ	33:1h:110:VAL:HG22	2.54	0.43
39:1n:92:ARG:HG3	39:1n:93:TYR:HD1	1.84	0.43
41:1p:26:PRO:HB2	41:1p:31:TYR:HE2	1.84	0.43
42:1q:17:HIS:O	42:1q:23:TYR:N	2.52	0.43
2:1B:45:LEU:O	2:1B:74:VAL:HA	2.19	0.43
3:1C:161:PRO:HA	3:1C:166:PHE:CG	2.54	0.43
6:1F:32:ARG:HB2	6:1F:34:LYS:HD2	2.01	0.43
9:1I:101:ASP:OD1	9:1I:102:GLY:N	2.52	0.43
9:1I:142:GLU:OE2	42:1q:119:GLY:N	2.52	0.43
10:1J:68:PHE:O	10:1J:72:THR:HG23	2.19	0.43
12:1L:55:MET:HE1	12:1L:471:ASN:HB3	2.01	0.43
12:1L:69:MET:HE2	12:1L:71:LEU:HD22	2.00	0.43
12:1L:581:LYS:HE2	24:1Y:43:LYS:HA	2.01	0.43
13:1M:25:ILE:H	13:1M:25:ILE:HD12	1.83	0.43
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.44	0.43
16:1P:144:ARG:HA	16:1P:147:ARG:HB3	2.01	0.43
16:1P:239:PHE:O	16:1P:243:GLN:HG3	2.18	0.43
17:1Q:37:ILE:HG22	17:1Q:56:LYS:O	2.19	0.43
17:1Q:55:TRP:HB2	17:1Q:86:PHE:HB2	2.01	0.43
17:1Q:116:LYS:HA	17:1Q:116:LYS:HD2	1.75	0.43
19:1S:53:LEU:HB3	19:1S:55:ARG:HE	1.83	0.43
21:1V:51:THR:H	21:1V:51:THR:HG1	1.62	0.43
21:1V:76:ILE:O	21:1V:80:ILE:HG13	2.19	0.43
25:1Z:99:LYS:HE2	25:1Z:99:LYS:HB3	1.89	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:86:ILE:HG22	30:1e:91:TYR:CD1	2.53	0.43
35:1j:27:PHE:O	35:1j:31:THR:HG22	2.19	0.43
40:1o:63:ILE:HD12	40:1o:64:GLN:N	2.33	0.43
42:1q:57:GLY:H	42:1q:59:HIS:HD2	1.67	0.43
43:1r:24:GLN:O	43:1r:25:LEU:HD23	2.19	0.43
2:1B:157:LEU:HD12	2:1B:157:LEU:HA	1.89	0.42
4:1D:59:HIS:HB3	4:1D:425:PHE:HZ	1.84	0.42
4:1D:62:LEU:HG	4:1D:64:LEU:HD21	2.01	0.42
4:1D:255:PHE:HB3	4:1D:259:MET:CB	2.49	0.42
4:1D:339:LYS:HE3	9:1I:127:PRO:O	2.19	0.42
7:1G:104:ASP:OD1	7:1G:104:ASP:N	2.51	0.42
7:1G:164:SER:OG	7:1G:165:GLU:OE1	2.25	0.42
7:1G:189:LYS:HG2	7:1G:190:MET:H	1.83	0.42
7:1G:380:VAL:HB	7:1G:453:LEU:HA	2.01	0.42
7:1G:589:PRO:O	22:1W:126:HIS:NE2	2.52	0.42
50:1L:701:3PE:H231	37:1l:88:ARG:HA	2.00	0.42
13:1M:270:ILE:HG13	13:1M:395:LEU:HD22	2.00	0.42
14:1N:89:MET:HE2	14:1N:98:MET:HE2	1.99	0.42
14:1N:112:HIS:NE2	14:1N:164:ILE:HG21	2.34	0.42
16:1P:14:SER:O	17:1Q:65:TRP:NE1	2.42	0.42
18:1R:59:CYS:SG	18:1R:84:CYS:HB2	2.58	0.42
20:1T:22:TYR:HB3	20:1T:25:ILE:HB	2.01	0.42
21:1V:100:GLU:HB2	21:1V:101:PRO:HD3	2.00	0.42
28:1c:31:LEU:HD23	29:1d:70:PHE:CD2	2.53	0.42
30:1e:78:ILE:O	30:1e:82:ARG:HB2	2.19	0.42
32:1g:66:PHE:HB2	33:1h:28:TYR:HE2	1.84	0.42
40:1o:7:ARG:HA	40:1o:15:GLU:HG3	2.01	0.42
52:1r:201:CDL:H182	52:1r:201:CDL:H321	2.01	0.42
3:1C:83:VAL:HG11	3:1C:86:ARG:HH21	1.84	0.42
3:1C:133:GLU:O	3:1C:137:MET:HB2	2.19	0.42
5:1E:9:HIS:HB3	7:1G:187:ILE:HA	2.00	0.42
5:1E:51:LEU:HD21	5:1E:84:ALA:HB2	2.01	0.42
6:1F:362:CYS:SG	6:1F:364:PRO:HD2	2.59	0.42
6:1F:430:MET:C	6:1F:430:MET:HE2	2.44	0.42
7:1G:247:VAL:HG13	7:1G:271:TYR:HB2	1.99	0.42
7:1G:296:TRP:HZ3	7:1G:561:LEU:HD22	1.84	0.42
8:1H:106:LEU:HD21	8:1H:146:LEU:HD23	2.00	0.42
9:1I:17:VAL:HG23	27:1b:13:ALA:HA	2.01	0.42
12:1L:100:ILE:HD12	12:1L:245:ALA:HB3	2.01	0.42
12:1L:135:ASN:O	12:1L:198:LEU:HG	2.18	0.42
12:1L:145:GLU:O	12:1L:149:ILE:HG22	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:213:LEU:HB3	12:1L:273:VAL:HG21	2.00	0.42
13:1M:221:VAL:HA	13:1M:283:LYS:HD3	2.00	0.42
13:1M:391:ILE:N	13:1M:391:ILE:HD12	2.34	0.42
15:1O:141:GLN:HG3	15:1O:198:TYR:HD1	1.84	0.42
15:1O:155:VAL:HA	15:1O:158:VAL:HG22	2.00	0.42
15:1O:308:TYR:HA	15:1O:317:ILE:HD11	2.01	0.42
16:1P:132:ILE:O	16:1P:149:LYS:NZ	2.52	0.42
17:1Q:19:ILE:HD11	17:1Q:98:LYS:HG3	2.01	0.42
18:1R:7:THR:O	18:1R:7:THR:OG1	2.30	0.42
20:1T:44:SER:O	20:1T:48:VAL:HG23	2.19	0.42
20:1T:50:ILE:HD12	20:1T:50:ILE:H	1.84	0.42
25:1Z:120:MET:HG3	25:1Z:122:GLY:H	1.83	0.42
33:1h:38:ILE:HD12	33:1h:38:ILE:H	1.84	0.42
34:1i:107:ASP:O	34:1i:116:ILE:HG22	2.19	0.42
39:1n:12:GLN:O	39:1n:16:LEU:HG	2.19	0.42
42:1q:141:SER:OG	42:1q:142:THR:N	2.51	0.42
1:1A:80:GLN:C	27:1b:45:ASN:HD21	2.27	0.42
2:1B:90:GLY:HA2	46:1B:201:SF4:S2	2.58	0.42
4:1D:146:ARG:NH2	4:1D:278:TYR:OH	2.53	0.42
6:1F:9:LYS:HG3	6:1F:244:SER:O	2.20	0.42
6:1F:74:PRO:HD2	6:1F:77:LEU:HD22	2.01	0.42
6:1F:347:ILE:HD13	6:1F:418:LEU:HG	2.01	0.42
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	2.01	0.42
8:1H:81:LEU:HD21	8:1H:111:LEU:HB3	2.01	0.42
8:1H:314:ILE:H	8:1H:314:ILE:HG13	1.68	0.42
13:1M:46:GLY:HA2	32:1g:84:ARG:CD	2.49	0.42
13:1M:51:ASN:HB2	33:1h:90:THR:OG1	2.19	0.42
13:1M:116:ILE:HG21	23:1X:167:PHE:HD1	1.84	0.42
13:1M:191:SER:HB2	51:1M:501:PGT:H12	2.00	0.42
13:1M:349:GLN:HA	13:1M:356:ALA:HB2	2.01	0.42
13:1M:423:ILE:HD13	13:1M:426:ILE:HD12	2.01	0.42
16:1P:106:PHE:CE2	16:1P:145:TYR:HA	2.51	0.42
20:1T:52:MET:HB3	22:1W:40:TYR:HE1	1.82	0.42
22:1W:54:ILE:HG13	22:1W:107:PHE:CD2	2.54	0.42
23:1X:112:ASP:OD1	23:1X:113:LYS:N	2.51	0.42
31:1f:42:LEU:HD11	41:1p:70:VAL:HG13	2.00	0.42
34:1i:58:ASN:OD1	34:1i:59:VAL:N	2.52	0.42
34:1i:71:VAL:HA	34:1i:75:LEU:HB2	2.01	0.42
38:1m:32:GLN:HA	38:1m:35:ARG:HG3	2.00	0.42
3:1C:93:VAL:HG22	3:1C:108:LYS:HB3	2.00	0.42
4:1D:413:ASP:O	4:1D:417:ILE:HG12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:84:ALA:HA	5:1E:90:TYR:HD2	1.84	0.42
6:1F:123:LEU:HD22	6:1F:161:LEU:O	2.19	0.42
6:1F:295:LEU:HD21	6:1F:343:ILE:HD11	2.01	0.42
6:1F:432:GLN:O	6:1F:436:GLN:HG3	2.18	0.42
7:1G:444:LYS:NZ	7:1G:476:ASN:O	2.52	0.42
7:1G:613:TYR:HD2	7:1G:622:ARG:HG3	1.83	0.42
9:1I:114:THR:HG21	9:1I:144:HIS:NE2	2.34	0.42
12:1L:546:GLN:HB2	13:1M:278:ARG:HH12	1.84	0.42
14:1N:113:PHE:O	14:1N:116:PRO:HD2	2.19	0.42
15:1O:165:PRO:HA	15:1O:166:PRO:HD3	1.92	0.42
16:1P:96:GLY:H	55:1P:501:NDP:C8A	2.32	0.42
16:1P:236:TYR:HB3	16:1P:241:LEU:HD21	2.00	0.42
19:1S:57:CYS:SG	19:1S:58:SER:N	2.91	0.42
20:1T:36:PHE:HB2	20:1T:37:MET:SD	2.60	0.42
22:1W:99:GLN:OE1	22:1W:99:GLN:HA	2.19	0.42
23:1X:113:LYS:HE2	23:1X:113:LYS:HB3	1.64	0.42
24:1Y:74:CYS:SG	24:1Y:75:ILE:N	2.92	0.42
25:1Z:76:GLN:O	25:1Z:80:ASP:HB2	2.19	0.42
25:1Z:110:VAL:HA	30:1e:70:LYS:NZ	2.34	0.42
41:1p:97:VAL:O	41:1p:101:ILE:HG12	2.19	0.42
2:1B:81:ARG:HB3	8:1H:216:ALA:HB2	2.00	0.42
4:1D:141:PHE:HE2	4:1D:184:VAL:HG21	1.83	0.42
5:1E:89:MET:CG	5:1E:90:TYR:H	2.33	0.42
5:1E:205:PRO:HA	5:1E:206:PRO:HD3	1.92	0.42
7:1G:400:LEU:HD12	7:1G:401:HIS:CE1	2.54	0.42
7:1G:411:SER:OG	7:1G:661:LEU:O	2.34	0.42
7:1G:537:LEU:HD11	42:1q:145:LYS:NZ	2.34	0.42
9:1I:43:ARG:HE	9:1I:43:ARG:HB2	1.70	0.42
9:1I:67:LEU:HD13	9:1I:154:LEU:HB3	2.01	0.42
9:1I:112:ASP:OD2	9:1I:112:ASP:C	2.61	0.42
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.19	0.42
12:1L:10:THR:HG21	34:1i:78:VAL:HG23	2.02	0.42
12:1L:161:ARG:HH21	39:1n:90:TYR:N	2.16	0.42
12:1L:304:PHE:CZ	12:1L:526:LEU:HD13	2.54	0.42
12:1L:306:THR:O	12:1L:309:GLN:N	2.52	0.42
14:1N:245:MET:SD	14:1N:249:LEU:HG	2.60	0.42
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.19	0.42
19:1S:12:LYS:HG3	19:1S:14:GLY:N	2.28	0.42
21:1V:30:ILE:CD1	21:1V:51:THR:HG23	2.50	0.42
23:1X:110:VAL:HB	23:1X:116:TRP:HB2	2.01	0.42
33:1h:56:PRO:HD2	33:1h:59:TYR:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:120:LYS:HZ2	40:1o:39:VAL:HG23	1.84	0.42
3:1C:160:HIS:HD2	3:1C:163:ARG:HE	1.66	0.42
4:1D:19:MET:HG2	14:1N:295:ARG:CZ	2.49	0.42
6:1F:263:ASN:ND2	6:1F:286:GLY:O	2.37	0.42
7:1G:32:LYS:HA	7:1G:32:LYS:HD2	1.84	0.42
7:1G:285:ARG:HD3	42:1q:144:TYR:CE1	2.53	0.42
9:1I:136:ASN:OD1	9:1I:138:GLU:N	2.51	0.42
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	2.01	0.42
11:1K:71:ALA:O	11:1K:75:LEU:HB2	2.19	0.42
12:1L:37:LYS:HD3	12:1L:98:TRP:HE1	1.84	0.42
12:1L:154:LEU:HB3	12:1L:243:VAL:CG1	2.48	0.42
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	2.00	0.42
14:1N:324:LYS:HE3	14:1N:324:LYS:HB3	1.79	0.42
52:1N:402:CDL:H152	52:1N:402:CDL:H402	2.02	0.42
15:1O:246:GLY:O	15:1O:249:PRO:HD2	2.18	0.42
20:1T:79:TYR:CE2	20:1T:83:LYS:HE2	2.55	0.42
25:1Z:97:ILE:HG12	30:1e:81:GLN:OE1	2.19	0.42
29:1d:9:VAL:HA	29:1d:10:PRO:HD3	1.89	0.42
29:1d:111:GLU:OE1	29:1d:111:GLU:N	2.53	0.42
30:1e:37:LYS:O	30:1e:41:GLU:HB3	2.20	0.42
35:1j:60:THR:HG22	35:1j:62:GLU:N	2.33	0.42
38:1m:28:THR:O	38:1m:32:GLN:HG2	2.19	0.42
3:1C:150:ARG:NH1	3:1C:154:GLY:O	2.52	0.42
4:1D:221:ARG:H	4:1D:221:ARG:HG2	1.67	0.42
7:1G:305:GLY:C	7:1G:306:MET:HE2	2.44	0.42
7:1G:343:LEU:HD13	7:1G:343:LEU:HA	1.92	0.42
7:1G:364:LEU:HD12	7:1G:491:ASN:ND2	2.34	0.42
8:1H:51:ASP:O	8:1H:55:LEU:HG	2.19	0.42
9:1I:27:TRP:CD1	45:1I:203:PC1:H222	2.55	0.42
10:1J:33:LEU:HD22	10:1J:65:LEU:HD11	2.02	0.42
12:1L:83:ASP:OD1	12:1L:84:TYR:N	2.53	0.42
12:1L:274:GLN:NE2	12:1L:318:GLY:O	2.53	0.42
12:1L:324:LEU:HB3	12:1L:395:ILE:HD11	2.01	0.42
12:1L:435:PRO:HD2	36:1k:51:ARG:O	2.19	0.42
12:1L:529:TYR:CE1	12:1L:533:MET:HG3	2.54	0.42
13:1M:113:THR:HG22	13:1M:175:ASN:ND2	2.35	0.42
14:1N:16:GLY:HA2	14:1N:35:MET:HE2	2.02	0.42
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.19	0.42
14:1N:313:MET:HE1	15:1O:103:SER:HA	2.01	0.42
16:1P:112:LYS:HD2	16:1P:112:LYS:HA	1.69	0.42
16:1P:131:HIS:HB3	16:1P:165:ILE:HD12	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:70:ASN:N	22:1W:70:ASN:OD1	2.53	0.42
23:1X:77:CYS:HB2	23:1X:80:PRO:HG2	2.01	0.42
44:1s:34:ASP:OD1	44:1s:34:ASP:N	2.52	0.42
2:1B:52:LEU:HD12	2:1B:89:ALA:O	2.20	0.42
5:1E:16:ASN:C	5:1E:16:ASN:OD1	2.63	0.42
6:1F:89:ARG:NH2	6:1F:219:PRO:HD3	2.34	0.42
6:1F:131:ALA:HB3	6:1F:173:PHE:CE1	2.55	0.42
6:1F:199:LYS:NZ	17:1Q:130:VAL:O	2.52	0.42
6:1F:387:ALA:HB1	43:1r:48:LEU:HD11	2.02	0.42
6:1F:403:THR:HB	46:1F:502:SF4:S2	2.60	0.42
8:1H:158:GLY:HA2	8:1H:315:PRO:HG2	2.02	0.42
9:1I:156:ASN:HD22	18:1R:34:GLU:HB3	1.85	0.42
12:1L:353:GLU:OE2	39:1n:79:TYR:OH	2.25	0.42
12:1L:597:ILE:O	12:1L:601:LEU:N	2.50	0.42
13:1M:209:LEU:O	13:1M:212:LEU:N	2.52	0.42
15:1O:143:PHE:N	15:1O:143:PHE:CD1	2.88	0.42
16:1P:31:GLY:O	16:1P:35:VAL:HG23	2.20	0.42
19:1S:74:LYS:HD3	19:1S:75:ASN:N	2.27	0.42
20:1T:21:LEU:H	20:1T:21:LEU:HD12	1.85	0.42
29:1d:46:ASN:HB3	29:1d:51:ARG:HB2	2.01	0.42
40:1o:30:PHE:HE1	40:1o:103:ARG:HD2	1.84	0.42
41:1p:136:LYS:HB2	41:1p:136:LYS:HE3	1.81	0.42
41:1p:139:GLN:O	41:1p:157:LYS:NZ	2.47	0.42
1:1A:71:LEU:HD21	11:1K:65:VAL:HG21	2.00	0.42
2:1B:101:ARG:NH1	2:1B:139:ILE:O	2.49	0.42
3:1C:42:VAL:HG12	3:1C:48:LEU:HB2	2.02	0.42
4:1D:34:ASN:ND2	15:1O:158:VAL:HA	2.34	0.42
6:1F:322:LEU:HD23	6:1F:322:LEU:HA	1.81	0.42
6:1F:363:THR:HG22	6:1F:366:ARG:HH21	1.84	0.42
6:1F:379:PHE:CE2	6:1F:392:LEU:HD13	2.55	0.42
7:1G:252:PRO:HB2	7:1G:261:GLU:C	2.44	0.42
7:1G:269:PHE:N	7:1G:269:PHE:HD1	2.17	0.42
7:1G:436:ASN:OD1	7:1G:436:ASN:N	2.52	0.42
8:1H:51:ASP:HA	8:1H:54:LYS:NZ	2.35	0.42
8:1H:140:ILE:HA	8:1H:143:GLU:OE2	2.19	0.42
10:1J:23:LYS:NZ	11:1K:18:GLY:O	2.53	0.42
12:1L:73:THR:CG2	12:1L:194:ASN:HD21	2.33	0.42
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.55	0.42
13:1M:425:ASN:ND2	38:1m:58:VAL:HG13	2.34	0.42
14:1N:258:SER:OG	14:1N:336:VAL:HG22	2.20	0.42
15:1O:130:SER:O	15:1O:133:VAL:HG22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:29:PHE:HB3	16:1P:30:LEU:H	1.65	0.42
16:1P:35:VAL:HA	16:1P:38:LEU:HB2	2.02	0.42
16:1P:81:ILE:O	16:1P:85:VAL:HG22	2.20	0.42
18:1R:30:ASP:O	18:1R:30:ASP:OD2	2.38	0.42
20:1T:11:ILE:HD12	20:1T:80:ILE:HD12	2.01	0.42
27:1b:9:LYS:HD3	27:1b:9:LYS:HA	1.86	0.42
34:1i:62:LYS:HB3	34:1i:62:LYS:HE3	1.86	0.42
37:1l:72:ASN:HD22	38:1m:39:ARG:HD2	1.85	0.42
37:1l:145:ASP:CG	37:1l:147:THR:HG1	2.25	0.42
42:1q:114:LYS:HD3	42:1q:114:LYS:HA	1.78	0.42
1:1A:77:TRP:CZ3	10:1J:51:PHE:HD2	2.34	0.42
2:1B:132:VAL:O	2:1B:134:ARG:NH1	2.52	0.42
4:1D:204:PRO:HA	9:1I:175:TYR:CZ	2.55	0.42
4:1D:216:LYS:HG3	25:1Z:19:ILE:HG22	2.02	0.42
5:1E:29:LYS:H	5:1E:29:LYS:HG3	1.74	0.42
5:1E:186:PRO:HB2	5:1E:190:ARG:O	2.20	0.42
6:1F:24:ASN:O	6:1F:113:HIS:HB3	2.19	0.42
6:1F:51:LYS:HE3	6:1F:55:TRP:NE1	2.35	0.42
7:1G:187:ILE:HD11	7:1G:189:LYS:HE2	2.02	0.42
7:1G:228:ILE:HG12	7:1G:581:GLN:HB3	2.02	0.42
7:1G:246:GLU:HG3	7:1G:248:MET:SD	2.60	0.42
11:1K:37:MET:HG2	11:1K:67:ALA:HB1	2.00	0.42
12:1L:154:LEU:HA	12:1L:154:LEU:HD23	1.83	0.42
12:1L:371:THR:O	12:1L:375:ILE:HG12	2.20	0.42
12:1L:546:GLN:O	12:1L:551:SER:HB3	2.20	0.42
13:1M:149:PHE:O	13:1M:153:THR:HG22	2.20	0.42
13:1M:378:GLU:O	13:1M:382:ILE:HG12	2.20	0.42
14:1N:3:PRO:HB3	15:1O:5:PRO:HB3	2.00	0.42
14:1N:152:ASN:O	14:1N:156:THR:HG23	2.20	0.42
15:1O:86:PRO:O	15:1O:93:SER:OG	2.36	0.42
16:1P:172:PHE:HB2	16:1P:179:LEU:HD23	2.02	0.42
19:1S:15:LEU:HD11	19:1S:18:ILE:HB	2.01	0.42
20:1T:22:TYR:HD1	20:1T:23:ASP:N	2.18	0.42
20:1U:69:LYS:HA	34:1i:2:GLY:N	2.35	0.42
21:1V:98:PRO:HD2	21:1V:99:TRP:CE2	2.54	0.42
26:1a:58:ASN:O	26:1a:59:ARG:HD3	2.19	0.42
29:1d:14:LEU:HD21	29:1d:77:LYS:HB3	2.01	0.42
32:1g:97:VAL:HG12	32:1g:101:GLU:OE1	2.20	0.42
32:1g:107:LEU:H	32:1g:107:LEU:HD22	1.85	0.42
34:1i:41:PRO:HA	34:1i:44:GLN:HE22	1.85	0.42
34:1i:93:PRO:HB3	41:1p:4:TRP:CE2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:59:TRP:HZ3	40:1o:102:GLU:HG3	1.85	0.42
38:1m:94:ILE:H	38:1m:94:ILE:CD1	2.29	0.42
39:1n:51:LYS:HE3	39:1n:51:LYS:HB3	1.69	0.42
42:1q:48:TYR:CG	42:1q:62:VAL:HG12	2.55	0.42
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.45	0.41
3:1C:137:MET:HE3	3:1C:152:LEU:HD22	2.01	0.41
4:1D:352:TYR:CD2	9:1I:86:VAL:HG21	2.55	0.41
5:1E:120:ILE:HD13	5:1E:120:ILE:HA	1.89	0.41
7:1G:410:GLY:CA	7:1G:661:LEU:HB2	2.50	0.41
7:1G:542:PHE:HA	7:1G:558:ASP:OD1	2.20	0.41
8:1H:117:LEU:HD23	8:1H:136:VAL:HG21	2.01	0.41
9:1I:126:CYS:HB2	46:1I:202:SF4:S3	2.58	0.41
10:1J:10:SER:O	10:1J:14:VAL:HG23	2.20	0.41
11:1K:30:LEU:HD13	11:1K:75:LEU:HD22	2.02	0.41
12:1L:3:PRO:HB3	41:1p:36:PHE:CZ	2.54	0.41
12:1L:54:PHE:CD1	12:1L:58:GLY:HA2	2.55	0.41
13:1M:106:LEU:HD21	13:1M:235:LEU:HD23	2.02	0.41
14:1N:158:ALA:HB1	14:1N:192:ALA:HB2	2.02	0.41
14:1N:243:LEU:O	14:1N:247:THR:HG22	2.20	0.41
15:1O:45:LYS:HE2	15:1O:45:LYS:HB2	1.81	0.41
16:1P:243:GLN:OE1	16:1P:244:TYR:N	2.53	0.41
17:1Q:126:LYS:HE2	17:1Q:126:LYS:HB2	1.66	0.41
20:1T:69:LYS:NZ	20:1T:79:TYR:HB2	2.34	0.41
20:1U:13:ASP:O	20:1U:17:TYR:HB2	2.20	0.41
25:1Z:121:MET:HE3	25:1Z:137:THR:HG21	2.02	0.41
32:1g:93:ALA:O	32:1g:97:VAL:HG23	2.20	0.41
32:1g:117:LYS:O	32:1g:118:ILE:HG12	2.20	0.41
35:1j:23:ILE:HA	35:1j:26:GLU:HB3	2.02	0.41
37:1l:30:ARG:NH1	38:1m:35:ARG:HG2	2.27	0.41
3:1C:139:GLY:HA3	3:1C:160:HIS:CG	2.54	0.41
3:1C:162:PHE:HZ	4:1D:88:GLU:HG2	1.83	0.41
4:1D:2:ARG:HD2	15:1O:287:HIS:CE1	2.55	0.41
4:1D:113:CYS:SG	4:1D:370:PRO:HD3	2.61	0.41
4:1D:136:TRP:CE3	4:1D:319:PRO:HG3	2.54	0.41
5:1E:160:TYR:HE1	44:1s:43:HIS:HE1	1.68	0.41
5:1E:184:PRO:C	5:1E:187:ARG:HH12	2.27	0.41
6:1F:295:LEU:N	6:1F:338:ASP:HA	2.30	0.41
7:1G:377:ILE:HG22	7:1G:379:LEU:HG	2.03	0.41
7:1G:387:GLU:HG3	7:1G:493:LEU:HD21	2.02	0.41
7:1G:539:LYS:HB2	7:1G:539:LYS:HE2	1.83	0.41
12:1L:384:PRO:HA	12:1L:389:PHE:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:548:SER:OG	12:1L:549:ALA:N	2.53	0.41
13:1M:278:ARG:O	38:1m:71:ARG:NH2	2.53	0.41
15:1O:104:ARG:NH2	15:1O:126:ARG:HE	2.18	0.41
16:1P:163:ALA:HB1	16:1P:165:ILE:HD11	2.01	0.41
17:1Q:37:ILE:HD12	17:1Q:37:ILE:O	2.19	0.41
17:1Q:70:MET:HE3	42:1q:126:PRO:HB3	2.02	0.41
20:1T:52:MET:HE3	22:1W:37:ARG:HD2	2.02	0.41
22:1W:20:ILE:HB	22:1W:80:ASP:OD2	2.20	0.41
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.51	0.41
38:1m:122:GLN:OE1	38:1m:122:GLN:N	2.54	0.41
40:1o:98:MET:HA	40:1o:101:PHE:HB3	2.02	0.41
41:1p:139:GLN:HA	41:1p:143:SER:HB3	2.02	0.41
1:1A:106:TRP:CE2	8:1H:291:LYS:HD2	2.55	0.41
4:1D:150:HIS:HD1	4:1D:150:HIS:H	1.68	0.41
4:1D:164:MET:O	4:1D:167:PHE:HB3	2.20	0.41
4:1D:334:LYS:O	4:1D:338:MET:N	2.50	0.41
5:1E:68:LYS:O	5:1E:71:GLU:HG3	2.19	0.41
5:1E:78:MET:HE3	5:1E:78:MET:HA	2.02	0.41
5:1E:202:LEU:HD21	6:1F:24:ASN:HA	2.02	0.41
6:1F:20:ARG:HB3	6:1F:269:GLU:HB3	2.03	0.41
6:1F:96:ASN:HD21	6:1F:187:GLY:C	2.28	0.41
6:1F:171:TYR:CE2	6:1F:173:PHE:HD1	2.38	0.41
7:1G:409:ILE:HG22	7:1G:422:LEU:HB3	2.01	0.41
7:1G:469:ALA:O	7:1G:473:ILE:HG12	2.20	0.41
9:1I:136:ASN:ND2	9:1I:161:TRP:HZ2	2.18	0.41
9:1I:162:GLU:O	9:1I:166:ALA:N	2.54	0.41
10:1J:51:PHE:O	10:1J:51:PHE:HD1	2.02	0.41
11:1K:59:MET:HE1	14:1N:75:ILE:HD11	2.02	0.41
12:1L:84:TYR:HA	12:1L:87:VAL:HG12	2.03	0.41
12:1L:194:ASN:O	12:1L:194:ASN:ND2	2.53	0.41
12:1L:203:MET:HE3	41:1p:120:TYR:HD2	1.85	0.41
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	2.02	0.41
12:1L:339:LEU:HD21	12:1L:376:GLY:HA3	2.02	0.41
12:1L:395:ILE:HD13	12:1L:395:ILE:HA	1.92	0.41
15:1O:112:LEU:HD12	15:1O:112:LEU:HA	1.85	0.41
16:1P:93:ASN:OD1	16:1P:94:LEU:N	2.54	0.41
19:1S:30:GLN:HA	19:1S:33:ARG:HB2	2.01	0.41
21:1V:3:LEU:HD12	21:1V:4:LEU:N	2.35	0.41
21:1V:80:ILE:HG13	21:1V:80:ILE:H	1.61	0.41
25:1Z:56:GLU:CD	25:1Z:59:ARG:HH21	2.28	0.41
34:1i:68:ILE:HG13	34:1i:69:PHE:N	2.34	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:131:LYS:HA	37:1l:131:LYS:HD3	1.61	0.41
1:1A:54:LYS:HD3	1:1A:114:ALA:O	2.21	0.41
1:1A:95:LEU:HD23	8:1H:302:MET:SD	2.60	0.41
3:1C:15:ASN:OD1	3:1C:15:ASN:C	2.63	0.41
5:1E:28:TYR:O	5:1E:31:ILE:HG13	2.20	0.41
5:1E:120:ILE:HD11	5:1E:169:ILE:HG13	2.03	0.41
6:1F:255:LEU:HA	6:1F:255:LEU:HD23	1.92	0.41
6:1F:259:SER:N	6:1F:334:VAL:O	2.50	0.41
8:1H:183:MET:H	8:1H:183:MET:HG2	1.70	0.41
12:1L:37:LYS:HB2	12:1L:101:MET:HG2	2.02	0.41
13:1M:24:TRP:O	13:1M:28:THR:OG1	2.30	0.41
13:1M:42:LEU:HD13	13:1M:42:LEU:HA	1.93	0.41
13:1M:342:MET:HE1	13:1M:409:TYR:CE2	2.55	0.41
51:1M:501:PGT:H131	51:1M:501:PGT:H361	2.01	0.41
14:1N:255:PRO:HG3	14:1N:260:PHE:CD1	2.55	0.41
15:1O:38:LEU:HD13	15:1O:228:ALA:HA	2.02	0.41
15:1O:157:LYS:O	15:1O:161:CYS:HB3	2.20	0.41
16:1P:209:ASP:N	16:1P:209:ASP:OD2	2.53	0.41
17:1Q:35:VAL:HG12	17:1Q:59:PHE:CE2	2.55	0.41
21:1V:37:ILE:CG2	21:1V:44:ARG:HG3	2.50	0.41
22:1W:68:MET:HA	22:1W:71:ALA:HB3	2.02	0.41
25:1Z:110:VAL:HA	30:1e:70:LYS:HZ1	1.86	0.41
25:1Z:121:MET:HE3	25:1Z:137:THR:CG2	2.51	0.41
33:1h:91:MET:HE2	41:1p:82:LEU:HD22	2.02	0.41
1:1A:97:LEU:HD23	1:1A:97:LEU:HA	1.82	0.41
1:1A:106:TRP:CZ2	8:1H:291:LYS:HD2	2.56	0.41
3:1C:195:ARG:HH21	9:1I:84:GLU:CD	2.28	0.41
4:1D:37:ASP:OD1	14:1N:51:ARG:NE	2.52	0.41
4:1D:80:ILE:HD12	4:1D:81:GLY:N	2.36	0.41
4:1D:170:MET:HE1	4:1D:304:MET:HE1	2.01	0.41
4:1D:381:ASP:HB3	4:1D:387:TYR:CD2	2.50	0.41
5:1E:38:TYR:HA	6:1F:135:TYR:OH	2.21	0.41
5:1E:155:GLN:HA	5:1E:160:TYR:HA	2.02	0.41
5:1E:162:GLU:OE2	6:1F:108:ARG:NH2	2.49	0.41
6:1F:374:LYS:HB3	7:1G:132:GLU:HG3	2.03	0.41
7:1G:386:PHE:CE1	7:1G:668:ILE:HD13	2.56	0.41
8:1H:87:VAL:HG22	8:1H:88:PRO:HD3	2.03	0.41
9:1I:67:LEU:O	9:1I:158:GLY:HA3	2.20	0.41
10:1J:84:VAL:HG13	10:1J:85:SER:N	2.36	0.41
12:1L:88:MET:C	12:1L:91:PRO:HD2	2.45	0.41
12:1L:108:MET:HE2	12:1L:108:MET:HB2	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.54	0.41
13:1M:452:LYS:NZ	32:1g:83:TYR:HB3	2.35	0.41
19:1S:20:ILE:HD12	19:1S:20:ILE:HA	1.96	0.41
23:1X:78:ALA:O	23:1X:82:THR:HG23	2.20	0.41
23:1X:111:LEU:HD12	23:1X:112:ASP:N	2.35	0.41
33:1h:15:GLY:O	33:1h:19:ARG:HG2	2.20	0.41
33:1h:19:ARG:HA	33:1h:19:ARG:NH1	2.35	0.41
33:1h:52:LEU:HD23	41:1p:62:TYR:CZ	2.56	0.41
33:1h:64:TRP:CE2	33:1h:77:ARG:HD3	2.55	0.41
34:1i:70:ALA:O	34:1i:74:VAL:HB	2.20	0.41
40:1o:112:LYS:HE2	40:1o:112:LYS:HB2	1.92	0.41
2:1B:45:LEU:O	2:1B:46:TRP:HD1	2.03	0.41
3:1C:51:PHE:N	3:1C:51:PHE:HD1	2.19	0.41
3:1C:105:ILE:HD12	3:1C:105:ILE:HA	1.95	0.41
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.55	0.41
5:1E:176:LEU:HD23	5:1E:181:ILE:HD13	2.02	0.41
6:1F:89:ARG:CZ	6:1F:219:PRO:HD3	2.50	0.41
6:1F:101:GLU:O	6:1F:104:THR:OG1	2.37	0.41
6:1F:157:TYR:CE2	44:1s:58:LEU:HD11	2.56	0.41
7:1G:296:TRP:CD2	22:1W:122:PHE:HE2	2.37	0.41
8:1H:201:THR:HA	8:1H:207:LEU:HD12	2.02	0.41
12:1L:306:THR:OG1	12:1L:307:SER:N	2.53	0.41
13:1M:94:LEU:HD23	50:1N:401:3PE:H351	2.03	0.41
14:1N:114:TRP:O	14:1N:118:VAL:HG22	2.21	0.41
14:1N:170:LEU:O	14:1N:295:ARG:NH1	2.54	0.41
16:1P:3:HIS:NE2	42:1q:136:GLU:HG2	2.35	0.41
16:1P:5:LEU:HD12	16:1P:5:LEU:HA	1.92	0.41
16:1P:256:TYR:CE2	16:1P:258:LEU:HB2	2.55	0.41
18:1R:37:GLU:H	18:1R:37:GLU:CD	2.28	0.41
20:1T:33:ASN:O	20:1T:72:CYS:HB3	2.20	0.41
22:1W:71:ALA:C	22:1W:72:HIS:HD1	2.29	0.41
23:1X:142:HIS:HB2	25:1Z:115:ARG:HB2	2.03	0.41
27:1b:40:TYR:O	27:1b:44:ILE:HG23	2.20	0.41
35:1j:66:ILE:HG23	40:1o:107:LEU:HG	2.02	0.41
37:1l:156:TYR:HA	40:1o:35:GLU:HA	2.02	0.41
38:1m:55:ARG:HE	38:1m:55:ARG:HB3	1.51	0.41
41:1p:69:ARG:NE	41:1p:69:ARG:HA	2.36	0.41
2:1B:52:LEU:HD21	2:1B:96:MET:HG2	2.03	0.41
2:1B:91:THR:HA	2:1B:119:CYS:HB3	2.03	0.41
2:1B:125:TYR:OH	4:1D:98:GLN:O	2.39	0.41
4:1D:59:HIS:HB3	4:1D:425:PHE:CZ	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:209:ASP:OD1	25:1Z:16:TYR:OH	2.29	0.41
5:1E:24:THR:O	5:1E:28:TYR:N	2.51	0.41
6:1F:53:PRO:HB3	6:1F:128:ALA:HA	2.03	0.41
6:1F:65:LEU:HG	6:1F:242:PHE:CE2	2.56	0.41
6:1F:250:ASN:HD22	6:1F:318:ASP:HB2	1.84	0.41
6:1F:344:VAL:HG21	6:1F:429:ARG:HG2	2.03	0.41
7:1G:534:ARG:HA	42:1q:145:LYS:NZ	2.36	0.41
7:1G:595:GLU:OE1	7:1G:598:LYS:HE2	2.21	0.41
7:1G:615:THR:O	7:1G:619:VAL:HG23	2.21	0.41
8:1H:169:GLN:OE1	8:1H:244:GLY:N	2.44	0.41
9:1I:123:GLN:HE22	9:1I:133:GLU:HG2	1.85	0.41
16:1P:210:VAL:O	16:1P:214:ILE:HD12	2.21	0.41
19:1S:83:ALA:HA	19:1S:86:VAL:HG22	2.02	0.41
34:1i:120:LYS:HG2	34:1i:121:GLU:N	2.36	0.41
37:1l:14:PRO:HA	37:1l:19:GLU:OE1	2.21	0.41
40:1o:20:ARG:HA	40:1o:20:ARG:HD2	1.67	0.41
40:1o:51:MET:HA	41:1p:118:GLU:HG3	2.02	0.41
2:1B:65:PRO:O	9:1I:47:THR:HA	2.21	0.41
4:1D:270:ARG:NH2	4:1D:303:GLU:OE2	2.43	0.41
5:1E:172:ILE:HG13	5:1E:173:ILE:N	2.35	0.41
6:1F:226:GLU:O	6:1F:230:VAL:HG22	2.20	0.41
7:1G:150:MET:HE2	7:1G:183:VAL:O	2.20	0.41
7:1G:462:ASP:N	7:1G:462:ASP:OD1	2.53	0.41
7:1G:537:LEU:HD11	42:1q:145:LYS:HZ2	1.85	0.41
8:1H:314:ILE:HD12	8:1H:314:ILE:O	2.21	0.41
12:1L:44:PHE:O	12:1L:48:LEU:HD23	2.21	0.41
12:1L:434:LYS:HG3	36:1k:52:TYR:CE2	2.56	0.41
12:1L:599:MET:HA	12:1L:599:MET:HE3	2.02	0.41
13:1M:200:ILE:HD13	13:1M:200:ILE:HA	1.91	0.41
15:1O:113:GLU:HB2	15:1O:263:VAL:HG11	2.03	0.41
16:1P:110:PHE:O	16:1P:152:GLY:HA3	2.21	0.41
17:1Q:35:VAL:HB	17:1Q:57:MET:HE2	2.03	0.41
17:1Q:129:ARG:HD2	44:1s:73:PRO:HG3	2.01	0.41
20:1U:50:ILE:HD13	20:1U:50:ILE:HA	1.82	0.41
21:1V:45:LYS:HE3	43:1r:91:LYS:HE3	2.02	0.41
22:1W:40:TYR:HE2	22:1W:60:ARG:NH1	2.19	0.41
22:1W:54:ILE:HG23	22:1W:58:GLN:NE2	2.35	0.41
29:1d:106:LYS:HD3	29:1d:106:LYS:C	2.46	0.41
32:1g:68:ILE:HD12	32:1g:72:LEU:HD12	2.03	0.41
33:1h:114:MET:SD	33:1h:120:GLY:HA3	2.60	0.41
34:1i:79:TRP:HD1	41:1p:40:VAL:HG13	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:176:ARG:HD3	39:1n:176:ARG:HA	1.88	0.41
42:1q:72:ASP:C	42:1q:72:ASP:OD2	2.63	0.41
1:1A:63:LEU:HD22	10:1J:67:VAL:HG21	2.02	0.41
2:1B:104:TYR:CE1	2:1B:111:ARG:HD2	2.56	0.41
3:1C:173:GLU:HB3	3:1C:188:VAL:HA	2.02	0.41
4:1D:37:ASP:OD2	14:1N:51:ARG:HG2	2.21	0.41
4:1D:90:LEU:HD12	4:1D:90:LEU:H	1.86	0.41
4:1D:133:ARG:HB3	4:1D:322:GLU:O	2.21	0.41
4:1D:251:LEU:HD13	4:1D:251:LEU:C	2.46	0.41
4:1D:415:VAL:HA	4:1D:418:ILE:HD12	2.02	0.41
5:1E:27:ASN:HB3	5:1E:53:LEU:HD11	2.03	0.41
5:1E:172:ILE:HG13	5:1E:173:ILE:HG23	2.03	0.41
6:1F:21:ILE:HG21	6:1F:230:VAL:HG12	2.03	0.41
6:1F:82:MET:HG3	6:1F:221:THR:HG22	2.03	0.41
6:1F:188:GLU:HG3	6:1F:190:THR:H	1.86	0.41
6:1F:307:ILE:HG23	6:1F:311:VAL:HB	2.02	0.41
7:1G:261:GLU:HB2	17:1Q:44:ASN:ND2	2.31	0.41
7:1G:391:PHE:CD2	7:1G:395:ILE:HD11	2.56	0.41
7:1G:474:ALA:HB1	7:1G:489:VAL:HB	2.03	0.41
7:1G:601:ARG:HG2	7:1G:611:LEU:HB2	2.02	0.41
8:1H:66:SER:HA	8:1H:122:ALA:O	2.21	0.41
8:1H:85:MET:O	8:1H:88:PRO:HD2	2.21	0.41
8:1H:142:TYR:CE1	8:1H:289:LEU:HD12	2.56	0.41
9:1I:3:LYS:HD2	9:1I:3:LYS:C	2.45	0.41
11:1K:10:MET:HE2	11:1K:10:MET:N	2.36	0.41
11:1K:38:LEU:O	11:1K:41:PHE:N	2.53	0.41
12:1L:128:MET:O	12:1L:132:VAL:HG23	2.21	0.41
12:1L:232:TRP:HZ3	12:1L:252:MET:HE1	1.86	0.41
12:1L:287:PHE:CZ	12:1L:527:GLY:HA3	2.55	0.41
12:1L:372:ALA:HA	12:1L:458:LEU:HD11	2.03	0.41
13:1M:50:LEU:HA	33:1h:86:ASN:HD21	1.86	0.41
13:1M:60:SER:HB2	32:1g:84:ARG:HH12	1.86	0.41
13:1M:310:MET:HE2	13:1M:459:TYR:HA	2.03	0.41
13:1M:361:MET:HA	13:1M:364:LEU:HG	2.03	0.41
14:1N:163:LEU:HD23	14:1N:167:TRP:CZ3	2.56	0.41
14:1N:268:GLN:HG3	23:1X:167:PHE:HZ	1.86	0.41
14:1N:274:GLU:OE1	24:1Y:139:LYS:HD3	2.21	0.41
14:1N:290:LEU:HA	14:1N:293:TYR:CD2	2.56	0.41
14:1N:296:LEU:HD13	14:1N:296:LEU:HA	1.95	0.41
15:1O:236:GLU:H	15:1O:236:GLU:HG3	1.74	0.41
15:1O:242:LYS:HE3	15:1O:244:ASP:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:46:ILE:H	16:1P:46:ILE:HG13	1.73	0.41
16:1P:139:ILE:HG13	16:1P:147:ARG:HG3	2.02	0.41
21:1V:97:LYS:HD2	21:1V:99:TRP:CZ3	2.56	0.41
22:1W:54:ILE:HD13	22:1W:54:ILE:HA	1.92	0.41
24:1Y:72:THR:HA	24:1Y:75:ILE:HG22	2.02	0.41
30:1e:20:GLN:HG2	30:1e:36:GLU:OE2	2.20	0.41
31:1f:11:TRP:O	31:1f:14:ILE:HG22	2.21	0.41
32:1g:110:SER:O	41:1p:161:ARG:NH1	2.45	0.41
36:1k:52:TYR:HH	39:1n:34:ASP:H	1.68	0.41
36:1k:59:ASN:HD22	36:1k:60:VAL:H	1.68	0.41
40:1o:99:LYS:HB3	40:1o:99:LYS:HE3	1.86	0.41
42:1q:39:VAL:HB	42:1q:50:GLU:OE1	2.20	0.41
42:1q:48:TYR:HE2	42:1q:86:TRP:HB3	1.86	0.41
42:1q:87:HIS:HE1	42:1q:91:HIS:CE1	2.39	0.41
43:1r:2:SER:HB3	43:1r:3:ALA:H	1.64	0.41
43:1r:20:GLN:OE1	43:1r:20:GLN:HA	2.21	0.41
2:1B:79:SER:OG	8:1H:209:SER:OG	2.12	0.41
4:1D:184:VAL:HG23	4:1D:185:SER:N	2.36	0.41
4:1D:194:ILE:HD13	4:1D:194:ILE:HA	1.96	0.41
6:1F:68:ARG:O	6:1F:68:ARG:HG2	2.20	0.41
7:1G:257:ASP:HA	7:1G:394:ARG:HH12	1.86	0.41
7:1G:285:ARG:NH2	7:1G:289:GLY:O	2.45	0.41
8:1H:221:ALA:O	8:1H:225:MET:HB2	2.20	0.41
10:1J:150:GLY:HA2	30:1e:16:TRP:CH2	2.56	0.41
11:1K:66:PHE:CE2	14:1N:31:ILE:HD12	2.56	0.41
12:1L:7:LEU:O	12:1L:11:THR:HG23	2.22	0.41
12:1L:317:ILE:HD13	12:1L:322:PRO:HA	2.03	0.41
13:1M:13:PRO:HB3	50:1N:401:3PE:H2C2	2.02	0.41
13:1M:14:MET:HE1	13:1M:30:HIS:ND1	2.36	0.41
13:1M:302:MET:HE3	13:1M:302:MET:HB3	1.97	0.41
14:1N:27:LEU:O	14:1N:31:ILE:HG12	2.21	0.41
15:1O:224:SER:HB3	15:1O:226:ARG:HH21	1.86	0.41
16:1P:32:ARG:HD2	16:1P:33:TYR:CE1	2.56	0.41
23:1X:73:ILE:HD11	26:1a:66:LEU:HD11	2.02	0.41
23:1X:165:ARG:O	33:1h:104:ARG:NH1	2.54	0.41
26:1a:39:ALA:HA	26:1a:44:GLN:HB3	2.03	0.41
29:1d:10:PRO:HG2	30:1e:7:LYS:HB3	2.02	0.41
33:1h:105:LEU:HD23	33:1h:105:LEU:HA	1.93	0.41
41:1p:69:ARG:CZ	41:1p:90:GLN:HE22	2.34	0.41
41:1p:73:ILE:HD12	41:1p:87:ALA:CB	2.50	0.41
44:1s:55:ASN:OD1	44:1s:55:ASN:C	2.63	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:73:LEU:HB3	10:1J:51:PHE:CZ	2.55	0.40
2:1B:63:ALA:HA	2:1B:69:MET:SD	2.61	0.40
3:1C:49:GLU:HB3	3:1C:51:PHE:HE1	1.85	0.40
3:1C:101:PHE:HE1	43:1r:99:PRO:HG3	1.86	0.40
3:1C:137:MET:SD	3:1C:162:PHE:CE1	3.14	0.40
3:1C:155:TYR:CE1	22:1W:97:TRP:HB3	2.56	0.40
4:1D:151:ILE:HG12	4:1D:304:MET:HE2	2.02	0.40
4:1D:178:PHE:HE1	4:1D:188:ARG:C	2.28	0.40
4:1D:222:ILE:HA	4:1D:222:ILE:HD12	1.69	0.40
7:1G:13:VAL:HG23	7:1G:79:ILE:HG12	2.03	0.40
7:1G:405:LYS:HZ3	17:1Q:127:ARG:HH22	1.68	0.40
9:1I:39:SER:C	9:1I:43:ARG:HH21	2.29	0.40
12:1L:176:ARG:C	13:1M:401:MET:HE1	2.46	0.40
12:1L:384:PRO:HG3	12:1L:491:LEU:HD13	2.03	0.40
12:1L:503:GLU:O	12:1L:507:THR:OG1	2.39	0.40
14:1N:59:TYR:CZ	14:1N:63:GLN:HG3	2.56	0.40
14:1N:96:THR:HG23	14:1N:153:LEU:HD11	2.03	0.40
14:1N:239:VAL:O	14:1N:243:LEU:HD12	2.22	0.40
15:1O:21:THR:HA	15:1O:23:LYS:NZ	2.36	0.40
16:1P:34:VAL:O	16:1P:38:LEU:N	2.40	0.40
16:1P:242:VAL:HG12	16:1P:253:PHE:CE1	2.55	0.40
19:1S:15:LEU:CD1	19:1S:50:LEU:HD13	2.51	0.40
20:1U:12:LYS:O	20:1U:16:LEU:HB2	2.21	0.40
21:1V:4:LEU:HD11	21:1V:17:GLU:HA	2.03	0.40
23:1X:76:HIS:CD2	23:1X:113:LYS:HB3	2.56	0.40
32:1g:72:LEU:HD23	32:1g:72:LEU:HA	1.86	0.40
34:1i:43:GLU:HA	34:1i:46:TRP:CE3	2.56	0.40
36:1k:35:LEU:HD21	39:1n:38:TYR:HD1	1.85	0.40
39:1n:40:ALA:HA	39:1n:43:MET:HB3	2.03	0.40
42:1q:48:TYR:N	42:1q:48:TYR:CD1	2.89	0.40
1:1A:88:LEU:O	1:1A:92:LEU:HD23	2.21	0.40
3:1C:51:PHE:N	3:1C:51:PHE:CD1	2.88	0.40
3:1C:64:LEU:HD13	3:1C:70:ALA:HB1	2.02	0.40
3:1C:209:TYR:CD1	43:1r:64:PRO:HD3	2.56	0.40
4:1D:51:PHE:CD2	4:1D:58:ALA:HB2	2.56	0.40
6:1F:196:ILE:HD13	6:1F:196:ILE:HA	1.90	0.40
7:1G:237:ASN:N	7:1G:237:ASN:OD1	2.53	0.40
7:1G:575:ASN:OD1	7:1G:577:GLU:HG2	2.21	0.40
8:1H:31:MET:HG3	9:1I:41:LEU:HB2	2.04	0.40
8:1H:112:ALA:O	8:1H:115:SER:HB3	2.21	0.40
9:1I:78:ILE:O	9:1I:104:ARG:HD3	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1I:203:PC1:H142	45:1I:203:PC1:H111	1.92	0.40
11:1K:95:LEU:HB2	14:1N:54:GLU:OE2	2.21	0.40
12:1L:188:TRP:CG	12:1L:212:PRO:HG3	2.57	0.40
17:1Q:89:LYS:HE2	17:1Q:89:LYS:HB3	1.73	0.40
22:1W:23:ARG:HA	22:1W:23:ARG:HD2	1.86	0.40
22:1W:42:GLU:HG2	22:1W:90:LEU:CD2	2.47	0.40
23:1X:29:HIS:HE1	25:1Z:63:GLU:HG2	1.87	0.40
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	2.02	0.40
26:1a:2:TRP:NE1	52:1r:201:CDL:OB5	2.54	0.40
30:1e:36:GLU:HB3	30:1e:62:PHE:CE1	2.56	0.40
32:1g:33:GLU:OE1	32:1g:33:GLU:N	2.46	0.40
34:1i:47:ASN:HA	34:1i:50:LEU:HB2	2.03	0.40
52:1r:201:CDL:H312	52:1r:201:CDL:OB9	2.21	0.40
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.51	0.40
2:1B:175:ILE:O	2:1B:179:ARG:HG3	2.22	0.40
3:1C:118:GLU:OE2	3:1C:118:GLU:N	2.29	0.40
3:1C:132:ARG:HD2	3:1C:151:ILE:HB	2.04	0.40
4:1D:141:PHE:HZ	4:1D:184:VAL:HG11	1.86	0.40
4:1D:283:PHE:HA	4:1D:309:ARG:HH21	1.86	0.40
5:1E:65:ALA:O	5:1E:69:VAL:HG12	2.21	0.40
5:1E:123:LYS:HG3	5:1E:124:LEU:HD22	2.03	0.40
6:1F:142:PHE:HB3	6:1F:145:GLU:CG	2.51	0.40
7:1G:551:ASP:OD1	7:1G:552:VAL:N	2.50	0.40
9:1I:76:ARG:HB2	9:1I:130:ALA:HA	2.04	0.40
9:1I:168:ASN:N	42:1q:88:ARG:HH12	2.19	0.40
11:1K:59:MET:O	11:1K:63:LEU:N	2.49	0.40
12:1L:60:GLU:HB2	34:1i:99:ARG:HD3	2.04	0.40
12:1L:174:TYR:CD1	12:1L:229:LEU:HB3	2.55	0.40
15:1O:136:GLU:OE2	15:1O:140:ARG:NH2	2.35	0.40
19:1S:39:ARG:NH1	19:1S:84:ASP:HA	2.37	0.40
20:1U:37:MET:HE1	20:1U:42:LEU:C	2.47	0.40
23:1X:34:GLN:HG2	23:1X:116:TRP:CE2	2.56	0.40
27:1b:61:ASN:OD1	27:1b:61:ASN:C	2.64	0.40
30:1e:30:GLY:O	30:1e:32:CYS:N	2.54	0.40
34:1i:44:GLN:HA	34:1i:47:ASN:HD21	1.86	0.40
39:1n:136:VAL:HA	39:1n:139:LEU:HD12	2.02	0.40
3:1C:150:ARG:NH2	3:1C:156:GLY:H	2.20	0.40
4:1D:59:HIS:ND1	4:1D:59:HIS:O	2.55	0.40
4:1D:149:ASN:ND2	4:1D:370:PRO:O	2.55	0.40
5:1E:15:ASN:O	5:1E:63:ILE:HB	2.21	0.40
6:1F:156:ALA:O	6:1F:161:LEU:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:232:PRO:O	6:1F:236:ARG:NE	2.53	0.40
6:1F:424:PRO:HA	6:1F:427:GLU:HB2	2.04	0.40
7:1G:200:ILE:HD13	7:1G:210:SER:HB3	2.03	0.40
7:1G:295:THR:OG1	7:1G:297:GLU:OE1	2.30	0.40
7:1G:321:GLY:HA3	7:1G:496:ILE:HG12	2.04	0.40
7:1G:511:VAL:O	7:1G:515:ARG:HG3	2.21	0.40
7:1G:575:ASN:OD1	7:1G:579:ARG:N	2.51	0.40
45:1H:401:PC1:H141	9:1I:19:ASP:HB3	2.03	0.40
9:1I:78:ILE:HD11	9:1I:80:CYS:HB3	2.02	0.40
9:1I:99:ARG:HB3	9:1I:101:ASP:OD1	2.21	0.40
11:1K:12:PHE:CD1	14:1N:72:MET:HE3	2.56	0.40
12:1L:109:HIS:HD1	12:1L:109:HIS:H	1.69	0.40
12:1L:358:LYS:HD3	12:1L:358:LYS:HA	1.85	0.40
12:1L:486:MET:HE3	12:1L:486:MET:H	1.87	0.40
12:1L:557:TRP:O	12:1L:561:ILE:HG22	2.21	0.40
13:1M:196:TRP:HE3	13:1M:197:LEU:HD23	1.87	0.40
13:1M:200:ILE:HG23	13:1M:204:MET:HG3	2.02	0.40
15:1O:259:LEU:HA	15:1O:259:LEU:HD12	1.82	0.40
16:1P:243:GLN:OE1	16:1P:335:LYS:NZ	2.55	0.40
16:1P:244:TYR:O	16:1P:248:VAL:HG22	2.21	0.40
18:1R:29:SER:C	18:1R:31:ARG:H	2.29	0.40
20:1T:42:LEU:H	20:1T:42:LEU:HD22	1.86	0.40
20:1U:51:ILE:HG23	20:1U:62:ILE:HD12	2.03	0.40
21:1V:39:LYS:HA	21:1V:44:ARG:HD3	2.02	0.40
23:1X:144:ARG:HH22	30:1e:57:ILE:HD13	1.87	0.40
28:1c:41:GLU:HG2	29:1d:19:ARG:HB3	2.04	0.40
31:1f:35:THR:HA	31:1f:56:TRP:HH2	1.85	0.40
33:1h:142:ASP:OD1	33:1h:142:ASP:C	2.64	0.40
34:1i:106:GLY:N	34:1i:116:ILE:HG23	2.36	0.40
37:1l:43:GLY:HA3	38:1m:75:ILE:HG13	2.03	0.40
38:1m:38:ILE:HA	38:1m:41:ARG:HE	1.86	0.40
1:1A:68:GLU:HB3	1:1A:98:LEU:HD21	2.02	0.40
1:1A:72:LEU:O	8:1H:151:LEU:HD11	2.21	0.40
2:1B:30:VAL:HG13	2:1B:174:ARG:NH1	2.36	0.40
2:1B:174:ARG:O	2:1B:178:ARG:HG2	2.22	0.40
3:1C:54:PRO:C	3:1C:56:GLY:H	2.29	0.40
3:1C:137:MET:HE2	3:1C:137:MET:HA	2.04	0.40
4:1D:18:VAL:HB	14:1N:171:ASN:OD1	2.22	0.40
4:1D:95:THR:OG1	4:1D:96:TYR:N	2.55	0.40
5:1E:47:VAL:O	5:1E:51:LEU:HB2	2.21	0.40
6:1F:97:ALA:HB3	6:1F:138:ILE:HA	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:57:VAL:HG12	7:1G:68:ALA:HB2	2.04	0.40
7:1G:197:GLY:O	7:1G:268:ARG:NE	2.54	0.40
7:1G:386:PHE:HE1	7:1G:668:ILE:HD13	1.86	0.40
7:1G:533:THR:HG22	7:1G:536:ASP:OD1	2.22	0.40
8:1H:17:VAL:HG12	8:1H:225:MET:HG2	2.03	0.40
9:1I:54:LYS:HB3	42:1q:91:HIS:CD2	2.56	0.40
10:1J:109:LYS:HD3	10:1J:109:LYS:N	2.37	0.40
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.86	0.40
50:1L:702:3PE:H222	50:1L:702:3PE:O31	2.22	0.40
14:1N:230:LEU:HD23	14:1N:296:LEU:HD12	2.04	0.40
14:1N:232:HIS:HE2	15:1O:278:TYR:HH	1.68	0.40
16:1P:60:ARG:HG2	16:1P:70:PHE:HE1	1.86	0.40
18:1R:23:TYR:CE2	18:1R:24:ARG:HG3	2.56	0.40
20:1T:24:LYS:NZ	20:1T:40:LEU:HB3	2.37	0.40
21:1V:24:LYS:O	21:1V:28:THR:HG23	2.21	0.40
22:1W:43:VAL:N	22:1W:44:PRO:HD2	2.37	0.40
23:1X:61:LEU:HA	23:1X:61:LEU:HD13	1.95	0.40
37:1l:98:TRP:O	37:1l:101:MET:HB2	2.21	0.40
38:1m:22:TYR:HD2	39:1n:64:ARG:HG2	1.86	0.40
38:1m:119:LYS:HD3	38:1m:119:LYS:HA	1.88	0.40
40:1o:50:LEU:HD21	40:1o:59:ALA:HB1	2.03	0.40
40:1o:90:GLU:O	40:1o:94:TYR:HB2	2.22	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	1A	84/115 (73%)	81 (96%)	3 (4%)	0	100	100
2	1B	153/258 (59%)	142 (93%)	11 (7%)	0	100	100
3	1C	207/264 (78%)	191 (92%)	16 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	1D	427/476 (90%)	396 (93%)	31 (7%)	0	100	100
5	1E	212/249 (85%)	184 (87%)	28 (13%)	0	100	100
6	1F	430/464 (93%)	392 (91%)	37 (9%)	1 (0%)	43	72
7	1G	697/727 (96%)	637 (91%)	59 (8%)	1 (0%)	48	79
8	1H	316/318 (99%)	298 (94%)	15 (5%)	3 (1%)	14	46
9	1I	174/239 (73%)	159 (91%)	14 (8%)	1 (1%)	21	54
10	1J	173/175 (99%)	159 (92%)	12 (7%)	2 (1%)	10	41
11	1K	96/98 (98%)	87 (91%)	8 (8%)	1 (1%)	12	45
12	1L	604/606 (100%)	556 (92%)	47 (8%)	1 (0%)	43	72
13	1M	457/459 (100%)	444 (97%)	12 (3%)	1 (0%)	43	72
14	1N	345/347 (99%)	325 (94%)	20 (6%)	0	100	100
15	1O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	311 (92%)	29 (8%)	0	100	100
17	1Q	127/175 (73%)	113 (89%)	13 (10%)	1 (1%)	16	49
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
20	1U	84/156 (54%)	74 (88%)	10 (12%)	0	100	100
21	1V	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	4 (4%)	1 (1%)	14	46
23	1X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	128 (92%)	11 (8%)	0	100	100
26	1a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
28	1c	47/76 (62%)	45 (96%)	1 (2%)	1 (2%)	5	31
29	1d	117/123 (95%)	109 (93%)	6 (5%)	2 (2%)	7	35
30	1e	97/106 (92%)	89 (92%)	8 (8%)	0	100	100
31	1f	55/135 (41%)	48 (87%)	7 (13%)	0	100	100
32	1g	98/154 (64%)	91 (93%)	6 (6%)	1 (1%)	12	45
33	1h	136/189 (72%)	130 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	1i	124/128 (97%)	119 (96%)	5 (4%)	0	100	100
35	1j	69/105 (66%)	68 (99%)	1 (1%)	0	100	100
36	1k	79/98 (81%)	72 (91%)	7 (9%)	0	100	100
37	1l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100
38	1m	126/129 (98%)	117 (93%)	9 (7%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100
40	1o	120/137 (88%)	115 (96%)	5 (4%)	0	100	100
41	1p	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	11 (8%)	1 (1%)	18	51
43	1r	90/114 (79%)	83 (92%)	7 (8%)	0	100	100
44	1s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
All	All	8165/9744 (84%)	7582 (93%)	565 (7%)	18 (0%)	44	72

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	92	PRO
9	1I	162	GLU
10	1J	85	SER
12	1L	464	ALA
13	1M	207	MET
29	1d	3	SER
29	1d	53	VAL
42	1q	142	THR
6	1F	249	ARG
8	1H	208	VAL
10	1J	116	ILE
28	1c	2	PHE
11	1K	22	TYR
7	1G	696	GLN
8	1H	200	LEU
17	1Q	70	MET
22	1W	96	VAL
32	1g	24	ILE

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	1A	76/99 (77%)	76 (100%)	0	100	100
2	1B	131/212 (62%)	131 (100%)	0	100	100
3	1C	190/227 (84%)	188 (99%)	2 (1%)	65	74
4	1D	371/405 (92%)	369 (100%)	2 (0%)	81	80
5	1E	183/207 (88%)	179 (98%)	4 (2%)	45	65
6	1F	346/368 (94%)	346 (100%)	0	100	100
7	1G	588/610 (96%)	585 (100%)	3 (0%)	81	80
8	1H	274/274 (100%)	270 (98%)	4 (2%)	57	70
9	1I	151/201 (75%)	150 (99%)	1 (1%)	76	78
10	1J	140/140 (100%)	140 (100%)	0	100	100
11	1K	84/84 (100%)	83 (99%)	1 (1%)	63	73
12	1L	539/539 (100%)	532 (99%)	7 (1%)	61	72
13	1M	408/408 (100%)	405 (99%)	3 (1%)	76	78
14	1N	310/310 (100%)	308 (99%)	2 (1%)	78	79
15	1O	283/307 (92%)	283 (100%)	0	100	100
16	1P	296/323 (92%)	296 (100%)	0	100	100
17	1Q	117/152 (77%)	114 (97%)	3 (3%)	40	62
18	1R	79/97 (81%)	79 (100%)	0	100	100
19	1S	77/82 (94%)	77 (100%)	0	100	100
20	1T	79/133 (59%)	76 (96%)	3 (4%)	29	55
20	1U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	98 (98%)	2 (2%)	48	66
22	1W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	152 (99%)	1 (1%)	76	78
24	1Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	122 (99%)	1 (1%)	73	77

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
26	1a	58/58 (100%)	58 (100%)	0	100 100
27	1b	69/70 (99%)	68 (99%)	1 (1%)	59 71
28	1c	45/66 (68%)	44 (98%)	1 (2%)	45 65
29	1d	107/109 (98%)	107 (100%)	0	100 100
30	1e	87/94 (93%)	86 (99%)	1 (1%)	65 74
31	1f	54/113 (48%)	54 (100%)	0	100 100
32	1g	92/129 (71%)	92 (100%)	0	100 100
33	1h	121/158 (77%)	121 (100%)	0	100 100
34	1i	119/120 (99%)	119 (100%)	0	100 100
35	1j	62/84 (74%)	62 (100%)	0	100 100
36	1k	63/76 (83%)	63 (100%)	0	100 100
37	1l	141/161 (88%)	139 (99%)	2 (1%)	59 71
38	1m	113/114 (99%)	113 (100%)	0	100 100
39	1n	156/160 (98%)	156 (100%)	0	100 100
40	1o	110/120 (92%)	110 (100%)	0	100 100
41	1p	154/156 (99%)	152 (99%)	2 (1%)	61 72
42	1q	131/131 (100%)	131 (100%)	0	100 100
43	1r	85/98 (87%)	84 (99%)	1 (1%)	63 73
44	1s	44/351 (12%)	44 (100%)	0	100 100
All	All	7196/8272 (87%)	7149 (99%)	47 (1%)	73 78

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	1C	50	ILE
3	1C	129	TRP
4	1D	178	PHE
4	1D	222	ILE
5	1E	60	TRP
5	1E	74	GLN
5	1E	159	ASN
5	1E	203	THR
7	1G	315	VAL
7	1G	532	ILE
7	1G	662	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1H	129	LEU
8	1H	133	LEU
8	1H	146	LEU
8	1H	283	ASP
9	1I	50	TYR
11	1K	81	VAL
12	1L	229	LEU
12	1L	261	ILE
12	1L	295	GLN
12	1L	338	MET
12	1L	409	LEU
12	1L	576	MET
12	1L	597	ILE
13	1M	139	GLN
13	1M	207	MET
13	1M	222	GLU
14	1N	108	LEU
14	1N	176	ARG
17	1Q	82	LEU
17	1Q	101	TRP
17	1Q	110	VAL
20	1T	52	MET
20	1T	62	ILE
20	1T	86	VAL
21	1V	54	LYS
21	1V	93	MET
23	1X	43	MET
25	1Z	120	MET
27	1b	83	LEU
28	1c	16	LYS
30	1e	36	GLU
37	1l	82	ASP
37	1l	83	MET
41	1p	53	GLN
41	1p	63	TYR
43	1r	2	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	10	ASN
1	1A	83	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	1B	121	ASN
2	1B	162	GLN
3	1C	39	GLN
3	1C	88	ASN
3	1C	160	HIS
4	1D	266	GLN
4	1D	273	GLN
4	1D	316	ASN
5	1E	9	HIS
5	1E	55	GLN
5	1E	91	ASN
5	1E	159	ASN
6	1F	116	HIS
6	1F	148	ASN
6	1F	150	GLN
6	1F	293	ASN
6	1F	373	ASN
7	1G	117	GLN
7	1G	313	ASN
7	1G	383	ASN
7	1G	475	GLN
7	1G	491	ASN
7	1G	546	GLN
8	1H	212	ASN
8	1H	247	HIS
8	1H	304	HIS
9	1I	49	ASN
11	1K	50	ASN
12	1L	30	ASN
12	1L	139	GLN
12	1L	194	ASN
12	1L	295	GLN
12	1L	506	ASN
12	1L	580	GLN
13	1M	48	ASN
13	1M	83	HIS
14	1N	83	GLN
14	1N	174	GLN
15	1O	72	GLN
15	1O	107	GLN
16	1P	67	GLN
16	1P	131	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	1P	216	ASN
16	1P	234	ASN
16	1P	341	ASN
17	1Q	44	ASN
20	1U	74	GLN
21	1V	52	ASN
21	1V	110	GLN
22	1W	102	HIS
24	1Y	128	GLN
24	1Y	133	GLN
26	1a	27	HIS
27	1b	10	ASN
29	1d	46	ASN
30	1e	6	GLN
30	1e	24	GLN
32	1g	86	GLN
32	1g	103	ASN
33	1h	124	GLN
33	1h	135	HIS
34	1i	88	HIS
34	1i	127	HIS
36	1k	59	ASN
37	1l	55	GLN
40	1o	43	GLN
41	1p	53	GLN
41	1p	103	ASN
41	1p	133	GLN
42	1q	17	HIS
42	1q	46	ASN
42	1q	87	HIS
42	1q	116	ASN
42	1q	123	GLN
44	1s	40	ASN
44	1s	42	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	FME	1H	1	8	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
10	FME	1J	1	10	8,9,10	0.56	0	8,9,11	0.93	1 (12%)
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
1	FME	1A	1	1	8,9,10	0.55	0	8,9,11	1.00	1 (12%)
34	SAC	1i	1	-	7,8,9	0.57	0	7,9,11	1.15	1 (14%)
14	FME	1N	1	14	8,9,10	0.54	0	8,9,11	0.94	1 (12%)
12	FME	1L	1	12	8,9,10	0.54	0	8,9,11	0.93	1 (12%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	1.08	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	1H	1	8	-	1/7/9/11	-
10	FME	1J	1	10	-	2/7/9/11	-
13	FME	1M	1	13	-	2/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
14	FME	1N	1	14	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	1i	1	SAC	O-C-CA	-2.97	117.14	124.77
1	1A	1	FME	O-C-CA	-2.58	118.13	124.77
10	1J	1	FME	O-C-CA	-2.57	118.15	124.77
11	1K	1	FME	O-C-CA	-2.56	118.19	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	1M	1	FME	O-C-CA	-2.54	118.25	124.77
8	1H	1	FME	O-C-CA	-2.53	118.25	124.77
12	1L	1	FME	O-C-CA	-2.43	118.53	124.77
14	1N	1	FME	O-C-CA	-2.36	118.70	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O-C-CA-CB
10	1J	1	FME	O-C-CA-CB
13	1M	1	FME	O1-CN-N-CA
11	1K	1	FME	C-CA-CB-CG
10	1J	1	FME	N-CA-CB-CG
1	1A	1	FME	CB-CG-SD-CE
13	1M	1	FME	C-CA-CB-CG

There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	1H	1	FME	1	0
10	1J	1	FME	1	0
13	1M	1	FME	1	0
1	1A	1	FME	2	0
14	1N	1	FME	2	0
11	1K	1	FME	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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	$\#\|Z\| > 2$
53	GTP	1O	401	54	33,34,34	0.59	0	50,54,54	0.61	0
58	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.29	0
50	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.41	0
57	EHZ	1W	201	-	31,36,37	0.20	0	36,44,47	1.30	1 (2%)
45	PC1	1g	201	-	43,43,53	0.30	0	49,51,61	0.37	0
45	PC1	1A	201	-	34,34,53	0.32	0	40,42,61	0.41	0
50	3PE	1b	101	-	46,46,50	0.28	0	49,51,55	0.35	0
50	3PE	1Y	201	-	30,30,50	0.34	0	33,35,55	0.65	1 (3%)
46	SF4	1I	201	9	0,12,12	-	-	-		
50	3PE	1L	701	-	45,45,50	0.29	0	48,50,55	0.32	0
46	SF4	1G	802	7	0,12,12	-	-	-		
57	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.37	1 (2%)
46	SF4	1I	202	9	0,12,12	-	-	-		
50	3PE	1Y	202	-	50,50,50	0.27	0	53,55,55	0.40	0
47	FES	1E	301	5	0,4,4	-	-	-		
46	SF4	1G	801	7	0,12,12	-	-	-		
45	PC1	1I	203	-	53,53,53	0.27	0	59,61,61	0.30	0
52	CDL	1N	402	-	76,76,99	0.30	0	82,88,111	0.37	0
46	SF4	1F	502	6	0,12,12	-	-	-		
45	PC1	1H	401	-	43,43,53	0.29	0	49,51,61	0.33	0
51	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.50	0
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.66	1 (2%)
47	FES	1G	803	7	0,4,4	-	-	-		
50	3PE	1L	702	-	41,41,50	0.31	0	44,46,55	1.25	5 (11%)
45	PC1	1M	502	-	45,45,53	0.28	0	51,53,61	0.34	0
55	NDP	1P	501	-	51,52,52	0.52	0	71,80,80	0.80	2 (2%)
46	SF4	1B	201	2	0,12,12	-	-	-		
52	CDL	1r	201	-	60,60,99	0.33	0	66,72,111	0.41	0

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
53	GTP	1O	401	54	-	1/22/38/38	0/3/3/3
58	MYR	1l	201	-	-	0/12/12/13	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	3PE	1N	401	-	-	10/54/54/54	-
57	EHZ	1W	201	-	-	4/42/44/45	-
45	PC1	1g	201	-	-	5/47/47/57	-
45	PC1	1A	201	-	-	5/38/38/57	-
50	3PE	1b	101	-	-	4/50/50/54	-
50	3PE	1Y	201	-	-	5/34/34/54	-
57	EHZ	1n	201	-	-	3/42/44/45	-
50	3PE	1L	701	-	-	8/49/49/54	-
46	SF4	1G	802	7	-	-	0/6/5/5
46	SF4	1I	201	9	-	-	0/6/5/5
46	SF4	1I	202	9	-	-	0/6/5/5
50	3PE	1Y	202	-	-	8/54/54/54	-
47	FES	1E	301	5	-	-	0/1/1/1
46	SF4	1G	801	7	-	-	0/6/5/5
45	PC1	1I	203	-	-	3/57/57/57	-
52	CDL	1N	402	-	-	6/87/87/110	-
46	SF4	1F	502	6	-	-	0/6/5/5
45	PC1	1H	401	-	-	7/47/47/57	-
51	PGT	1M	501	-	-	23/55/55/55	-
48	FMN	1F	501	-	-	4/18/18/18	0/3/3/3
47	FES	1G	803	7	-	-	0/1/1/1
50	3PE	1L	702	-	-	6/45/45/54	-
45	PC1	1M	502	-	-	5/49/49/57	-
55	NDP	1P	501	-	-	4/34/77/77	0/5/5/5
46	SF4	1B	201	2	-	-	0/6/5/5
52	CDL	1r	201	-	-	9/71/71/110	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
57	1n	201	EHZ	C10-S1-C9	7.70	124.62	101.84
57	1W	201	EHZ	C10-S1-C9	7.10	122.83	101.84
50	1L	702	3PE	O21-C21-C22	6.06	124.60	111.48
55	1P	501	NDP	P2B-O2B-C2B	-4.53	111.32	123.43
50	1L	702	3PE	O21-C21-O22	-2.71	117.38	123.70
50	1L	702	3PE	C2-O21-C21	2.55	123.90	117.80
55	1P	501	NDP	O4D-C1D-C2D	-2.54	101.19	106.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	1Y	201	3PE	O21-C21-C22	2.47	116.82	111.48
50	1L	702	3PE	O21-C2-C3	2.27	116.48	108.34
50	1L	702	3PE	O21-C2-C1	2.15	116.05	108.34
48	1F	501	FMN	C4-N3-C2	-2.10	121.91	125.64

There are no chirality outliers.

All (120) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1A	201	PC1	C1-O11-P-O13
45	1H	401	PC1	C11-O13-P-O12
45	1H	401	PC1	C11-O13-P-O11
45	1I	203	PC1	C1-O11-P-O14
45	1M	502	PC1	O32-C31-O31-C3
45	1M	502	PC1	C32-C31-O31-C3
45	1g	201	PC1	C1-O11-P-O14
48	1F	501	FMN	C1'-C2'-C3'-C4'
50	1L	701	3PE	C1-O11-P-O12
50	1L	702	3PE	O22-C21-O21-C2
50	1L	702	3PE	C22-C21-O21-C2
50	1Y	201	3PE	C1-O11-P-O14
50	1Y	201	3PE	O32-C31-O31-C3
50	1Y	201	3PE	C32-C31-O31-C3
50	1Y	201	3PE	O22-C21-O21-C2
50	1Y	201	3PE	C22-C21-O21-C2
50	1Y	202	3PE	C1-O11-P-O14
50	1Y	202	3PE	C2-C1-O11-P
51	1M	501	PGT	O31-C31-O2-C2
51	1M	501	PGT	C1-O3P-P-O1P
51	1M	501	PGT	C1-O3P-P-O4P
51	1M	501	PGT	C4-O4P-P-O3P
51	1M	501	PGT	C4-O4P-P-O1P
52	1r	201	CDL	CA3-OA5-PA1-OA3
52	1r	201	CDL	CB2-OB2-PB2-OB3
52	1r	201	CDL	CB3-OB5-PB2-OB3
52	1r	201	CDL	CB4-CB3-OB5-PB2
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
51	1M	501	PGT	O11-C11-O3-C3
51	1M	501	PGT	C12-C11-O3-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	1M	501	PGT	C32-C31-O2-C2
57	1W	201	EHZ	C13-C12-N1-C11
57	1W	201	EHZ	O3-C12-N1-C11
55	1P	501	NDP	C2D-C1D-N1N-C2N
55	1P	501	NDP	C2D-C1D-N1N-C6N
45	1H	401	PC1	C31-C32-C33-C34
51	1M	501	PGT	C14-C15-C16-C17
51	1M	501	PGT	C40-C41-C42-C43
51	1M	501	PGT	C5-C4-O4P-P
51	1M	501	PGT	C15-C16-C17-C18
45	1I	203	PC1	C24-C25-C26-C27
51	1M	501	PGT	C34-C35-C36-C37
50	1Y	202	3PE	C3C-C3D-C3E-C3F
48	1F	501	FMN	O2'-C2'-C3'-C4'
51	1M	501	PGT	C21-C22-C23-C24
50	1L	702	3PE	O11-C1-C2-O21
50	1L	701	3PE	C38-C39-C3A-C3B
50	1b	101	3PE	O21-C2-C3-O31
52	1N	402	CDL	OA6-CA4-CA6-OA8
52	1r	201	CDL	CA4-CA3-OA5-PA1
50	1N	401	3PE	O31-C31-C32-C33
52	1N	402	CDL	CA3-CA4-CA6-OA8
50	1Y	202	3PE	O11-C1-C2-O21
52	1N	402	CDL	C76-C77-C78-C79
51	1M	501	PGT	C22-C23-C24-C25
50	1Y	202	3PE	C35-C36-C37-C38
51	1M	501	PGT	C33-C34-C35-C36
45	1I	203	PC1	O31-C31-C32-C33
51	1M	501	PGT	C45-C46-C47-C48
50	1N	401	3PE	C34-C35-C36-C37
50	1b	101	3PE	C1-C2-C3-O31
50	1N	401	3PE	C2-C3-O31-C31
50	1Y	202	3PE	C12-C11-O13-P
50	1b	101	3PE	C12-C11-O13-P
52	1r	201	CDL	OB6-CB4-CB6-OB8
45	1M	502	PC1	C2-C1-O11-P
45	1A	201	PC1	O13-C11-C12-N
55	1P	501	NDP	O4D-C1D-N1N-C2N
55	1P	501	NDP	O4D-C1D-N1N-C6N
48	1F	501	FMN	O2'-C2'-C3'-O3'
50	1L	702	3PE	C1-C2-C3-O31
51	1M	501	PGT	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	1A	201	PC1	C1-O11-P-O14
45	1H	401	PC1	C11-O13-P-O14
45	1M	502	PC1	C11-O13-P-O14
45	1g	201	PC1	C1-O11-P-O13
50	1L	701	3PE	C1-O11-P-O13
50	1L	701	3PE	C1-O11-P-O14
50	1N	401	3PE	C1-O11-P-O14
50	1N	401	3PE	C2-C1-O11-P
51	1M	501	PGT	C4-C5-C6-O6
50	1b	101	3PE	C33-C34-C35-C36
50	1L	701	3PE	C36-C37-C38-C39
50	1N	401	3PE	O21-C2-C3-O31
52	1r	201	CDL	C52-C51-CB5-OB6
50	1N	401	3PE	C39-C3A-C3B-C3C
51	1M	501	PGT	C2-C1-O3P-P
50	1L	702	3PE	C1-C2-O21-C21
52	1N	402	CDL	C55-C56-C57-C58
50	1N	401	3PE	O11-C1-C2-O21
50	1N	401	3PE	C3A-C3B-C3C-C3D
50	1Y	202	3PE	O11-C1-C2-C3
52	1r	201	CDL	CB3-CB4-CB6-OB8
45	1g	201	PC1	O11-C1-C2-C3
51	1M	501	PGT	C39-C40-C41-C42
45	1M	502	PC1	C35-C36-C37-C38
52	1N	402	CDL	C53-C54-C55-C56
51	1M	501	PGT	C41-C42-C43-C44
50	1L	701	3PE	C39-C3A-C3B-C3C
45	1g	201	PC1	O31-C31-C32-C33
52	1r	201	CDL	C12-C13-C14-C15
50	1L	701	3PE	O31-C31-C32-C33
45	1A	201	PC1	O21-C2-C3-O31
45	1H	401	PC1	O21-C2-C3-O31
45	1H	401	PC1	C22-C23-C24-C25
50	1L	702	3PE	C32-C33-C34-C35
50	1Y	202	3PE	C3F-C3G-C3H-C3I
45	1H	401	PC1	C32-C33-C34-C35
45	1A	201	PC1	C2-C1-O11-P
53	1O	401	GTP	C4'-C5'-O5'-PA
50	1N	401	3PE	O32-C31-C32-C33
52	1N	402	CDL	C37-C38-C39-C40
48	1F	501	FMN	O3'-C3'-C4'-C5'
45	1g	201	PC1	O32-C31-C32-C33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
50	1L	701	3PE	C2B-C2C-C2D-C2E
57	1n	201	EHZ	C1-C21-C22-C23
51	1M	501	PGT	C16-C17-C18-C19

There are no ring outliers.

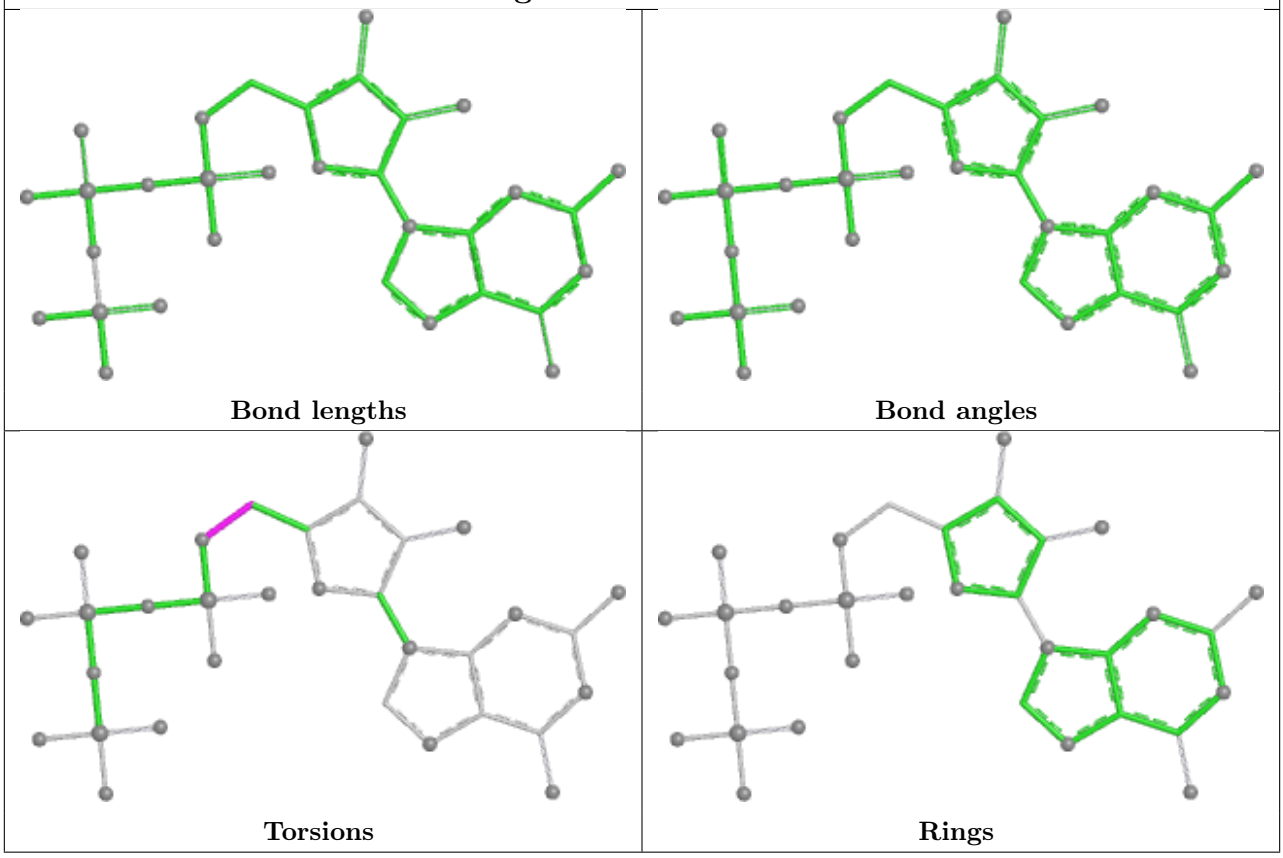
23 monomers are involved in 71 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1O	401	GTP	1	0
58	1l	201	MYR	1	0
50	1N	401	3PE	9	0
57	1W	201	EHZ	1	0
45	1A	201	PC1	2	0
50	1b	101	3PE	1	0
50	1Y	201	3PE	4	0
50	1L	701	3PE	3	0
57	1n	201	EHZ	2	0
46	1I	202	SF4	2	0
47	1E	301	FES	3	0
46	1G	801	SF4	1	0
45	1I	203	PC1	4	0
52	1N	402	CDL	4	0
46	1F	502	SF4	2	0
45	1H	401	PC1	5	0
51	1M	501	PGT	9	0
48	1F	501	FMN	2	0
50	1L	702	3PE	2	0
45	1M	502	PC1	3	0
55	1P	501	NDP	5	0
46	1B	201	SF4	2	0
52	1r	201	CDL	4	0

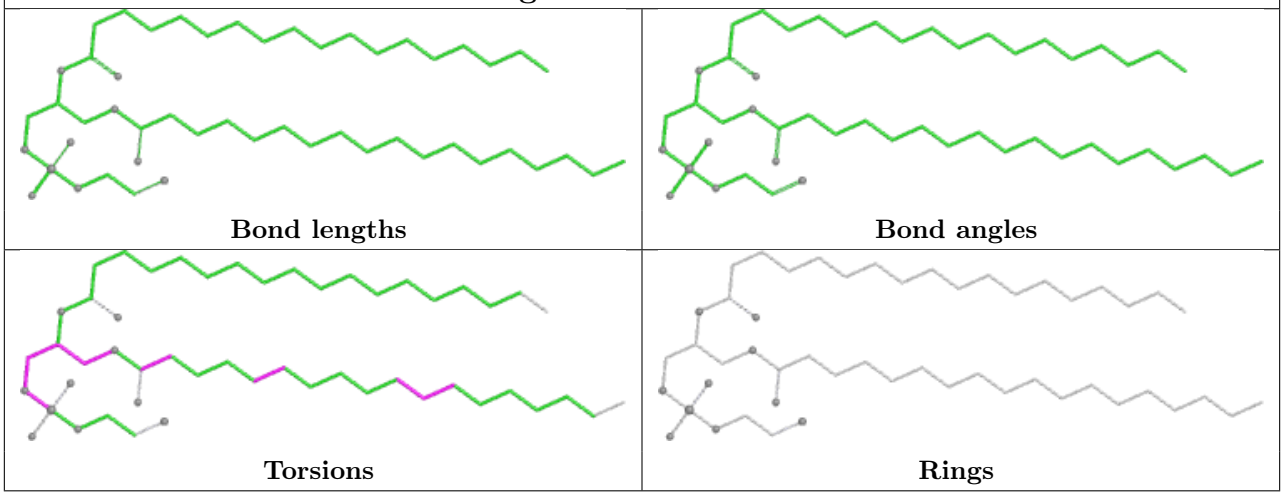
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

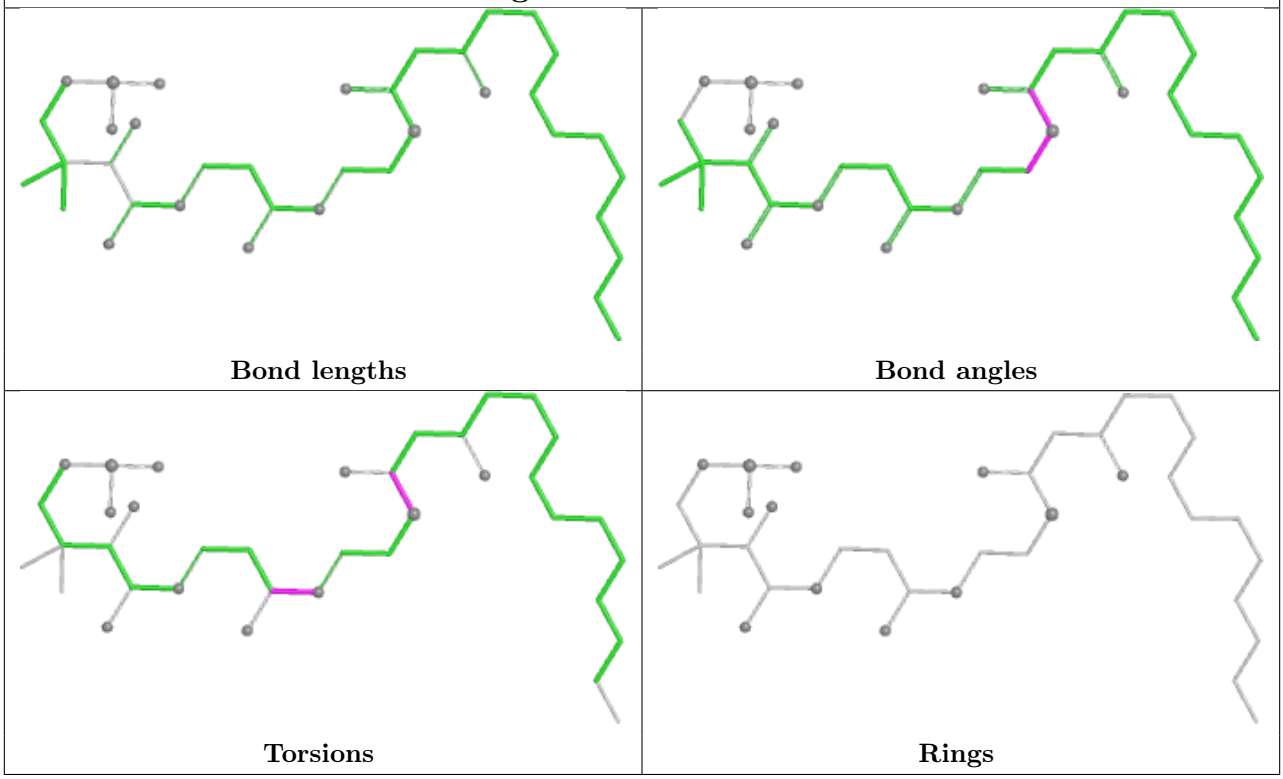
Ligand GTP 1O 401



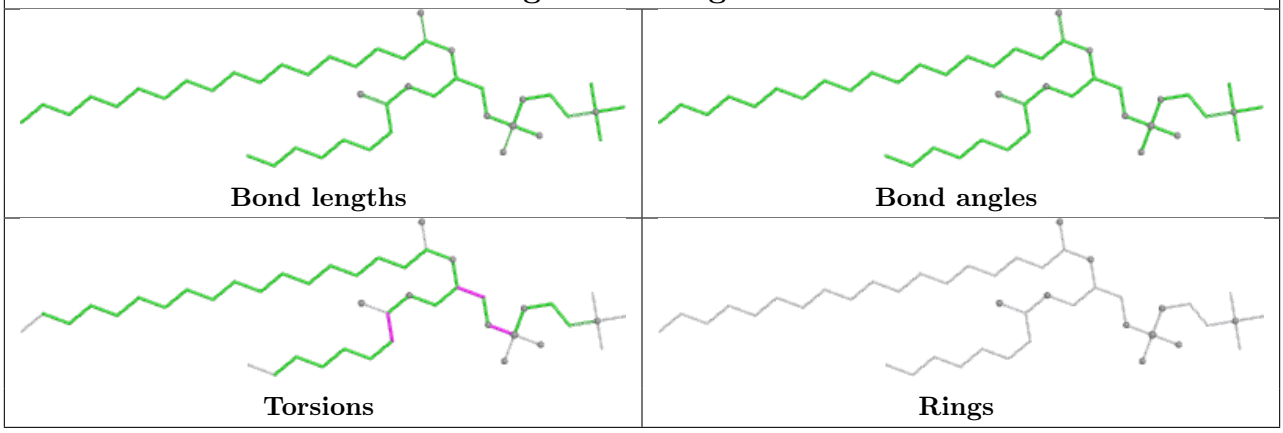
Ligand 3PE 1N 401



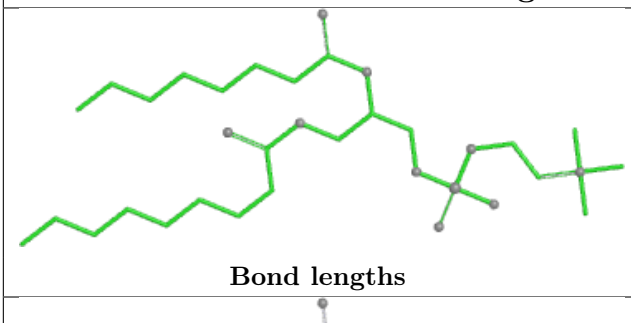
Ligand EHZ 1W 201



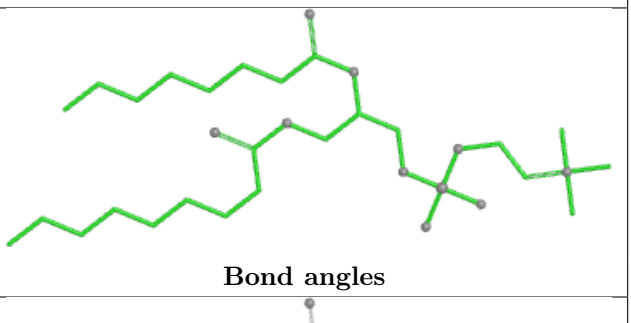
Ligand PC1 1g 201



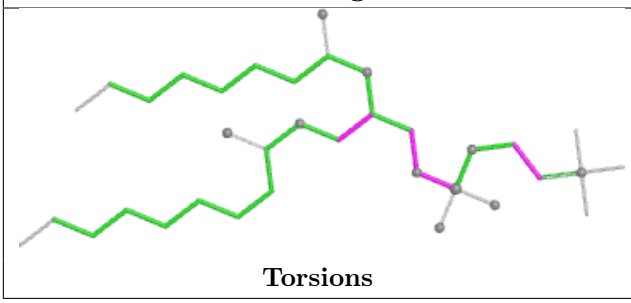
Ligand PC1 1A 201



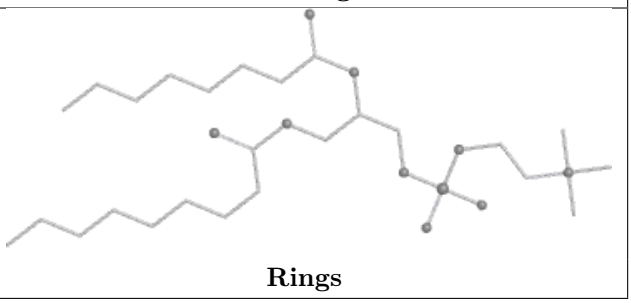
Bond lengths



Bond angles

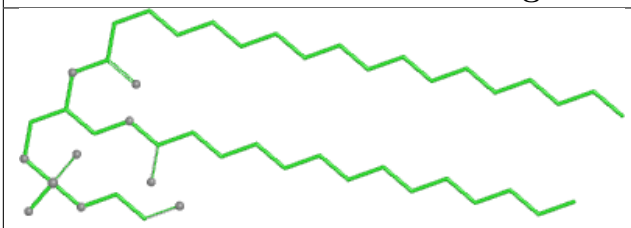


Torsions

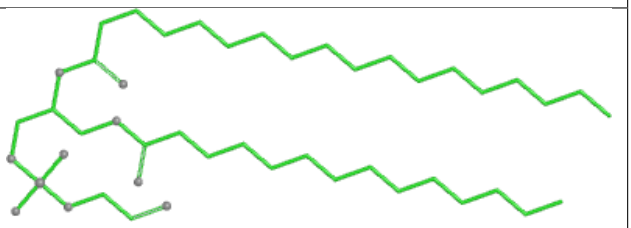


Rings

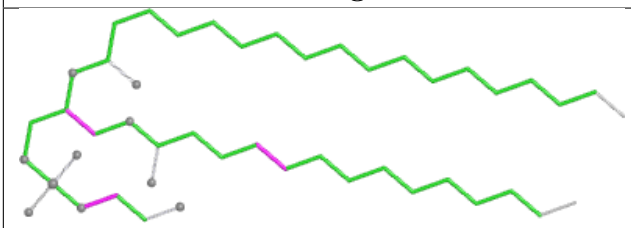
Ligand 3PE 1b 101



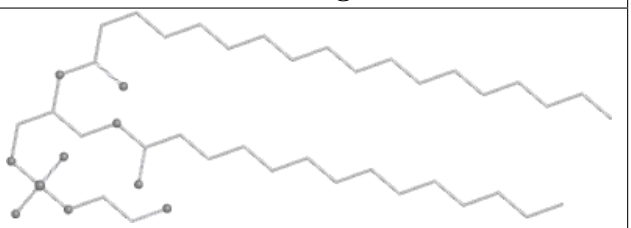
Bond lengths



Bond angles

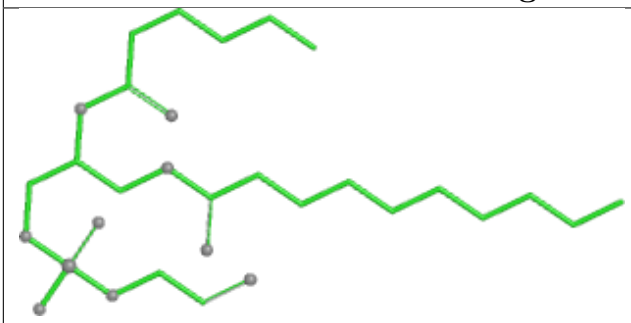


Torsions

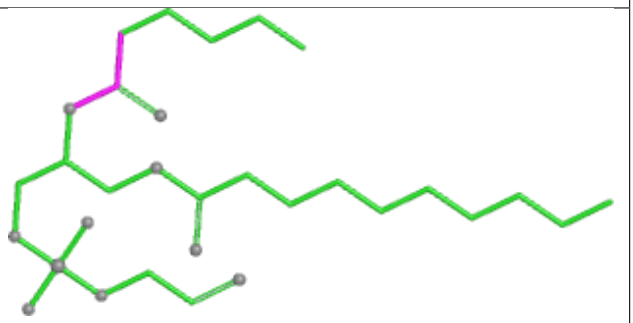


Rings

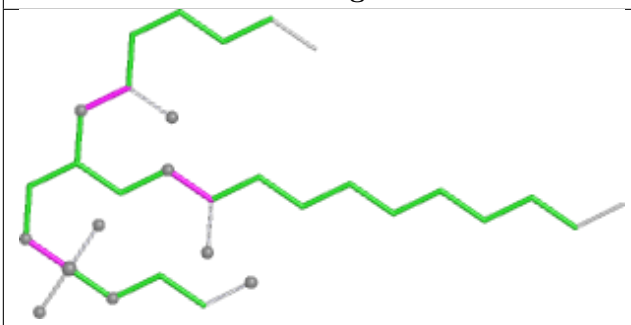
Ligand 3PE 1Y 201



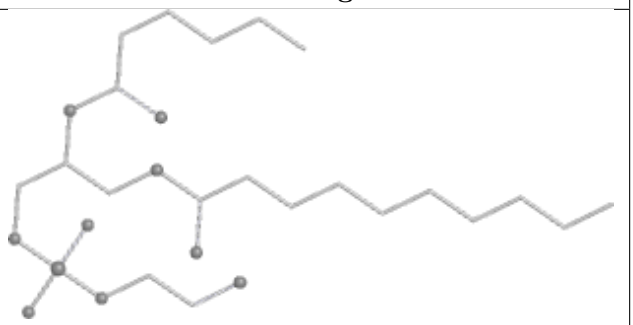
Bond lengths



Bond angles

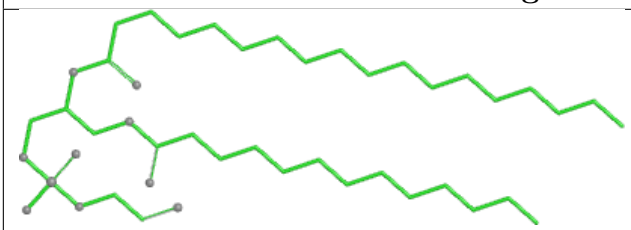


Torsions

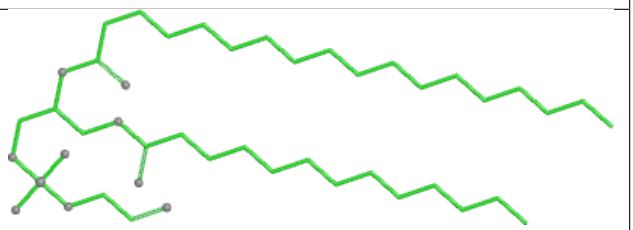


Rings

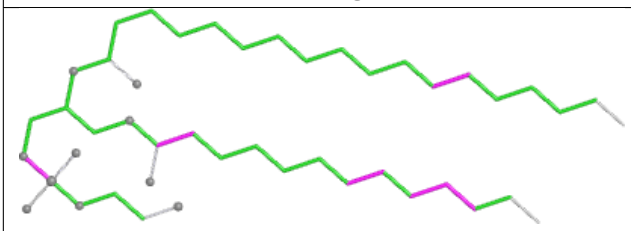
Ligand 3PE 1L 701



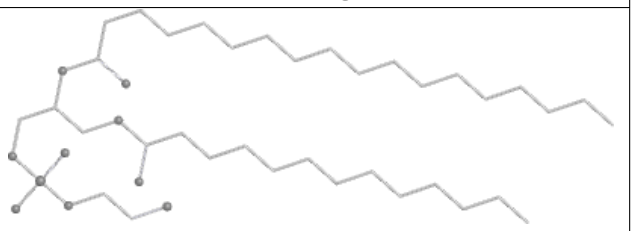
Bond lengths



Bond angles

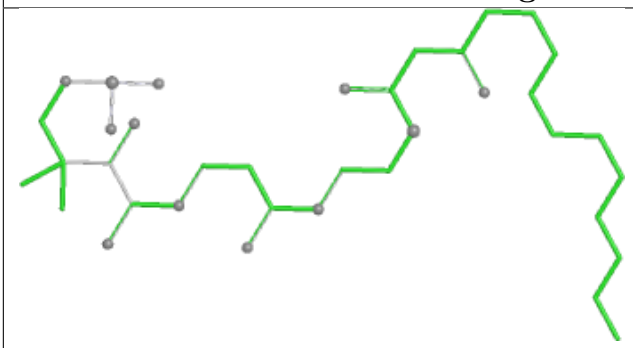


Torsions

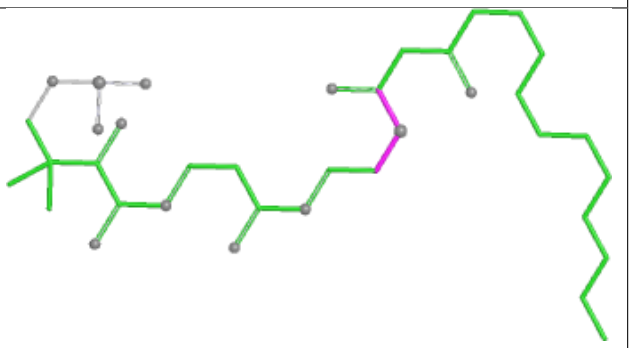


Rings

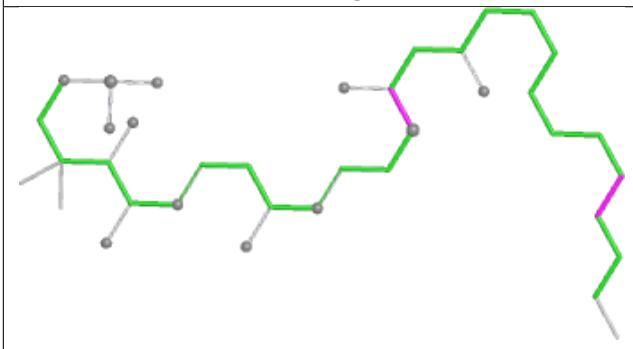
Ligand EHZ 1n 201



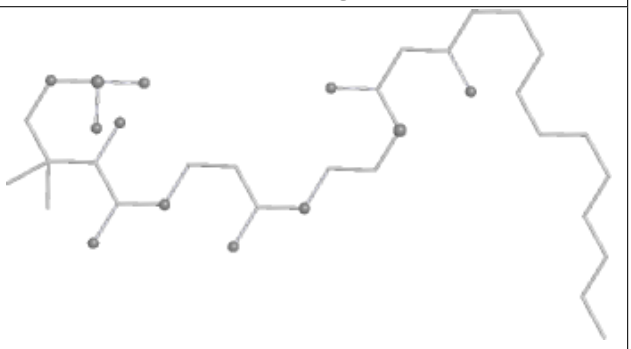
Bond lengths



Bond angles

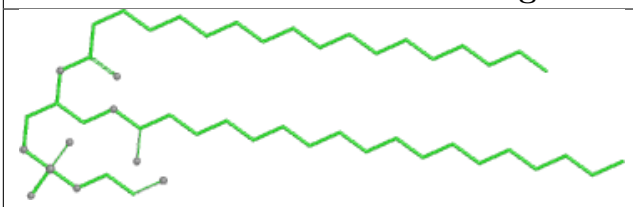


Torsions

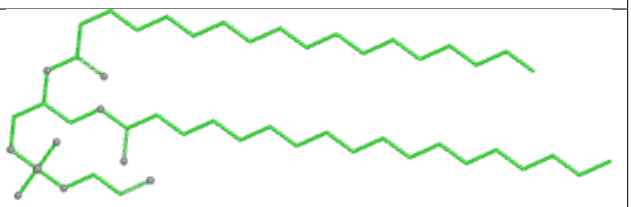


Rings

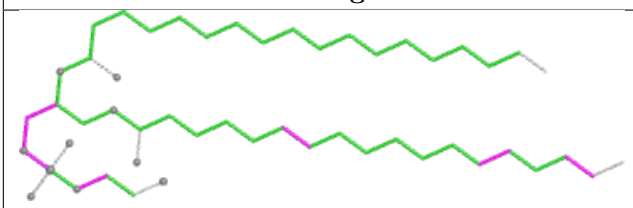
Ligand 3PE 1Y 202



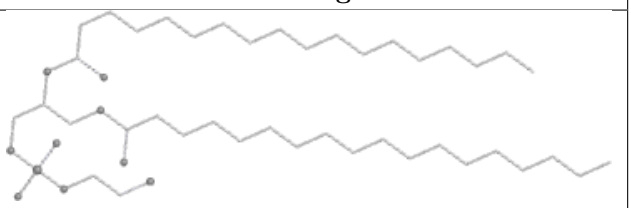
Bond lengths



Bond angles

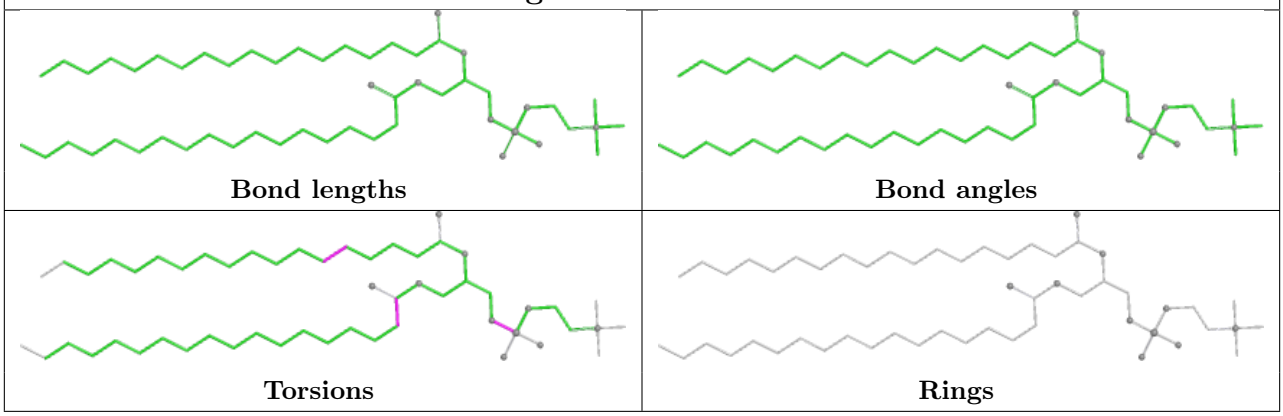


Torsions

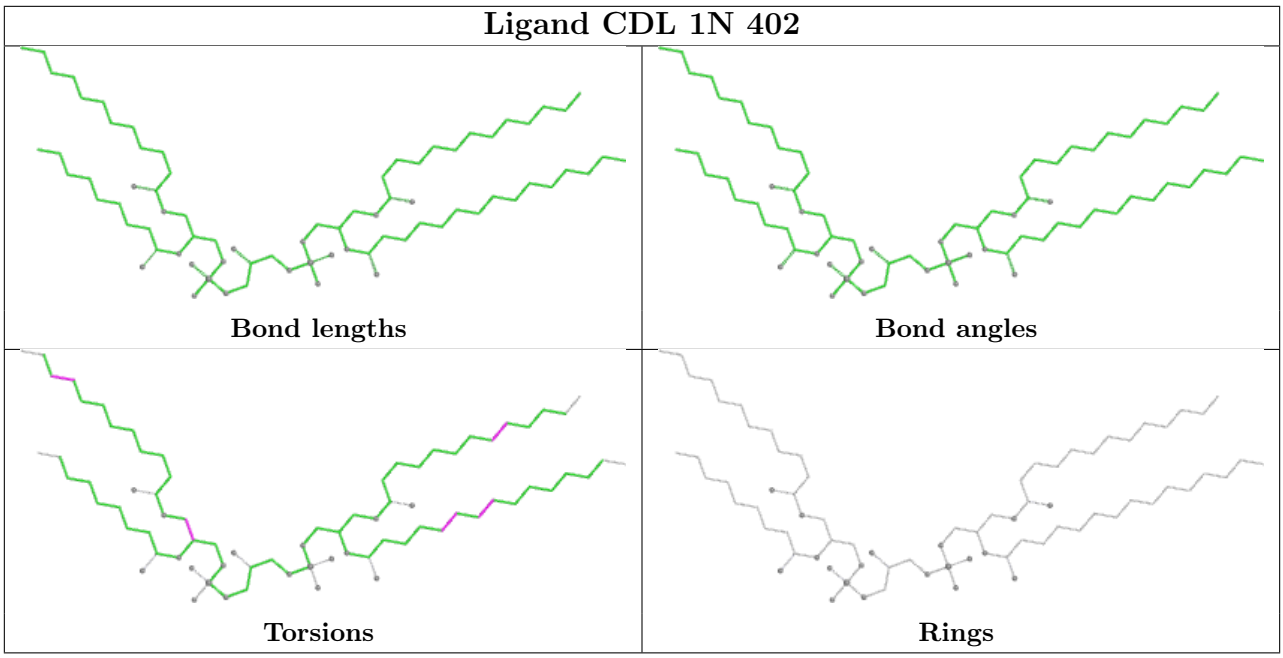


Rings

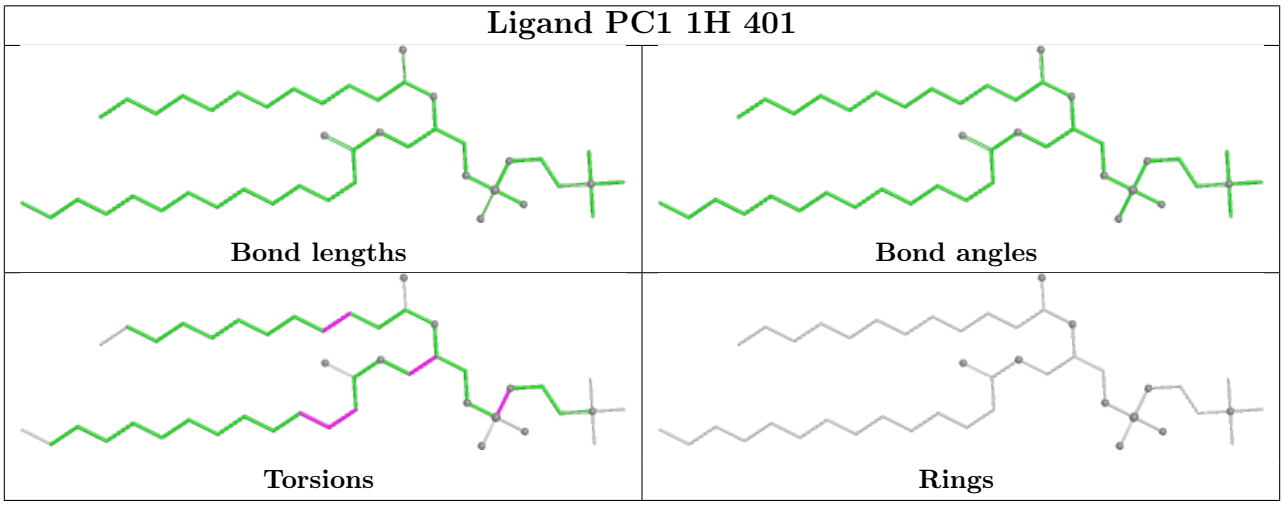
Ligand PC1 1I 203



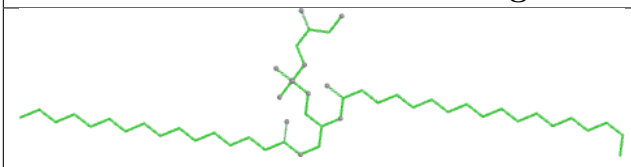
Ligand CDL 1N 402



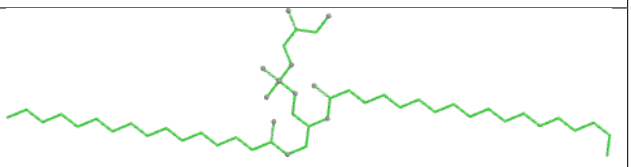
Ligand PC1 1H 401



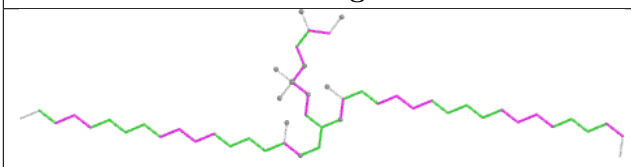
Ligand PGT 1M 501



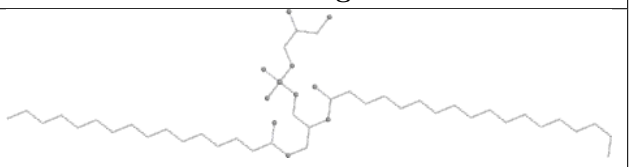
Bond lengths



Bond angles

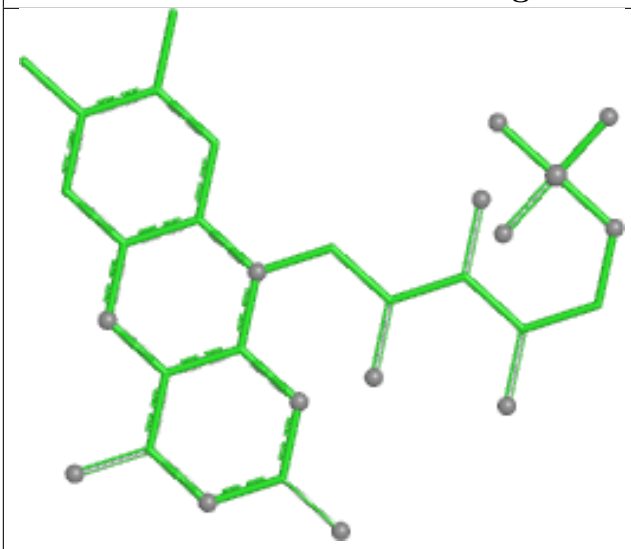


Torsions

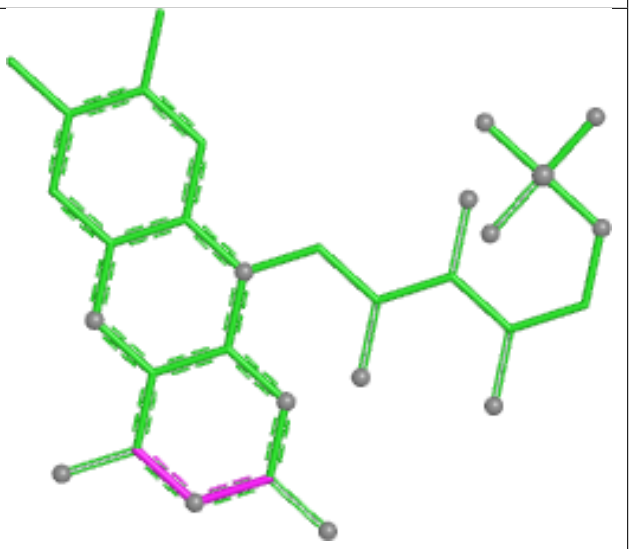


Rings

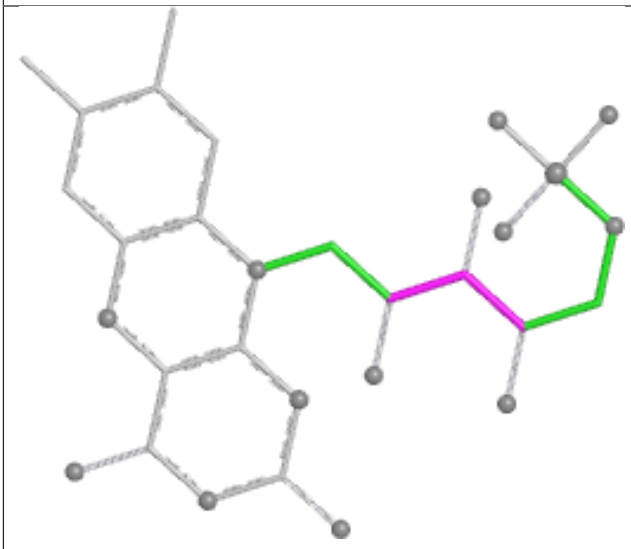
Ligand FMN 1F 501



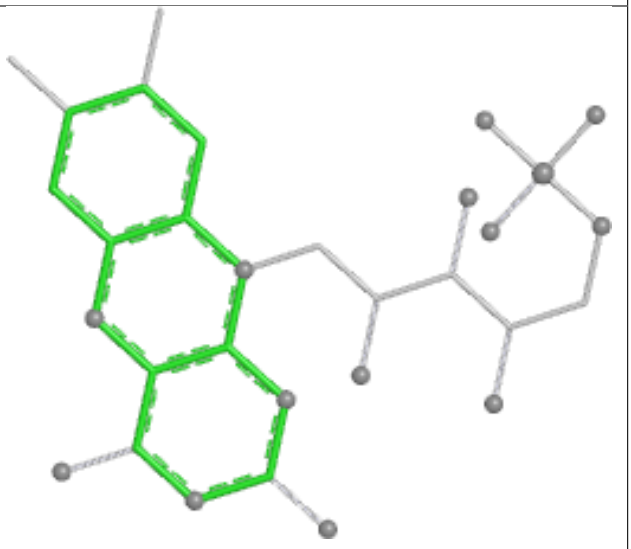
Bond lengths



Bond angles

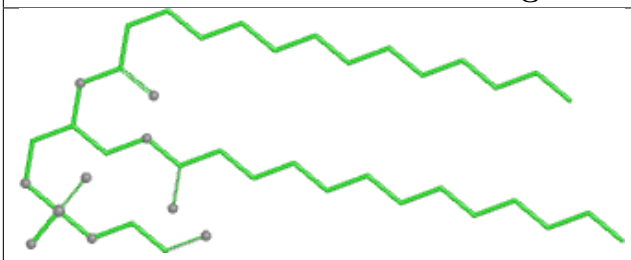


Torsions

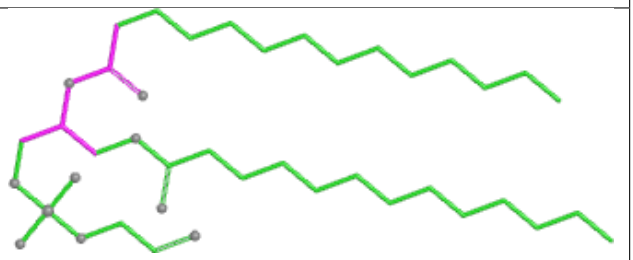


Rings

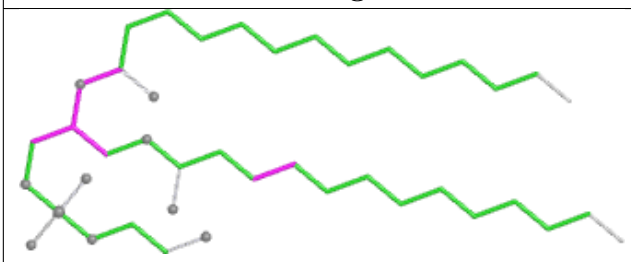
Ligand 3PE 1L 702



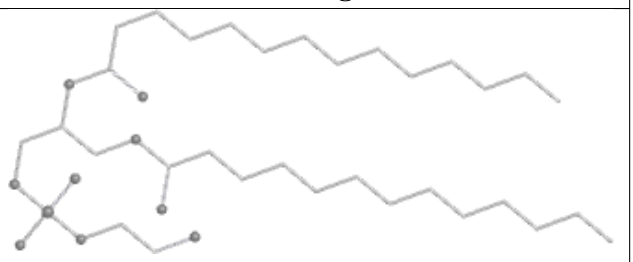
Bond lengths



Bond angles

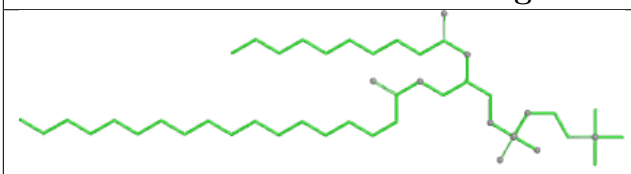


Torsions

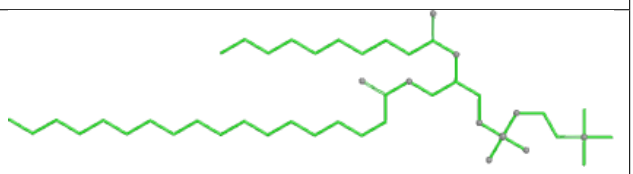


Rings

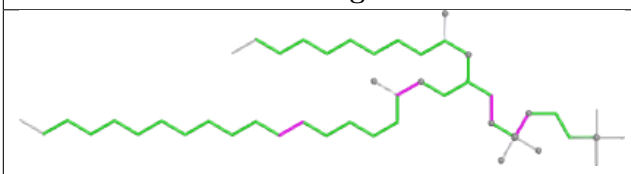
Ligand PC1 1M 502



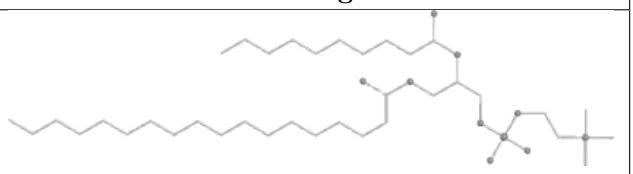
Bond lengths



Bond angles

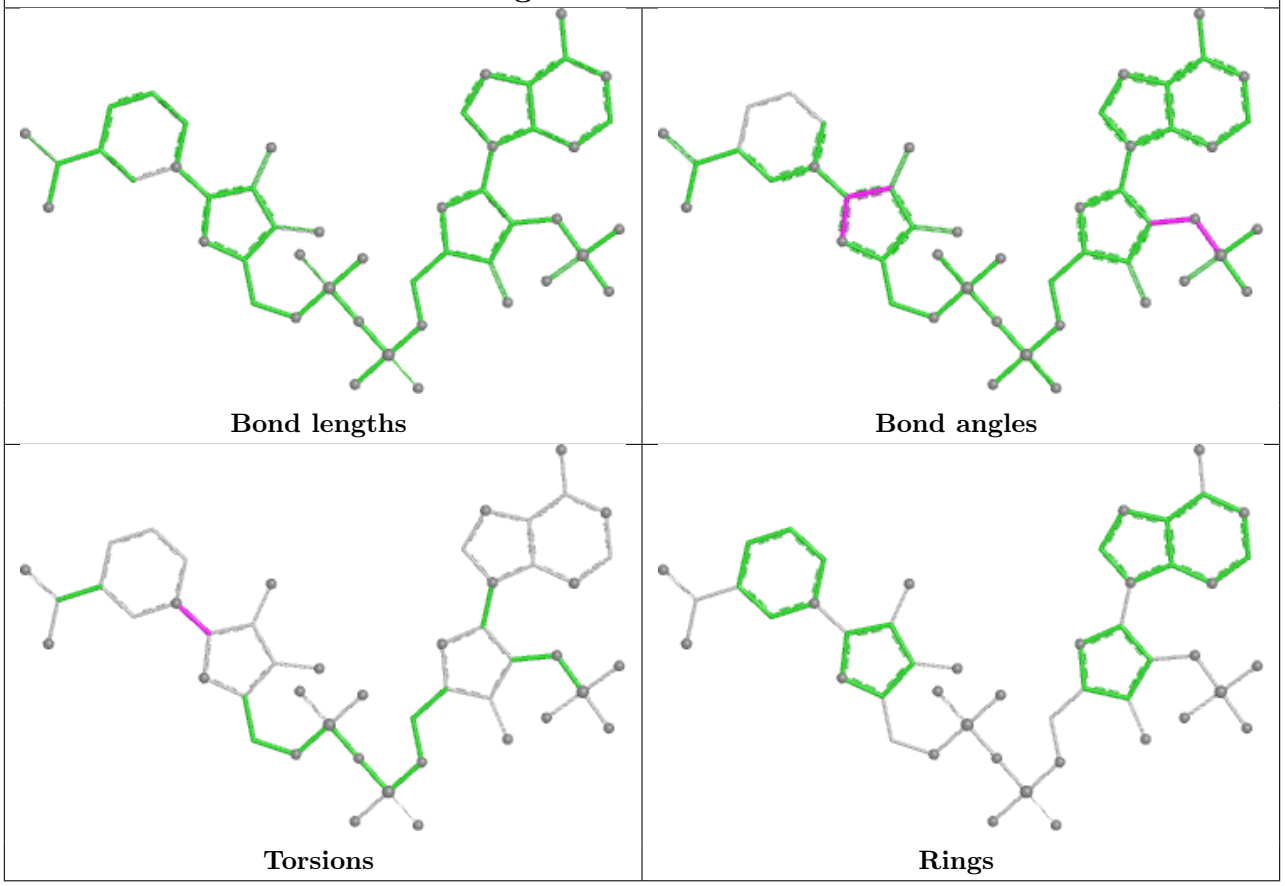


Torsions

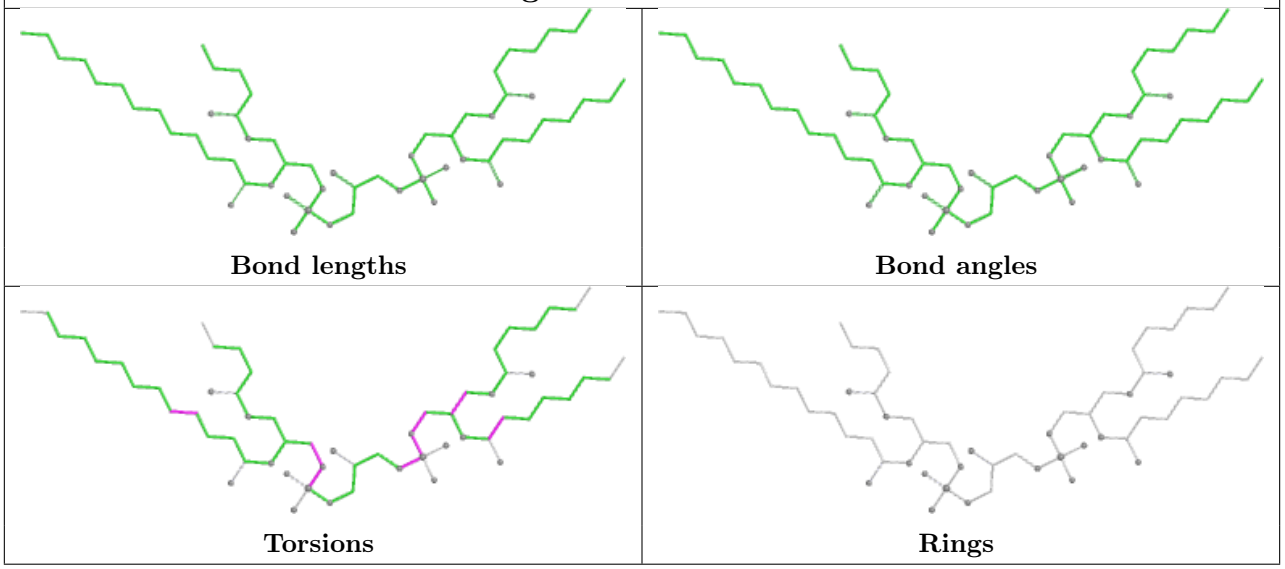


Rings

Ligand NDP 1P 501



Ligand CDL 1r 201



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1i	1
43	1r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	3.85
1	1r	1:ALA	C	2:SER	N	3.14

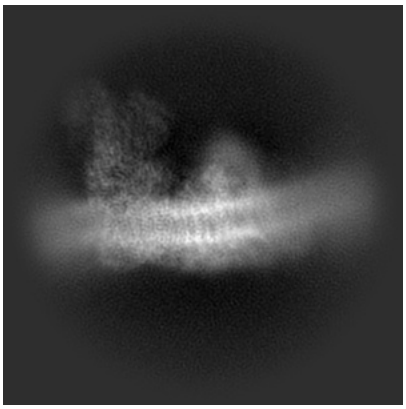
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-42171. These allow visual inspection of the internal detail of the map and identification of artifacts.

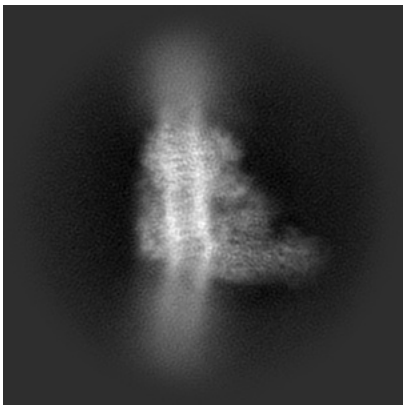
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

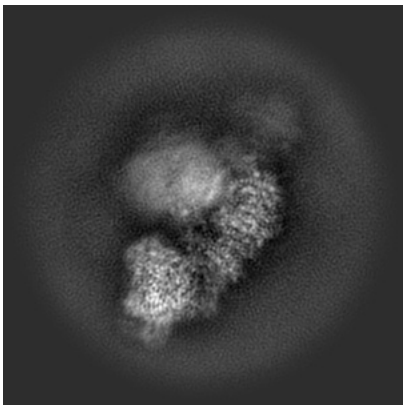
6.1.1 Primary map



X

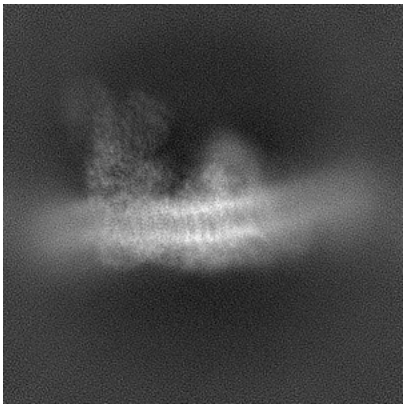


Y

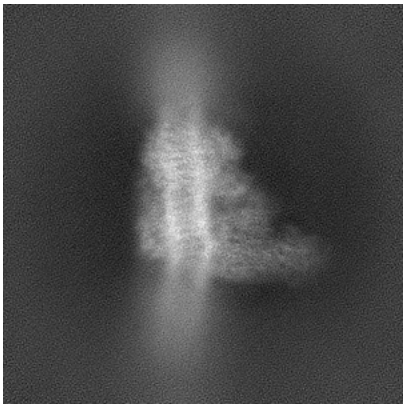


Z

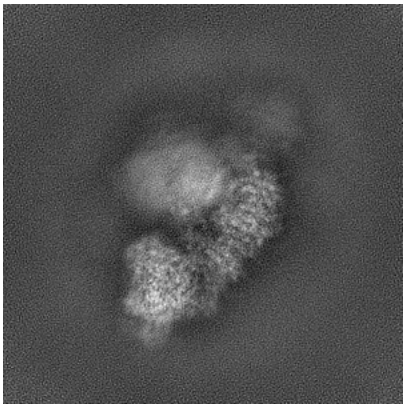
6.1.2 Raw map



X



Y

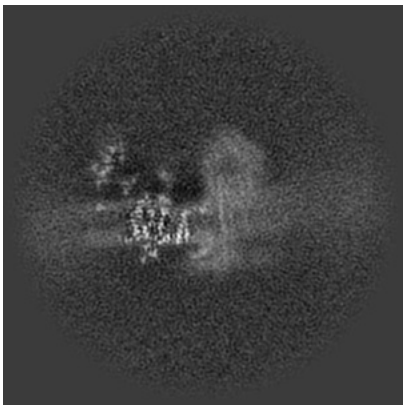


Z

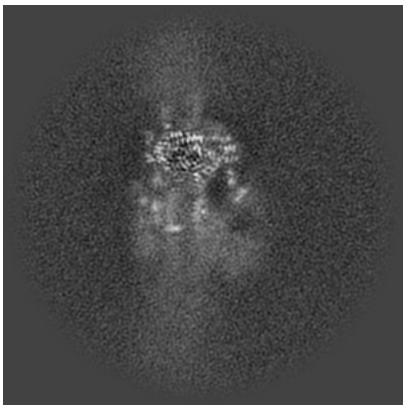
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

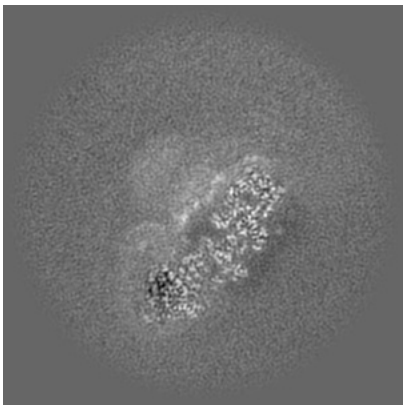
6.2.1 Primary map



X Index: 160

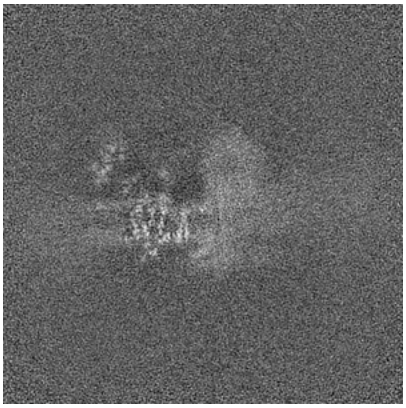


Y Index: 160

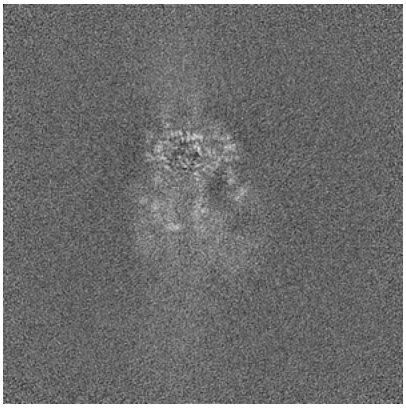


Z Index: 160

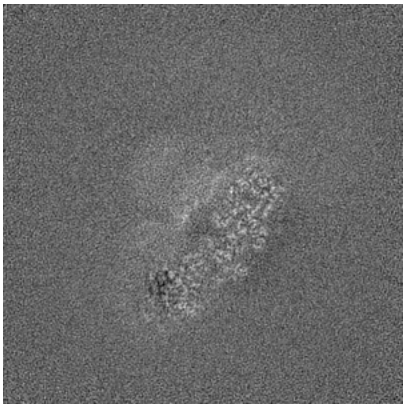
6.2.2 Raw map



X Index: 160



Y Index: 160

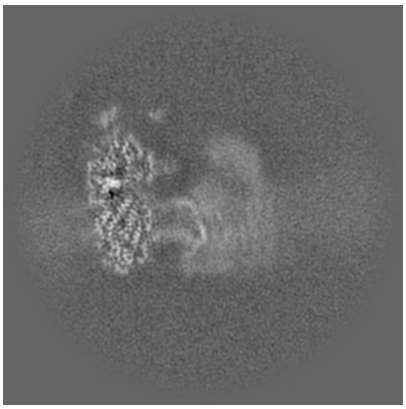


Z Index: 160

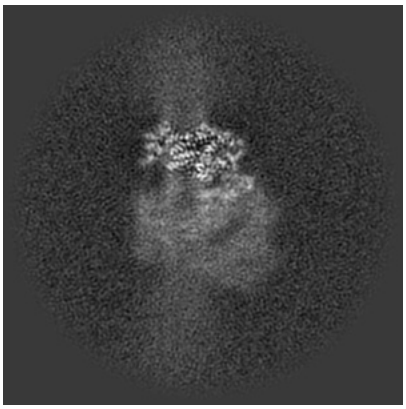
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

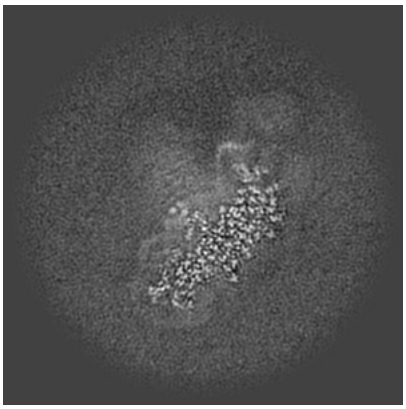
6.3.1 Primary map



X Index: 140

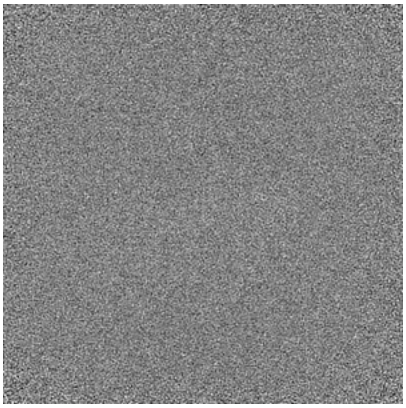


Y Index: 171

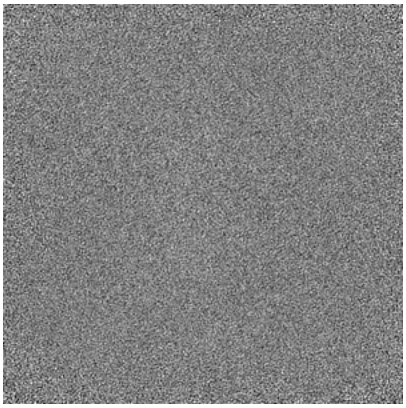


Z Index: 134

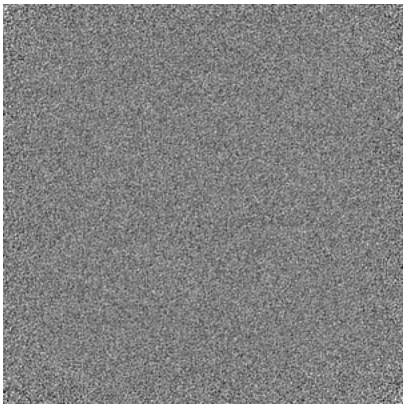
6.3.2 Raw map



X Index: 0



Y Index: 0

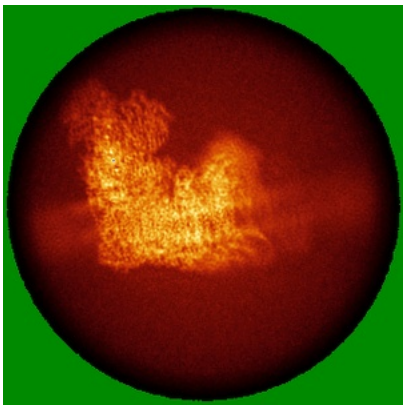


Z Index: 0

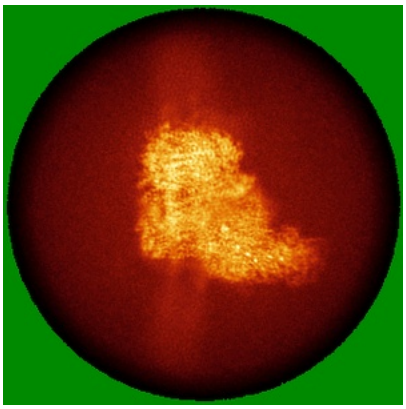
The images above show the largest variance slices of the map in three orthogonal directions.

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

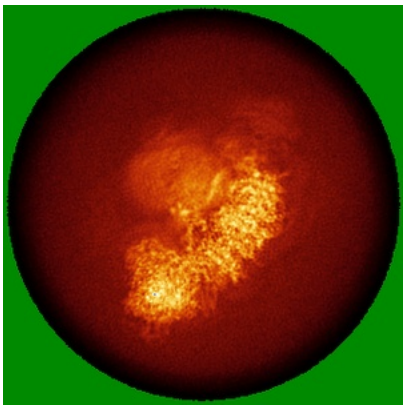
6.4.1 Primary map



X

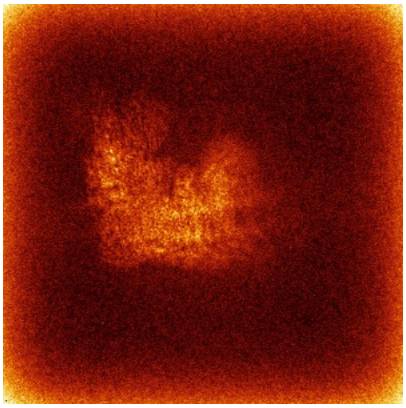


Y

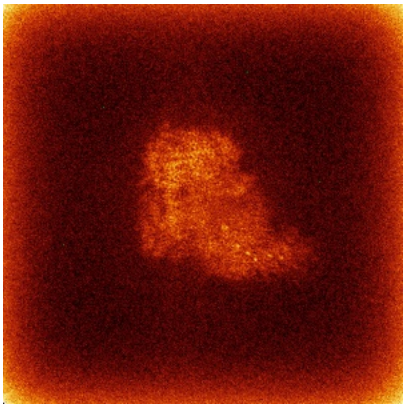


Z

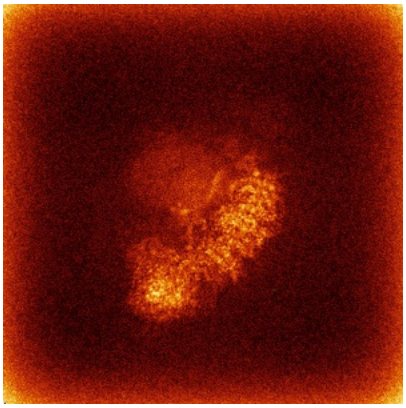
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

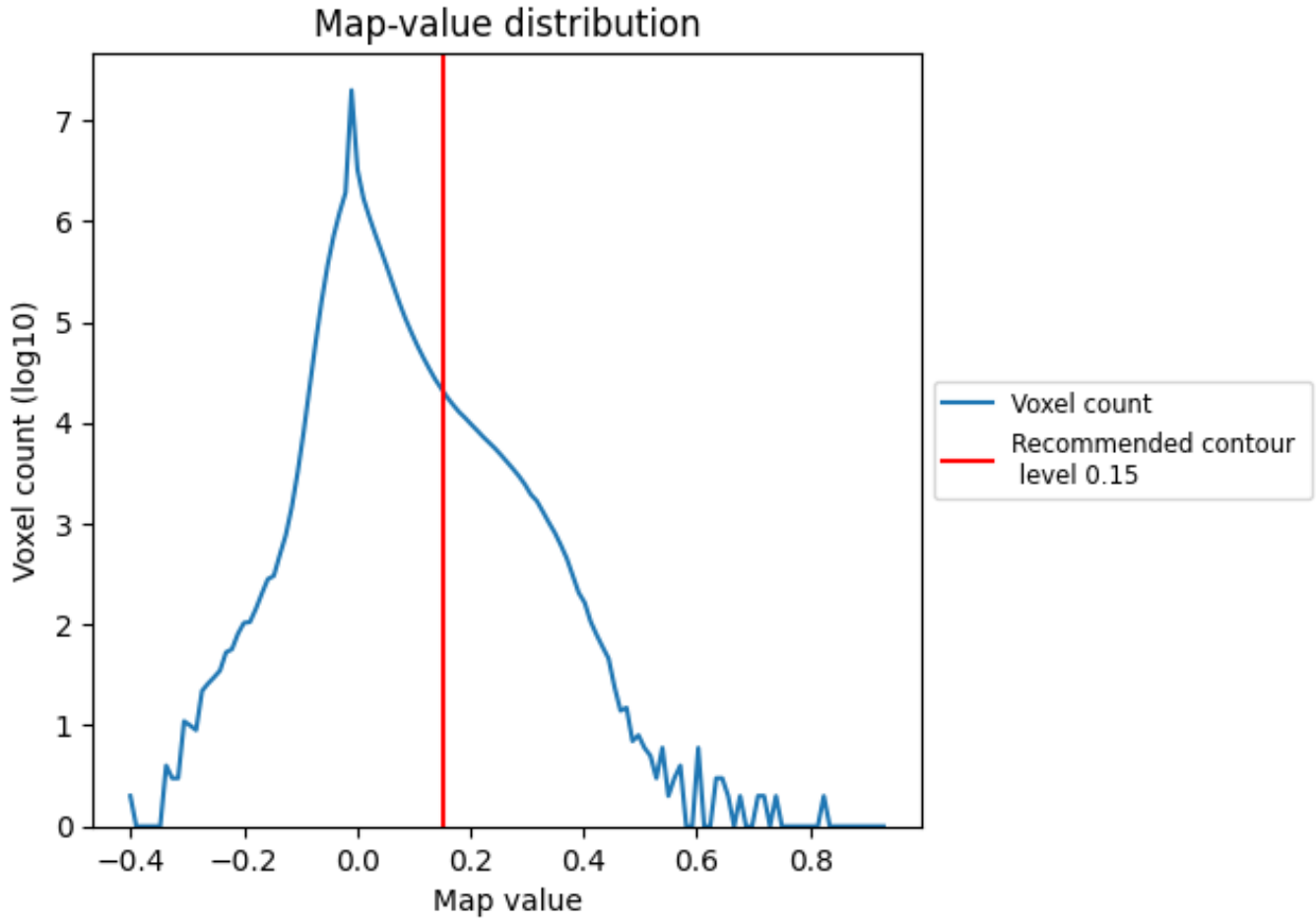
6.6 Mask visualisation (i)

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

7 Map analysis

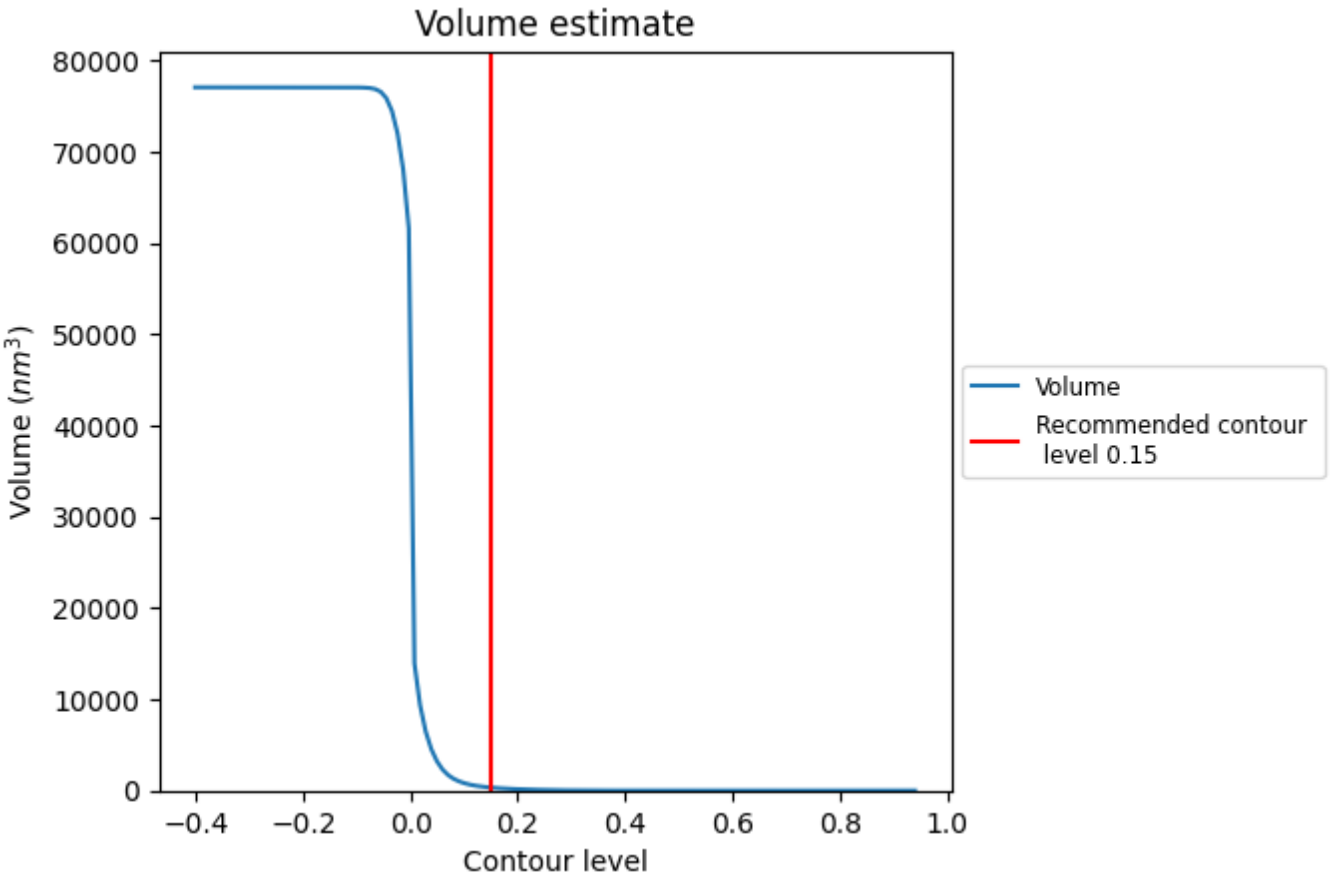
This section contains the results of statistical analysis of the map.

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.

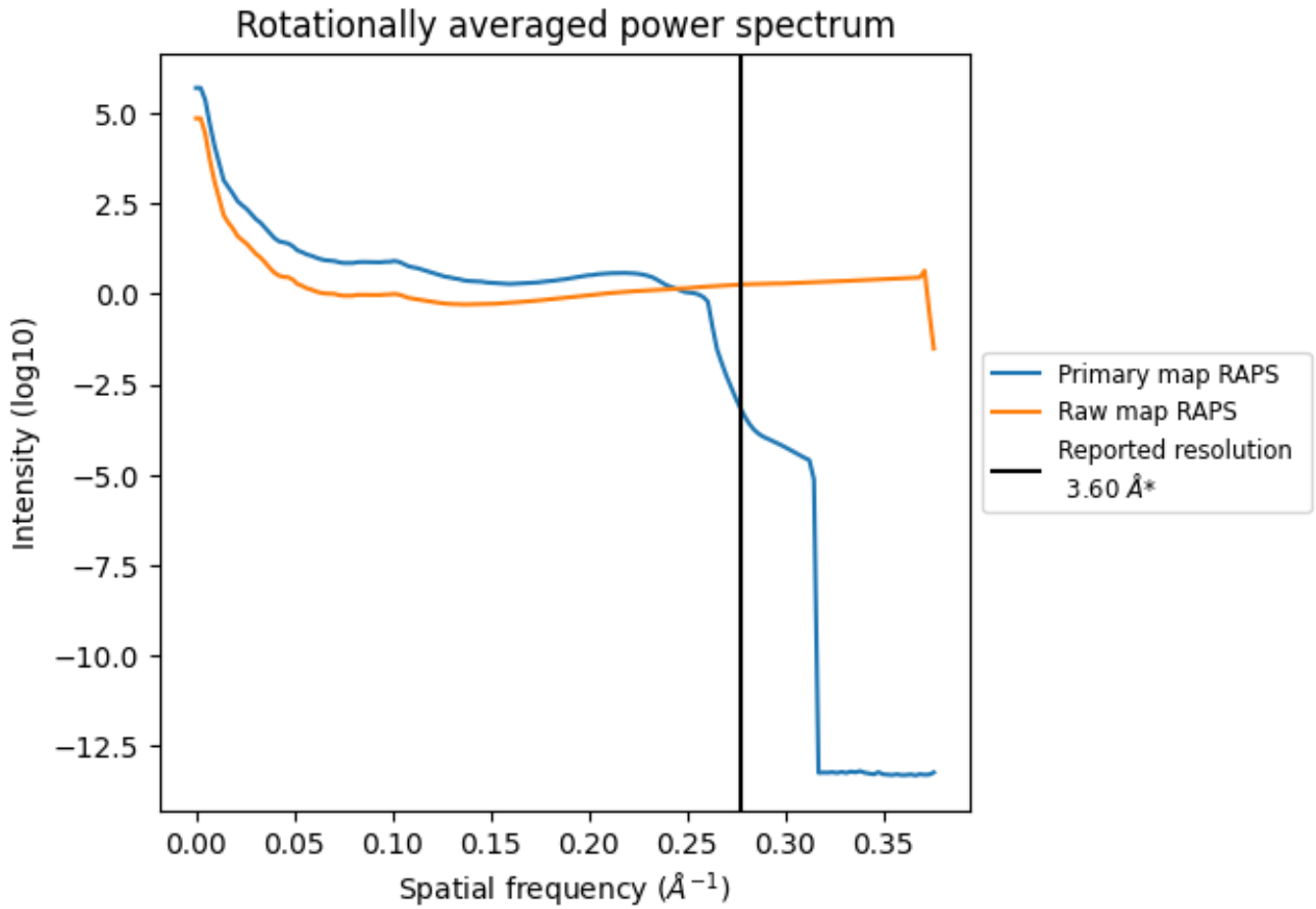
7.2 Volume estimate



The volume at the recommended contour level is 329 nm^3; this corresponds to an approximate mass of 297 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)

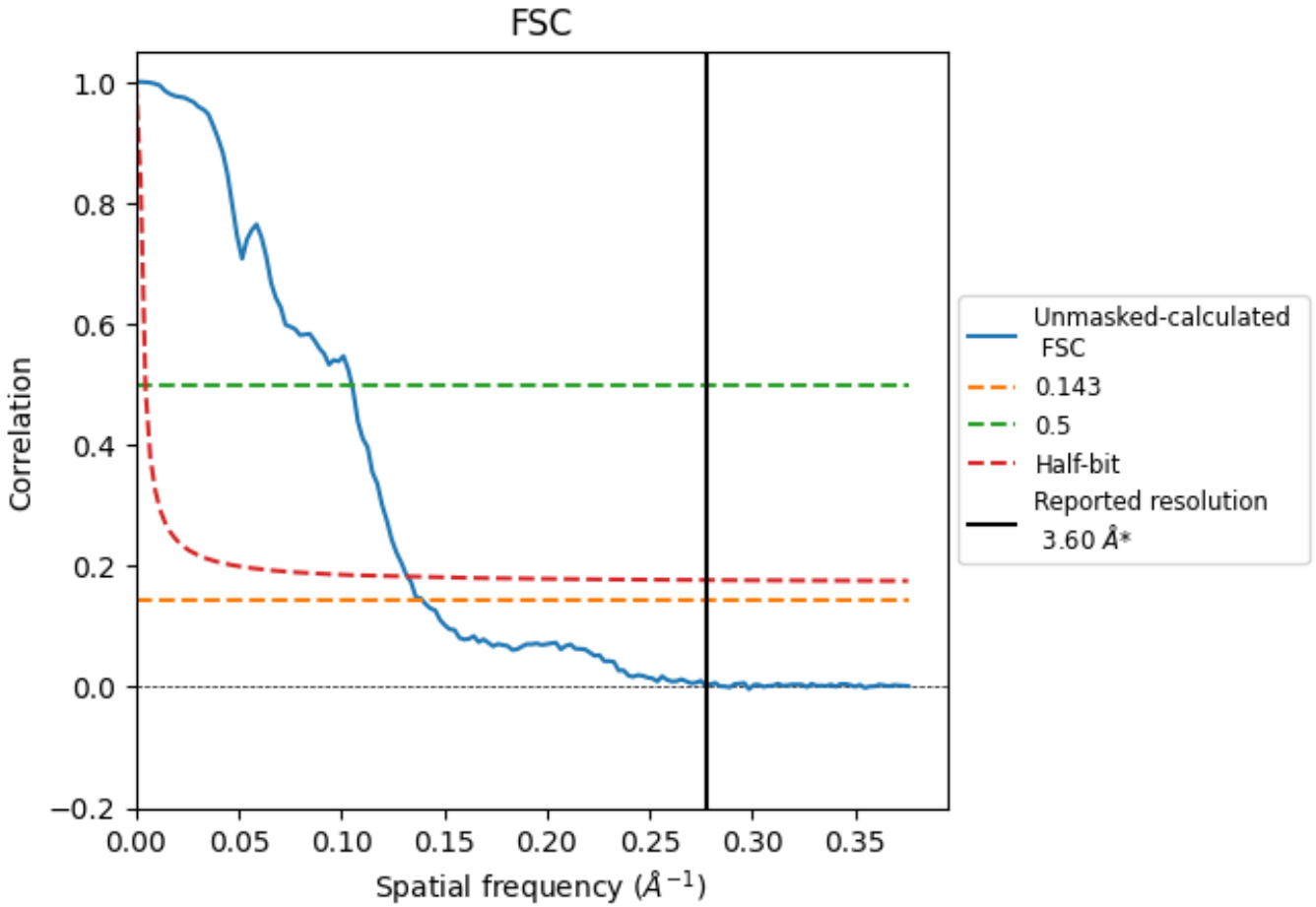


*Reported resolution corresponds to spatial frequency of 0.278 $Å^{-1}$

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

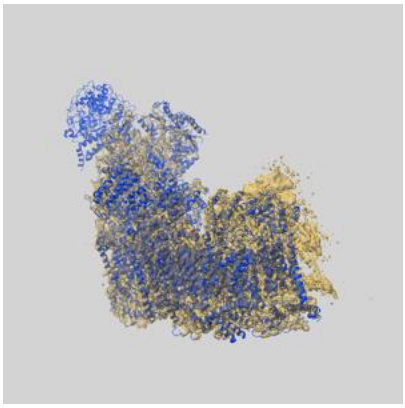
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.17	9.51	7.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.17 differs from the reported value 3.6 by more than 10 %

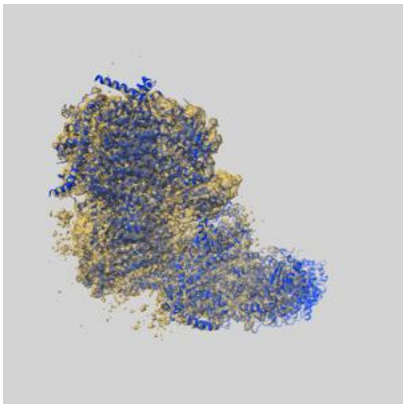
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-42171 and PDB model 8UEU. Per-residue inclusion information can be found in section 3 on page 21.

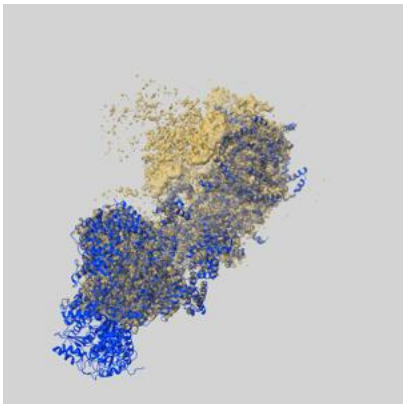
9.1 Map-model overlay



X



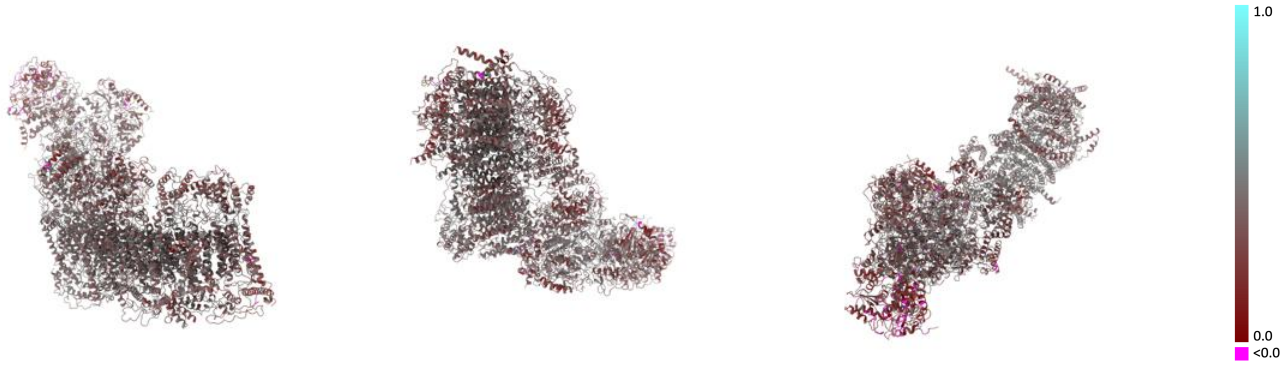
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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.

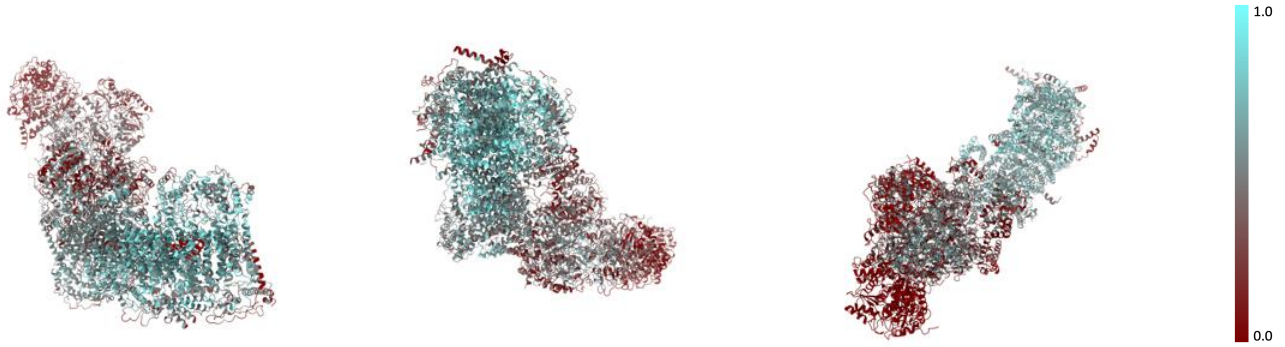
9.2 Q-score mapped to coordinate model (i)



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.

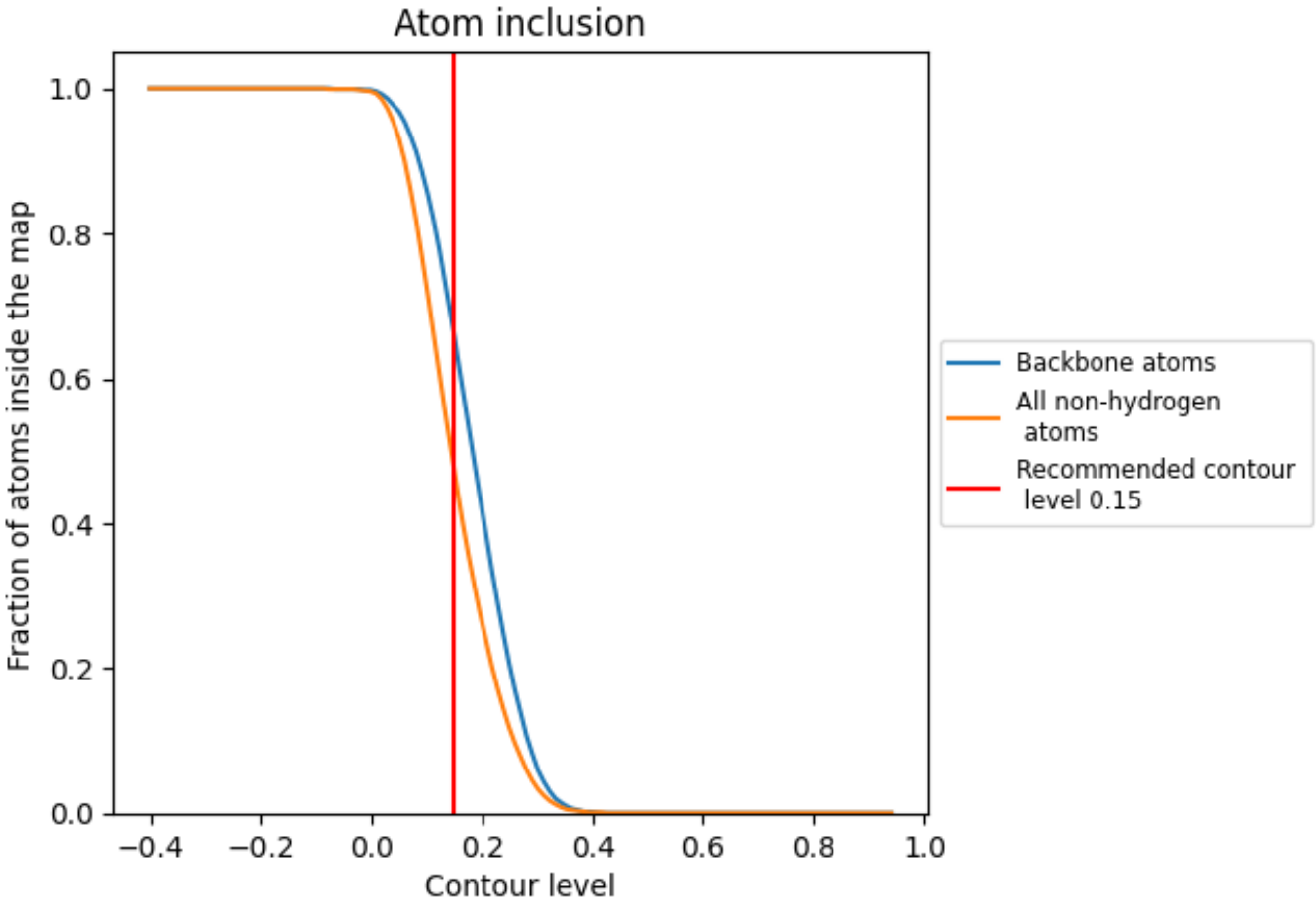
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.15).

9.4 Atom inclusion (i)



At the recommended contour level, 66% of all backbone atoms, 47% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4700	0.3710
1A	0.5100	0.3940
1B	0.5440	0.4170
1C	0.3790	0.4030
1D	0.4830	0.3910
1E	0.0210	0.2640
1F	0.0350	0.2430
1G	0.2770	0.3550
1H	0.5430	0.3880
1I	0.5620	0.4180
1J	0.5150	0.3800
1K	0.6090	0.3970
1L	0.7040	0.3990
1M	0.7470	0.4300
1N	0.6630	0.4130
1O	0.3890	0.3580
1P	0.2930	0.3360
1Q	0.2960	0.3780
1R	0.2880	0.3890
1S	0.1230	0.2940
1T	0.2060	0.2870
1U	0.6160	0.3480
1V	0.2130	0.3310
1W	0.3100	0.3290
1X	0.5310	0.3960
1Y	0.6440	0.3680
1Z	0.5490	0.4110
1a	0.6250	0.4080
1b	0.5050	0.3990
1c	0.4900	0.3790
1d	0.6760	0.4140
1e	0.5830	0.4140
1f	0.4830	0.3910
1g	0.5860	0.3820
1h	0.6600	0.4040

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1i	0.4100	0.3420
1j	0.5120	0.3480
1k	0.4910	0.3600
1l	0.6450	0.3910
1m	0.7020	0.3750
1n	0.6520	0.3640
1o	0.5250	0.3160
1p	0.6040	0.3850
1q	0.4360	0.4070
1r	0.3620	0.4010
1s	0.0000	0.2000