



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 12:28 AM EDT

PDB ID : 8UEO / pdb_00008ueo
EMDB ID : EMD-42165
Title : In-situ complex I (Active-Apo)
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 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) : 2.50

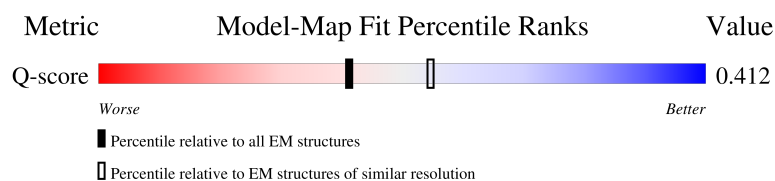
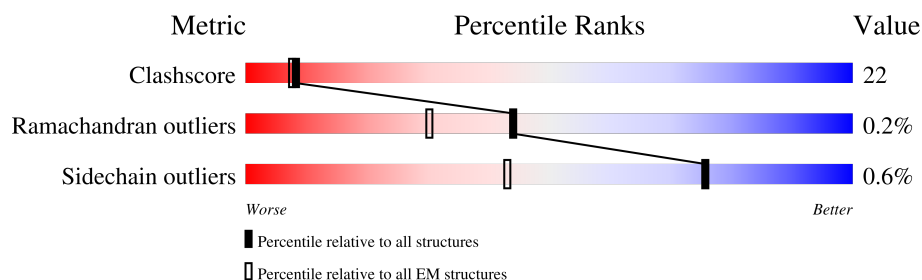
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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 $\leq 5\%$. 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	27% 49% 50% .
2	1B	258	9% 26% 33% 40%
3	1C	264	15% 42% 36% . 21%
4	1D	430	15% 54% 46%

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	122	
30	1e	106	
31	1f	58	
32	1g	154	
33	1h	189	
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	112	
44	1s	471	

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
47	SF4	1G	801	-	-	X	-
47	SF4	1I	201	-	-	X	-
48	FES	1E	301	-	-	X	-
48	FES	1G	803	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 68026 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
1	1A	115	Total	C	N	O	S	0	0
			914	615	134	158	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1C	209	Total	C	N	O	S	0	0
			1746	1128	299	317	2		

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

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

- 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	317	Total	C	N	O	S	0	0
			2494	1667	384	423	20		

- 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	173	Total	C	N	O	S	0	0
			1322	888	188	234	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	1K	97	Total	C	N	O	S	0	0
			740	488	112	127	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	1L	605	Total	C	N	O	S	0	0
			4808	3189	745	824	50		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	1M	458	Total	C	N	O	S	0	0
			3622	2405	571	608	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	1N	346	Total	C	N	O	S	0	0
			2702	1777	419	461	45		

- 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	119	Total	C	N	O	S	0	0
			985	641	171	168	5		

- 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.

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

- 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	128	Total	C	N	O	S	0	0
			1100	723	194	181	2		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1i	0	ACE	-	acetylation	UNP A0A4X1UIV8

- 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		
			1062	691	182	189	0	0

- 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		
			1495	956	273	258	8	0	0

- 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		
			1045	650	198	187	10	0	0

- 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		
			1449	908	263	270	8	0	0

- 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		
			1212	775	219	213	5	0	0

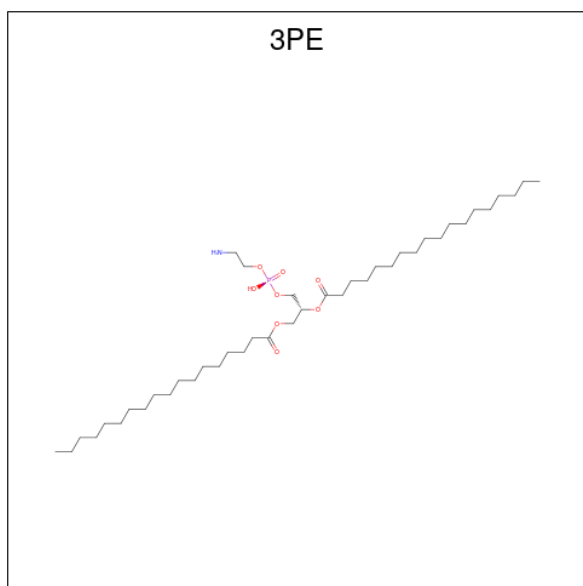
- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	1r	94	Total	C	N	O	S		
			759	478	143	135	3	0	0

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

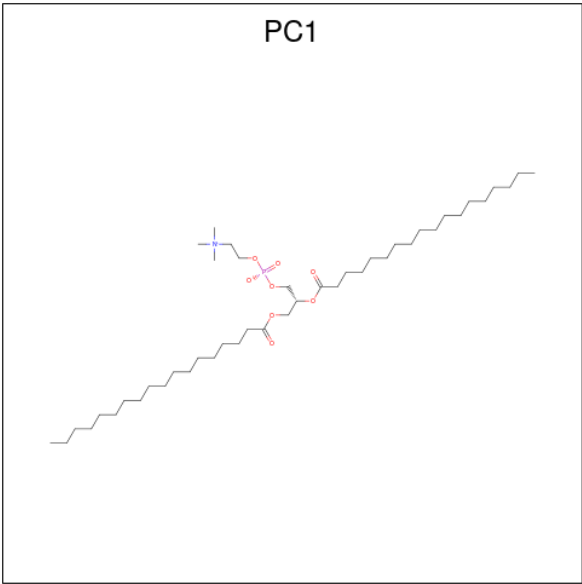
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1D	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1M	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	1M	1	Total	C	N	O	P	0
			38	28	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			40	30	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
45	1f	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P).



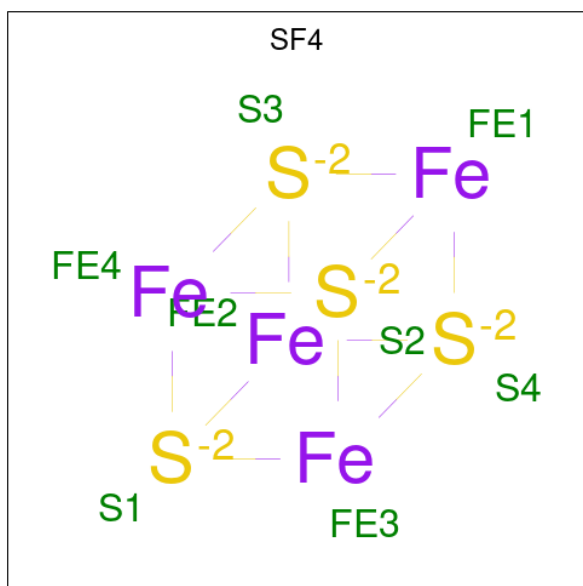
Mol	Chain	Residues	Atoms					AltConf
46	1A	1	Total	C	N	O	P	0
			27	17	1	8	1	
46	1B	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1B	1	Total	C	N	O	P	0
			48	38	1	8	1	
46	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1J	1	Total	C	N	O	P	0
			32	22	1	8	1	
46	1L	1	Total	C	N	O	P	0
			38	28	1	8	1	
46	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1Z	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1f	1	Total	C	N	O	P	0
			34	24	1	8	1	

Continued on next page...

Continued from previous page...

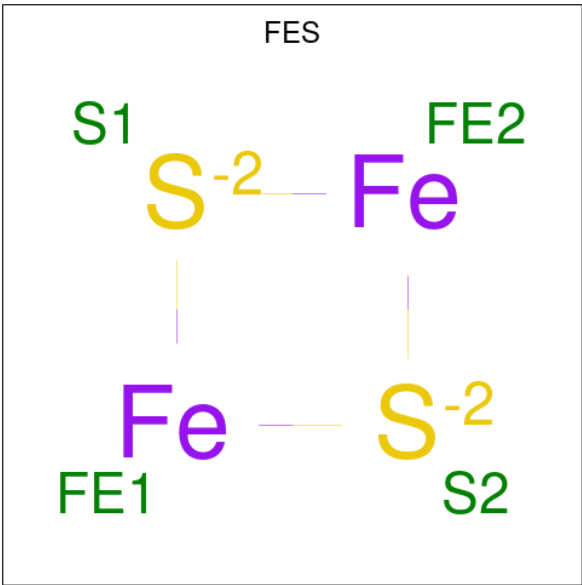
Mol	Chain	Residues	Atoms					AltConf
46	1h	1	Total	C	N	O	P	0
			47	37	1	8	1	

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



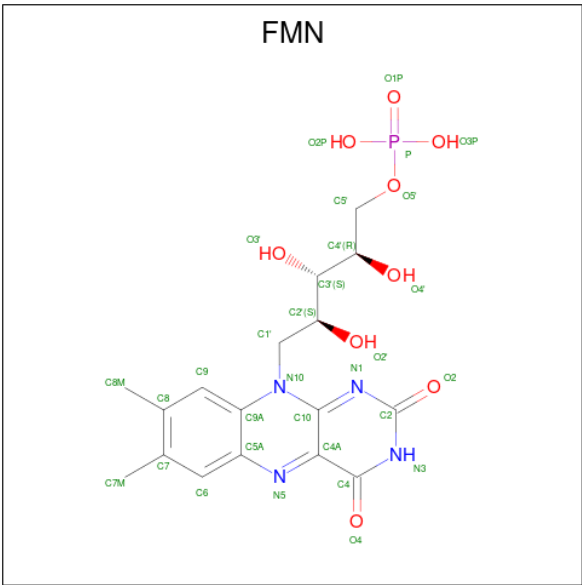
Mol	Chain	Residues	Atoms			AltConf
47	1B	1	Total	Fe	S	0
			8	4	4	
47	1F	1	Total	Fe	S	0
			8	4	4	
47	1G	1	Total	Fe	S	0
			8	4	4	
47	1G	1	Total	Fe	S	0
			8	4	4	
47	1I	1	Total	Fe	S	0
			8	4	4	
47	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
48	1E	1	Total	Fe	S	0
			4	2	2	
48	1G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

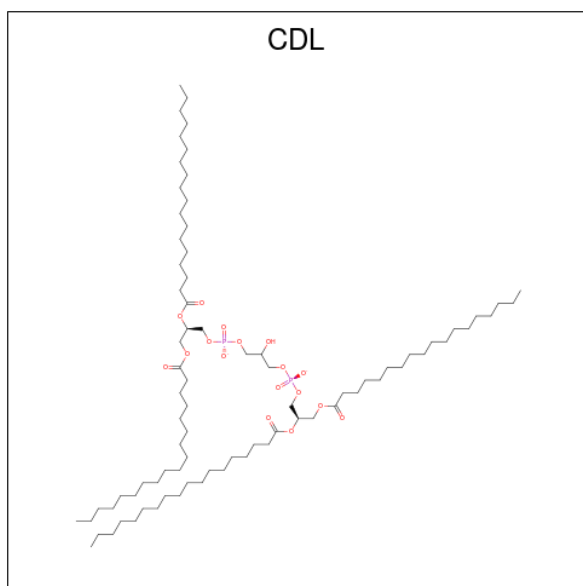


Mol	Chain	Residues	Atoms					AltConf
49	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is POTASSIUM ION (CCD ID: K) (formula: K).

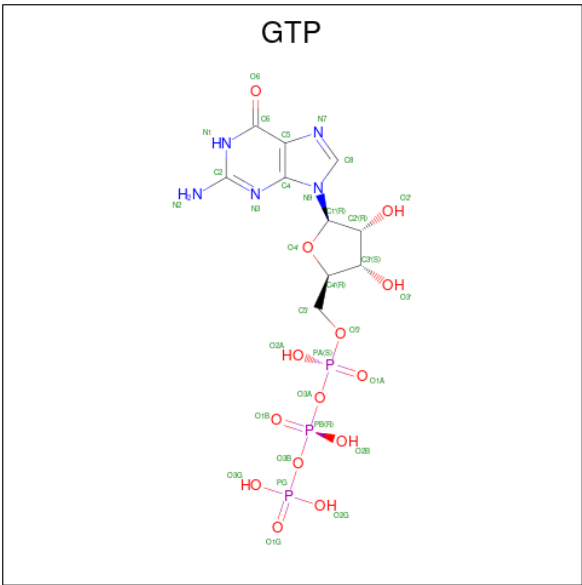
Mol	Chain	Residues	Atoms		AltConf
50	1G	1	Total	K	0
			1	1	

- Molecule 51 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total	C	O	P	0
			51	32	17	2	
51	1L	1	Total	C	O	P	0
			76	57	17	2	
51	1N	1	Total	C	O	P	0
			65	46	17	2	
51	1N	1	Total	C	O	P	0
			67	48	17	2	
51	1X	1	Total	C	O	P	0
			86	67	17	2	
51	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

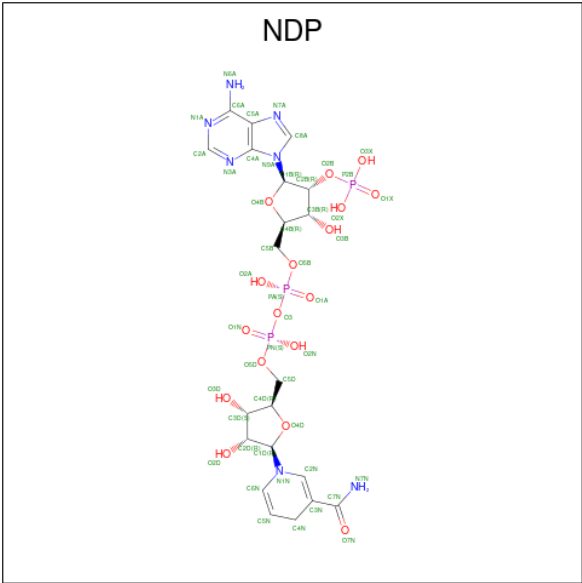


Mol	Chain	Residues	Atoms					AltConf
52	10	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	10	1	Total	Mg	0
			1	1	

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

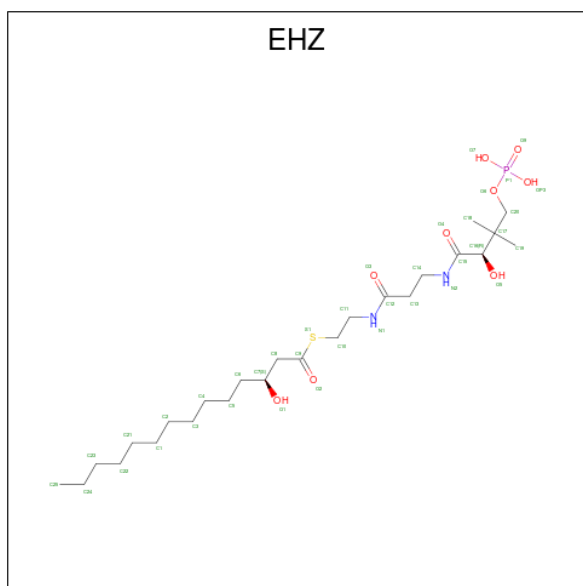


Mol	Chain	Residues	Atoms					AltConf
54	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

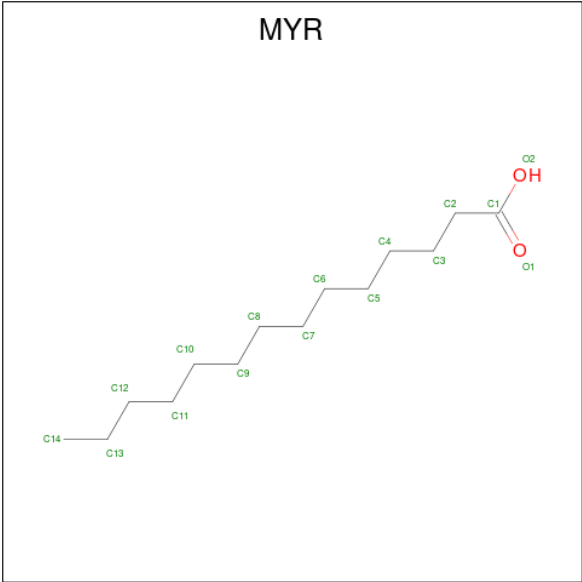
Mol	Chain	Residues	Atoms		AltConf
55	1R	1	Total	Zn	0
			1	1	

- Molecule 56 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: C₂₅H₄₉N₂O₉PS).



Mol	Chain	Residues	Atoms						AltConf
56	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 57 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

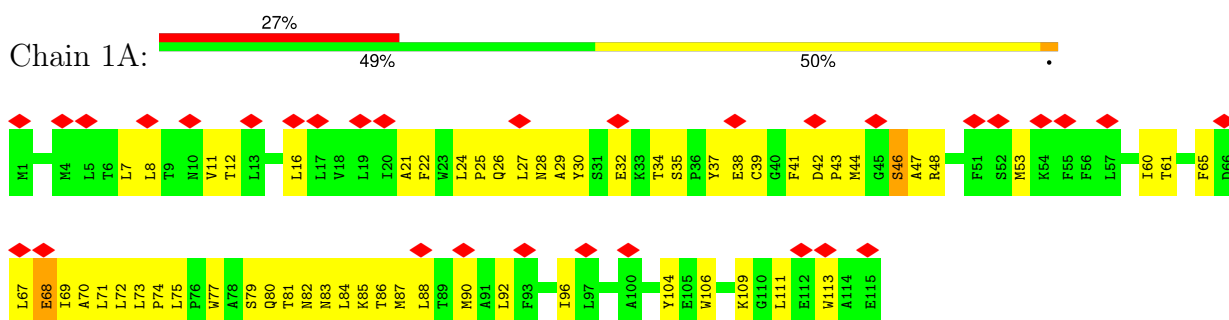


Mol	Chain	Residues	Atoms			AltConf
57	1l	1	Total	C	O	0
			15	14	1	

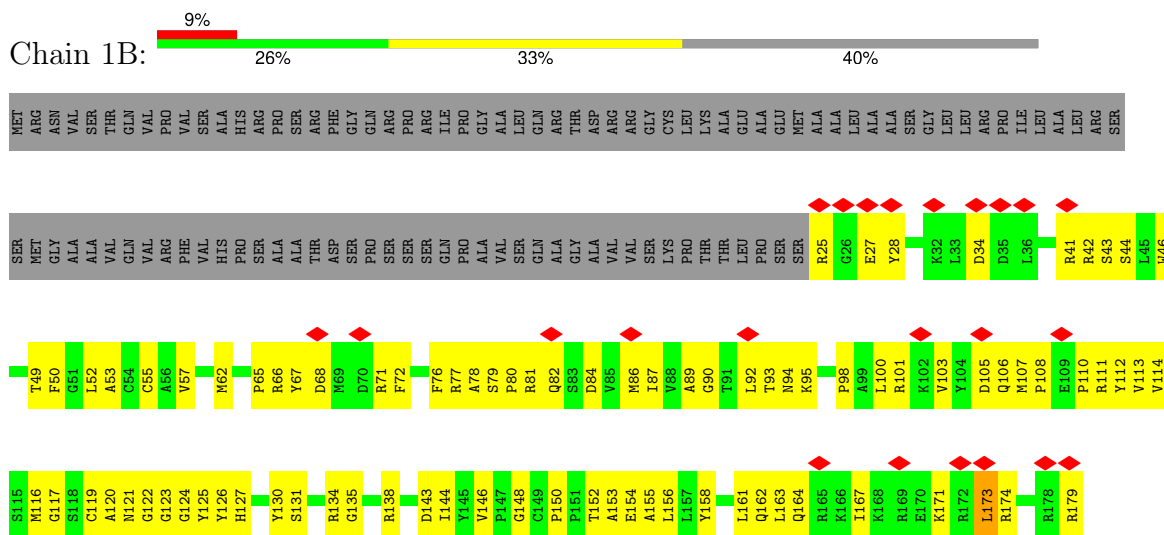
3 Residue-property plots

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

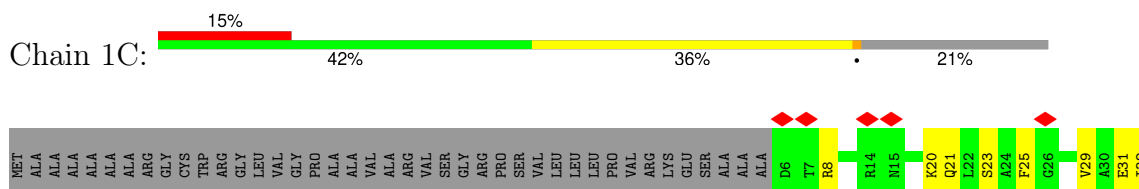
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

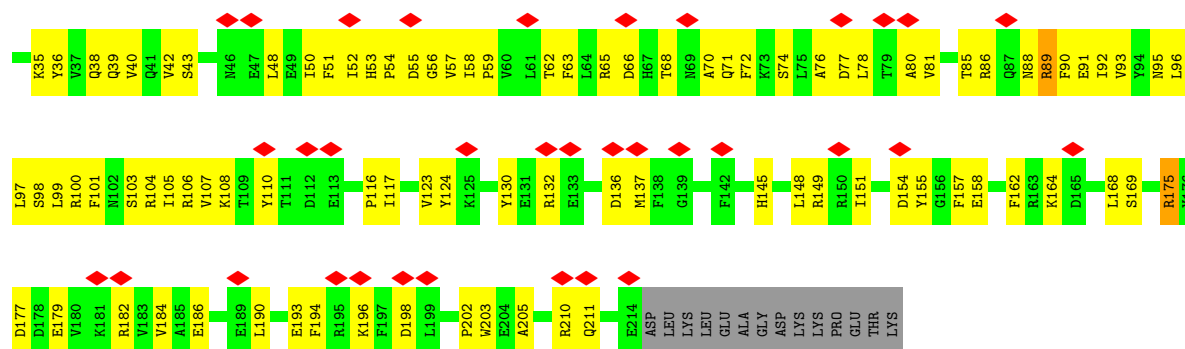


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

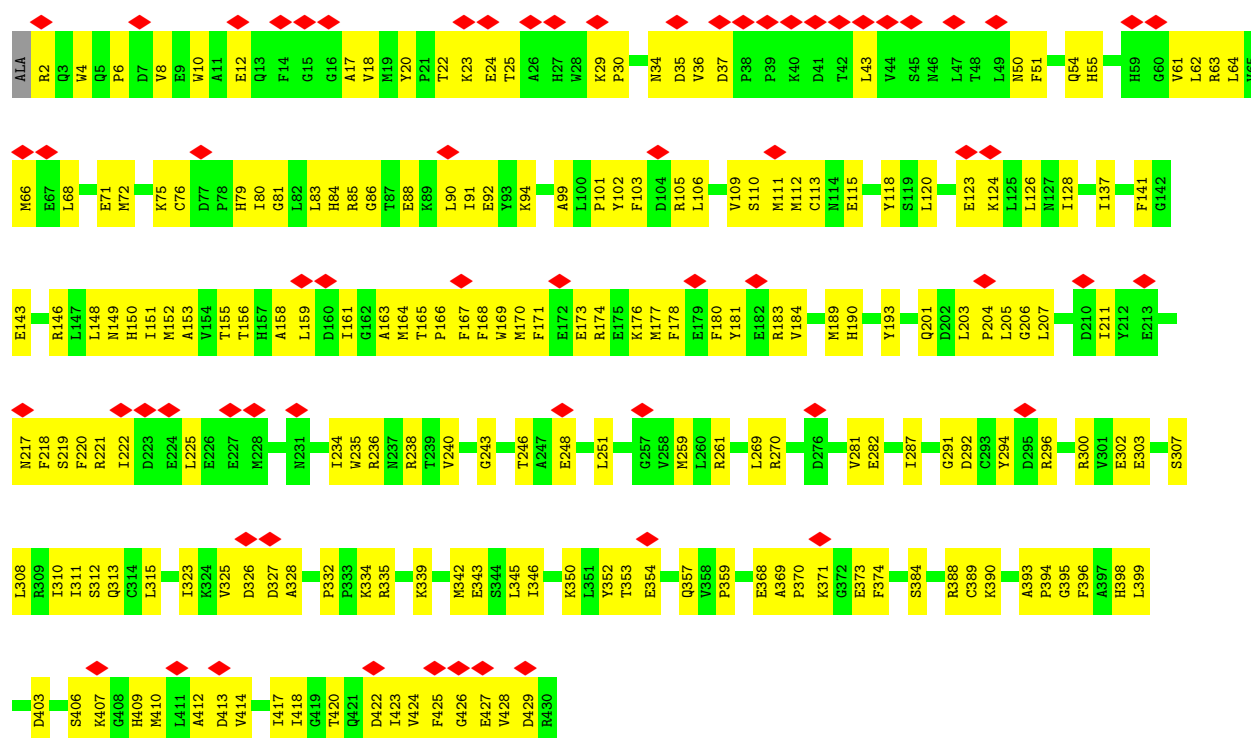


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

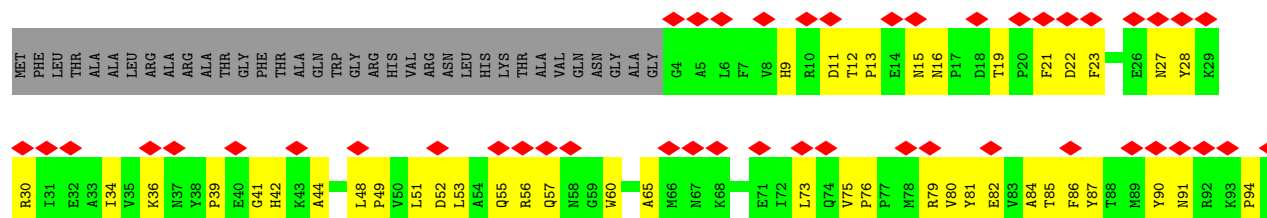
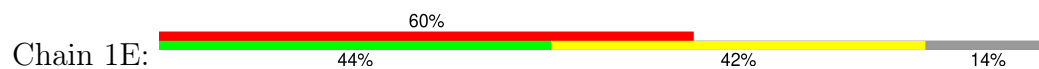




- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial



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

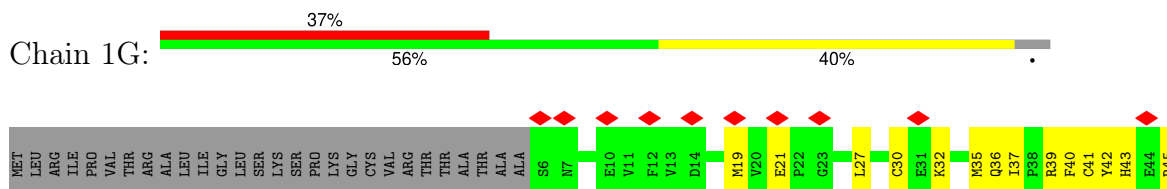


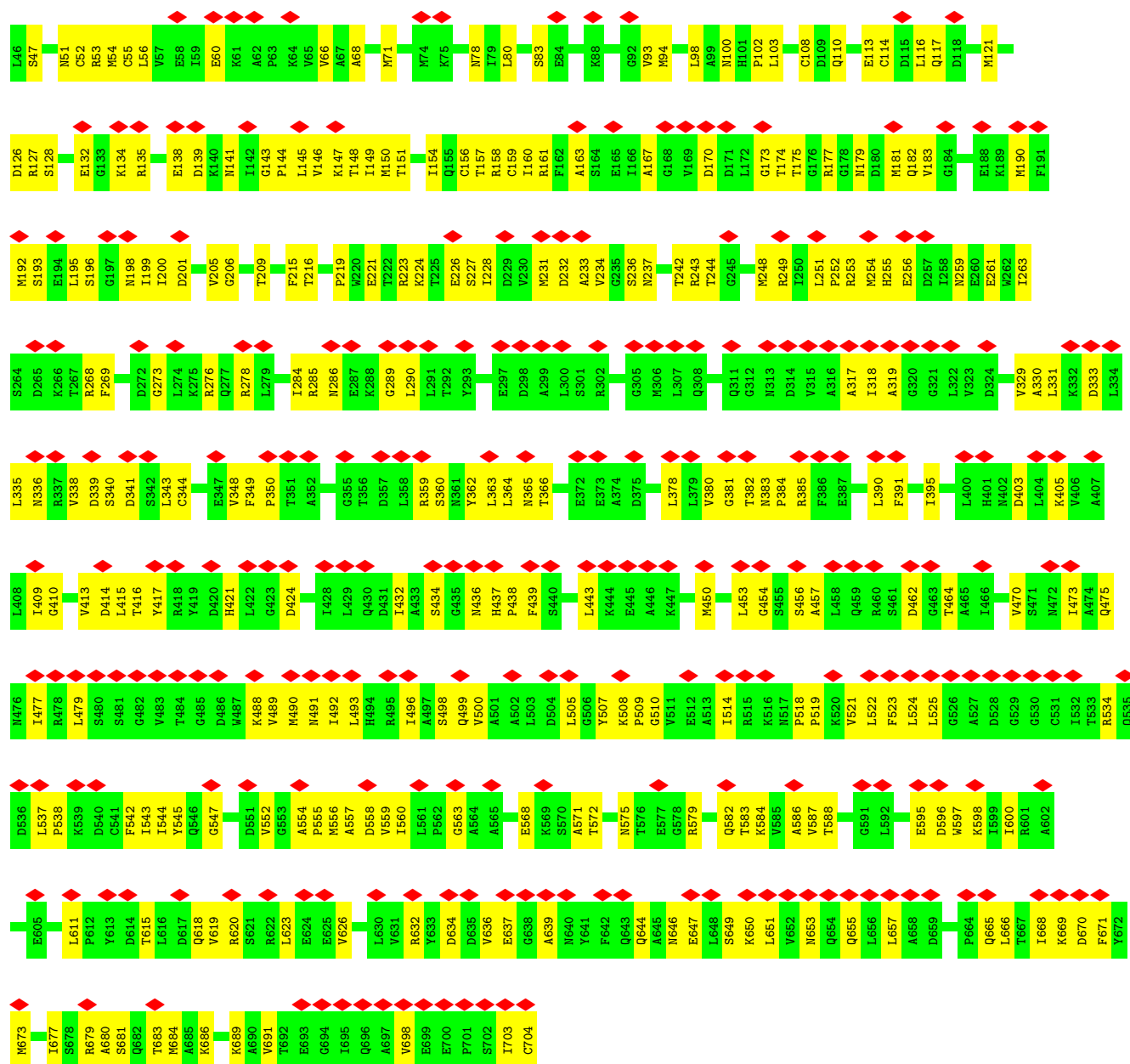


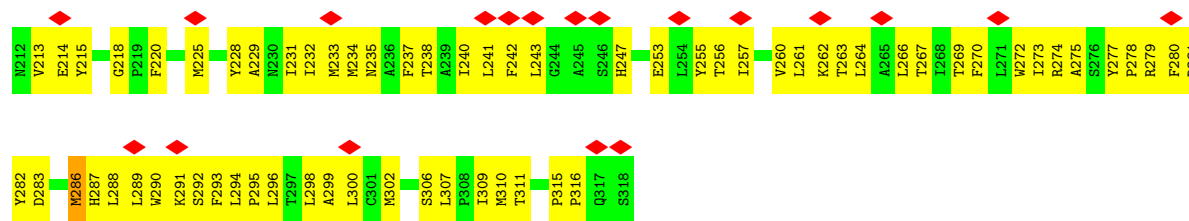
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



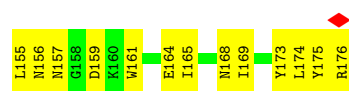
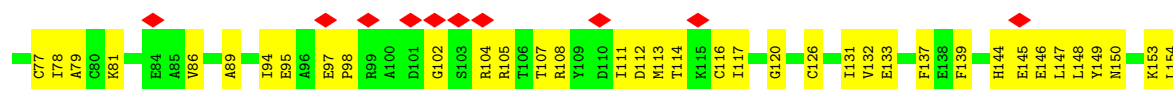
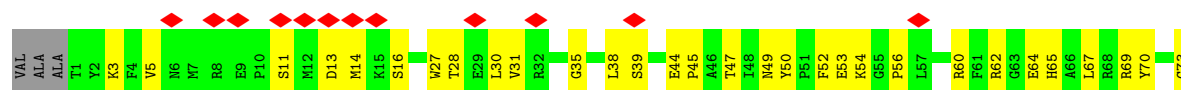
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



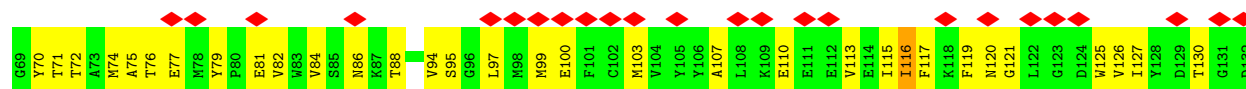
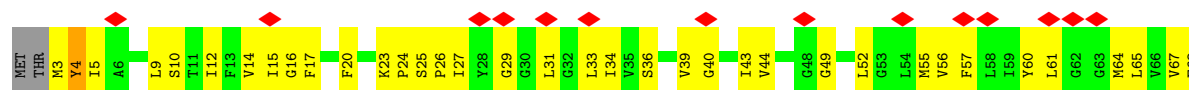




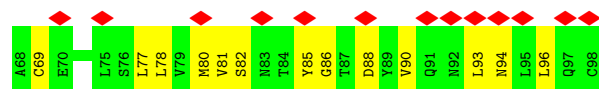
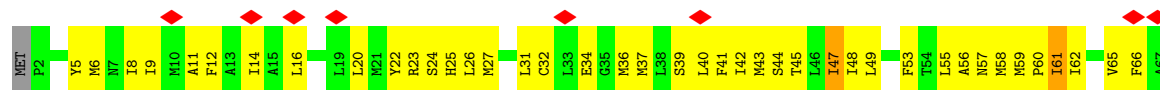
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



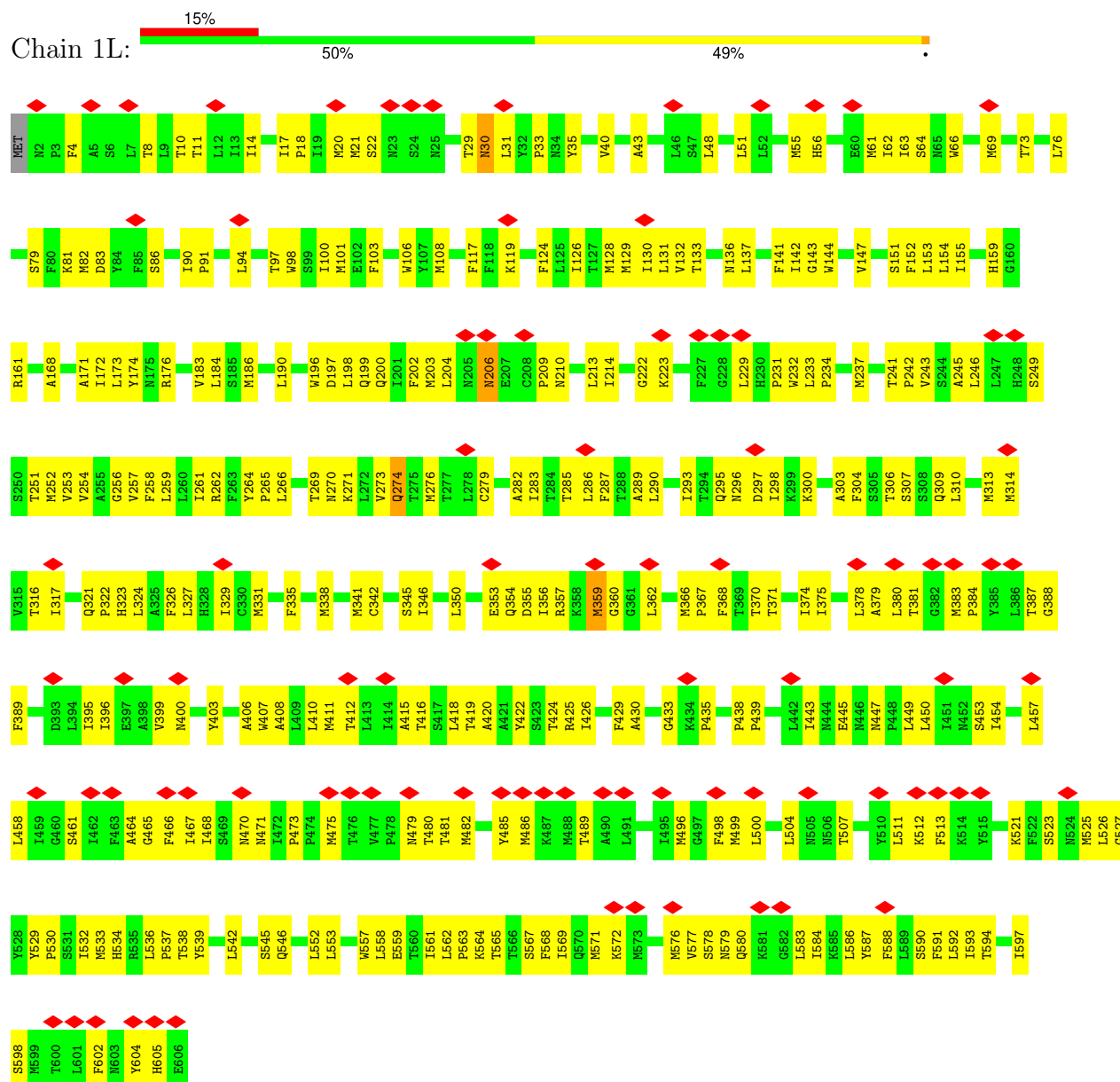
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



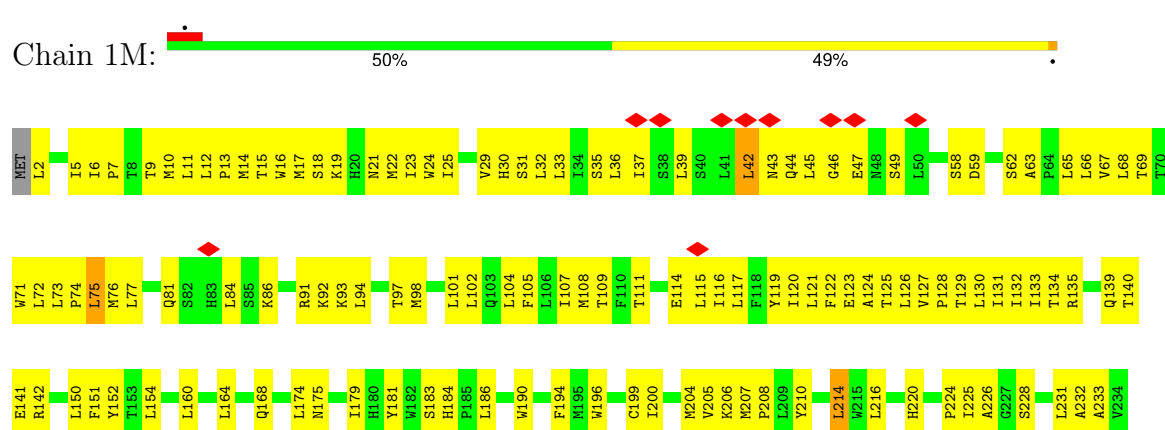
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

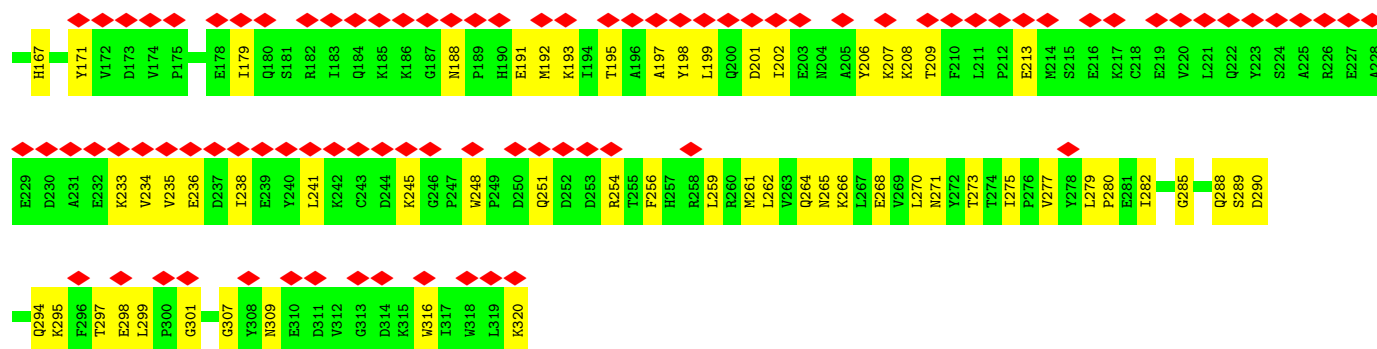


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

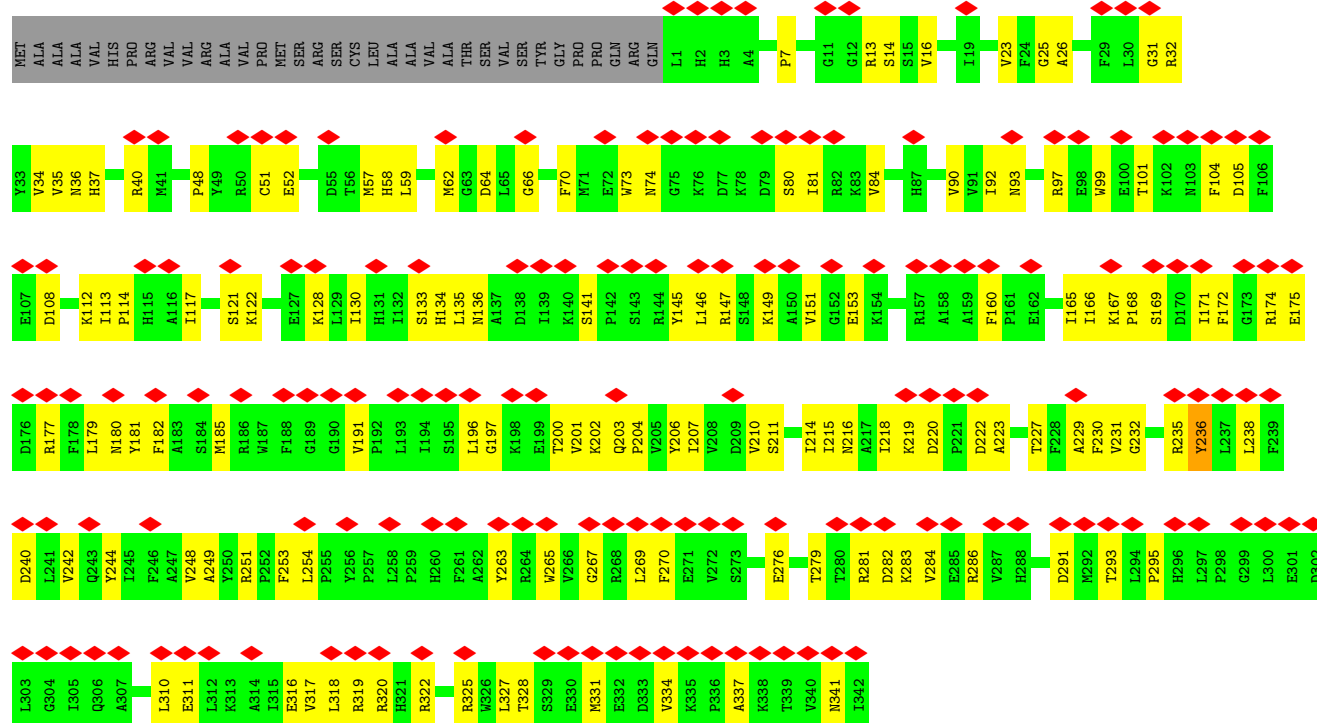


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

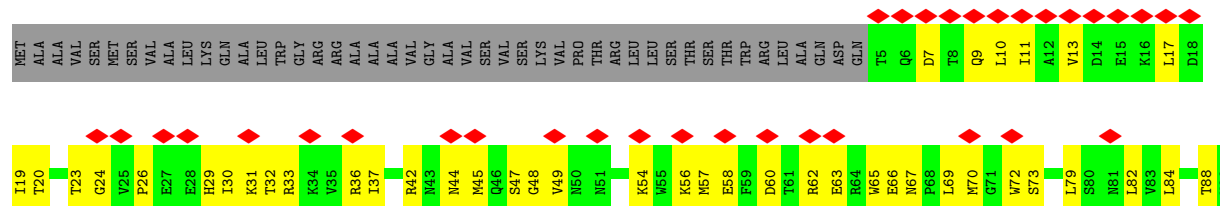


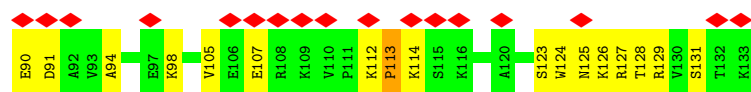


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

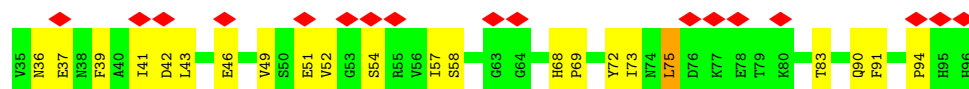
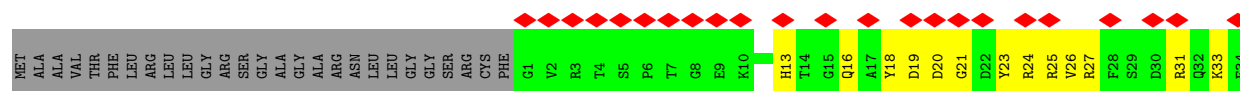


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

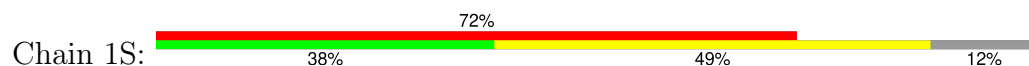




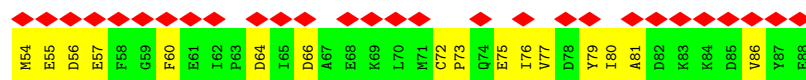
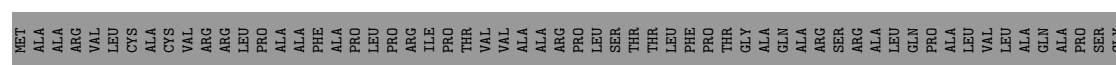
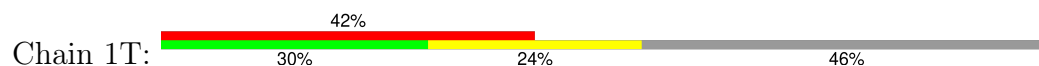
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



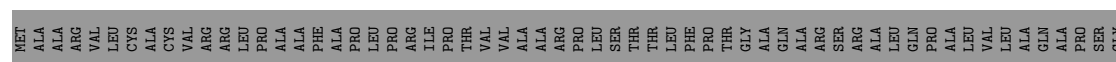
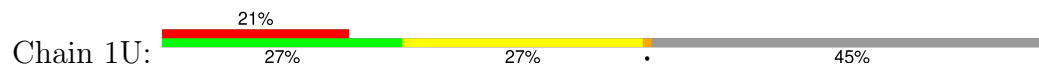
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

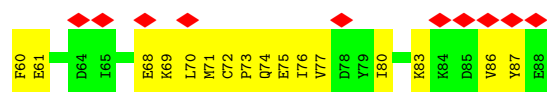


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



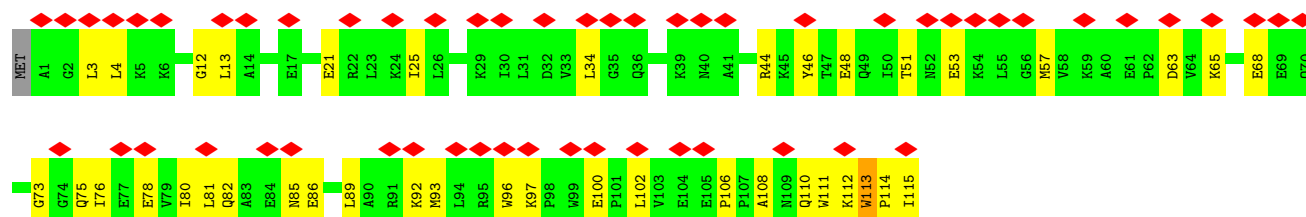
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1





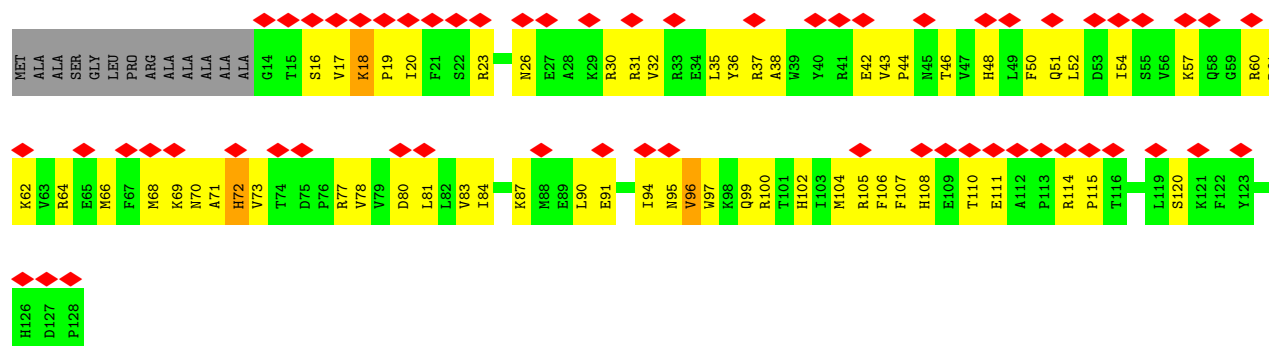
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

Chain 1V: ..



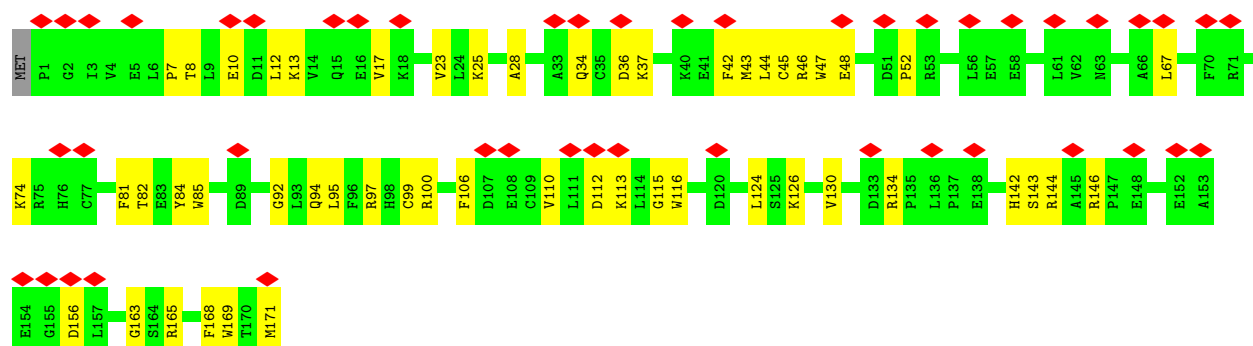
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain 1W: •



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

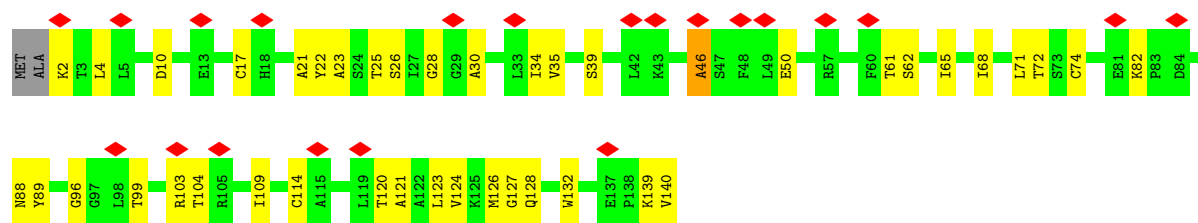
Chain 1X: •



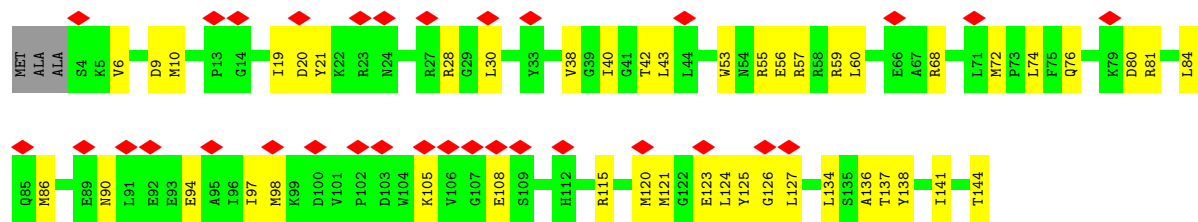
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y: ..

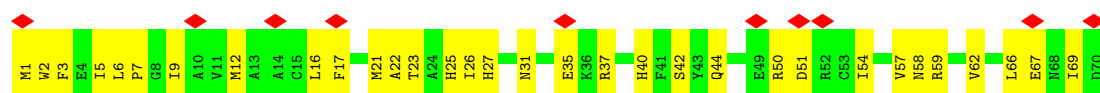




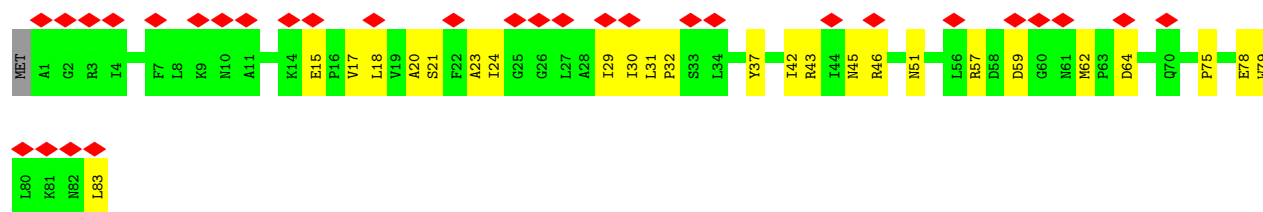
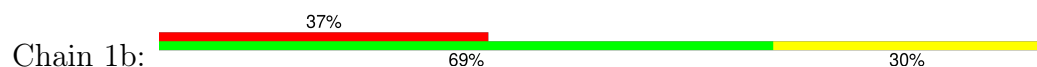
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



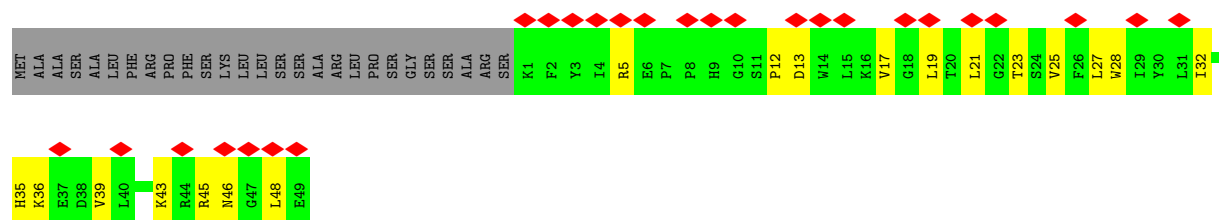
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



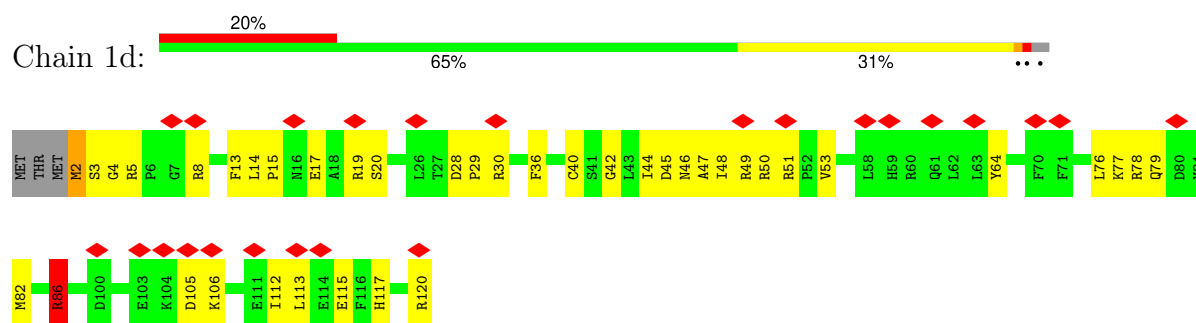
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



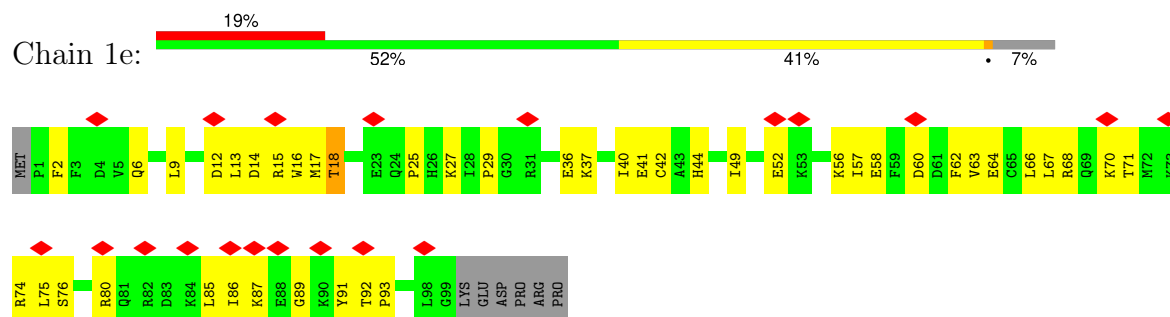
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



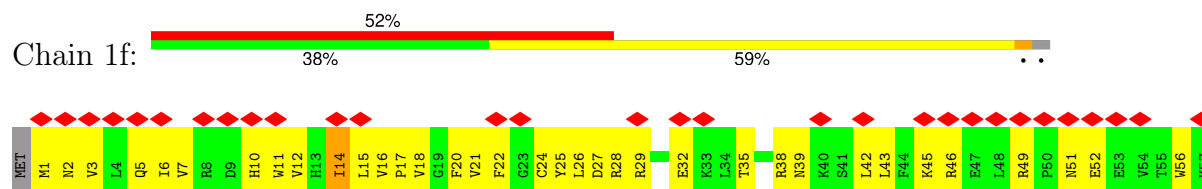
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



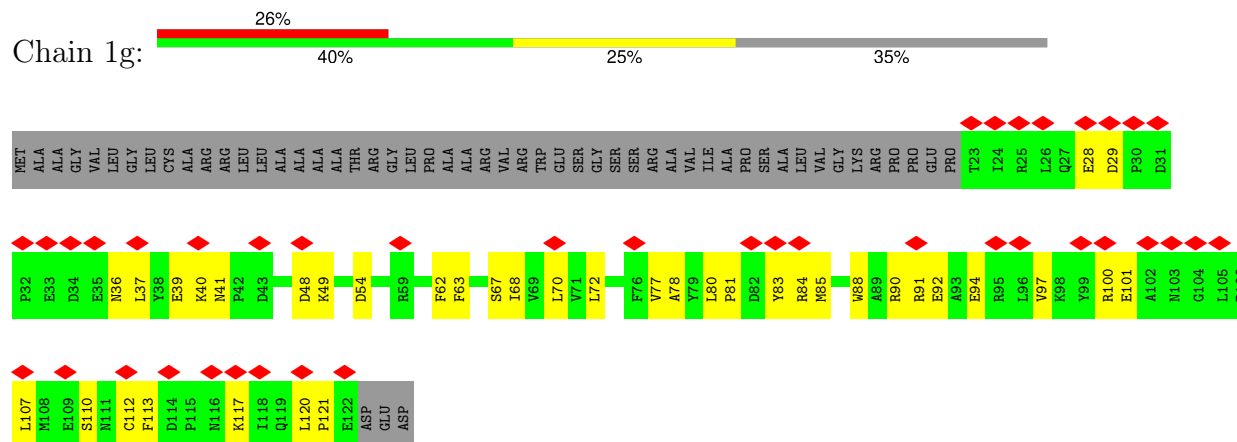
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



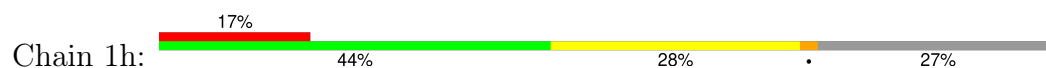
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

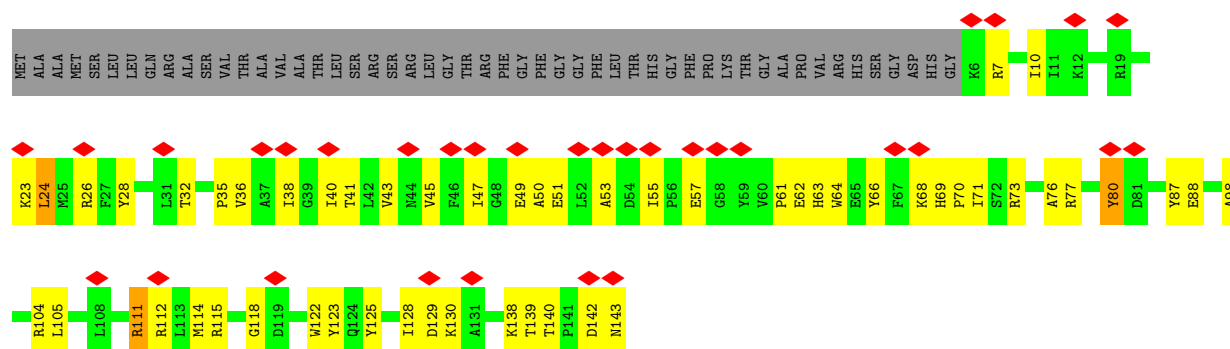


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

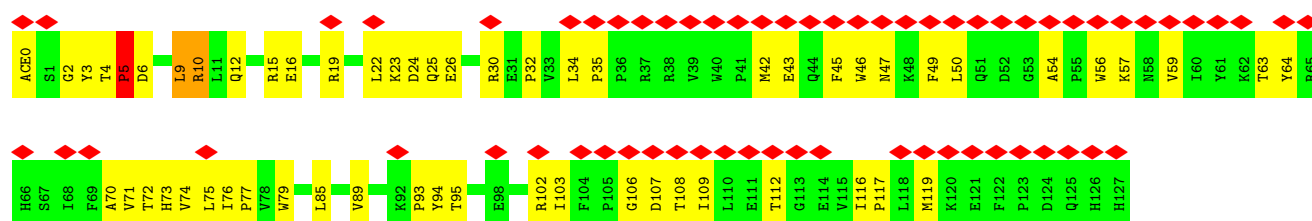


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

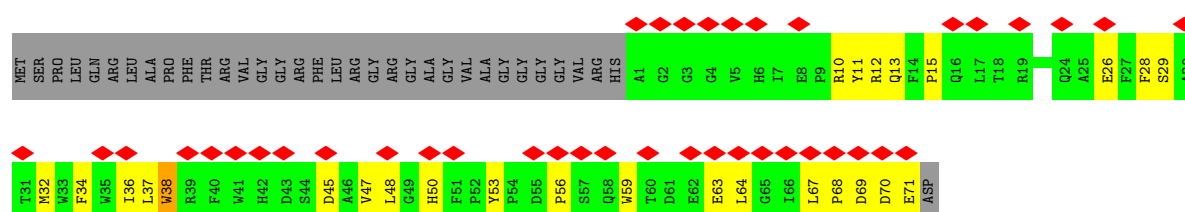
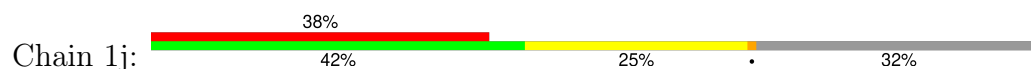




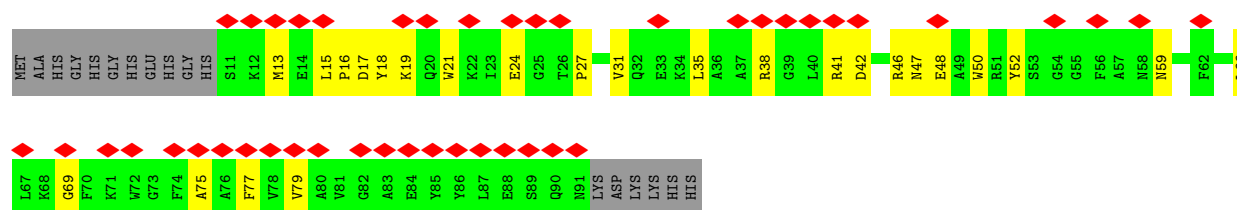
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

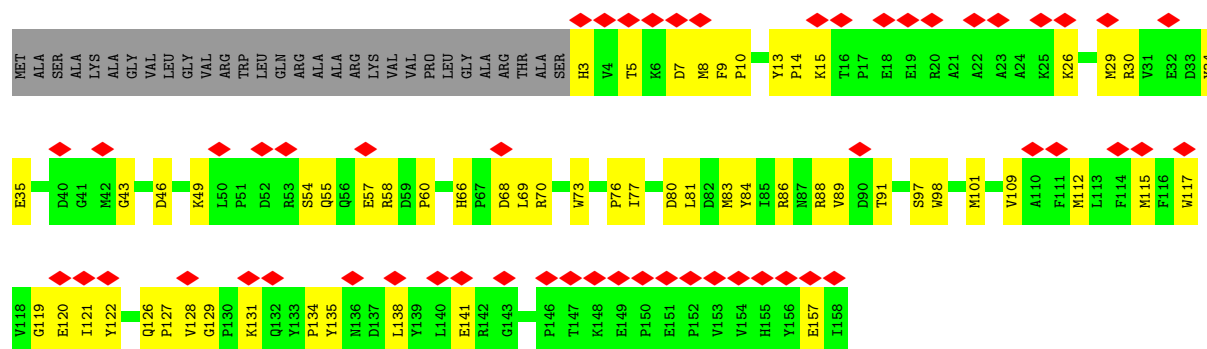


• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

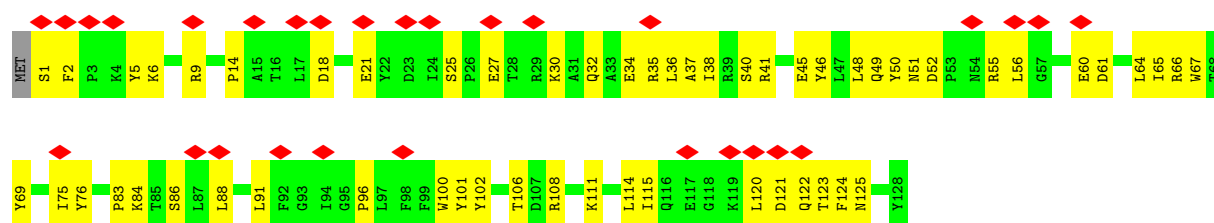


• Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

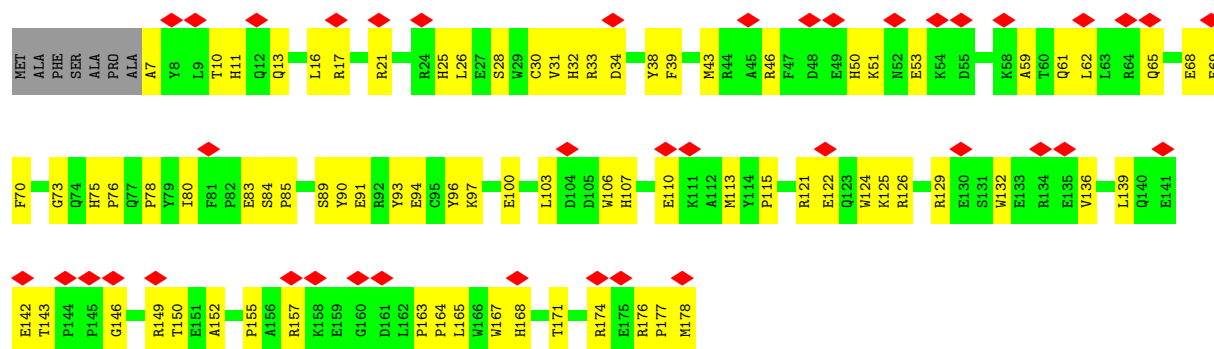




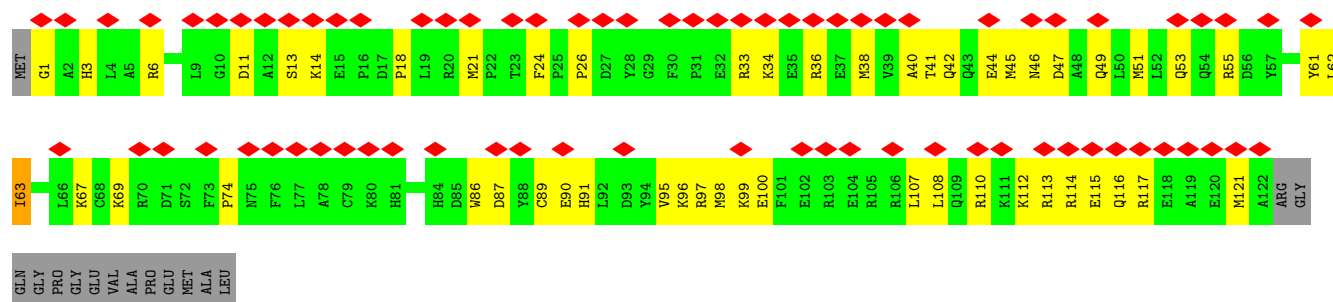
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



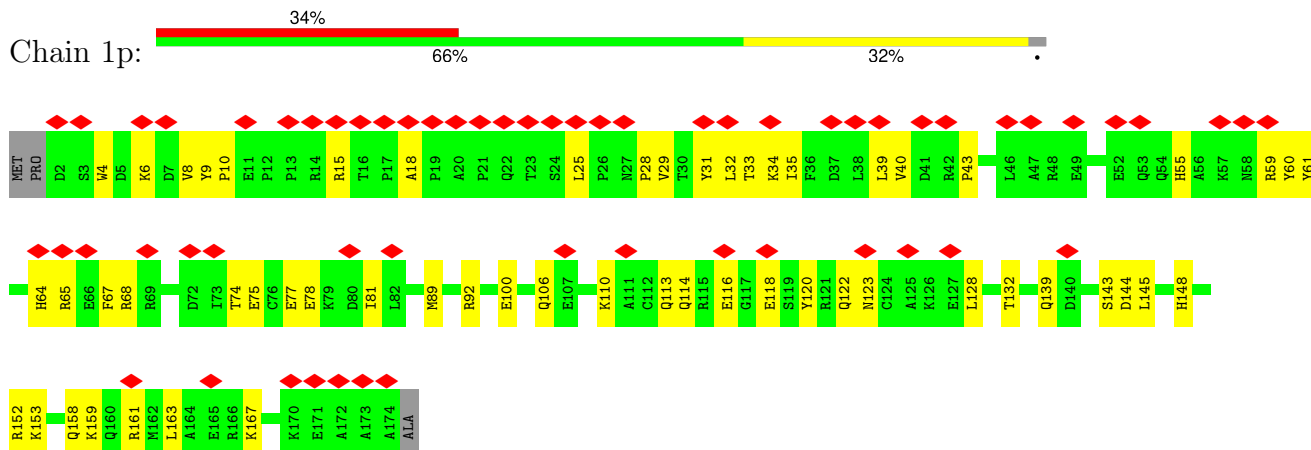
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



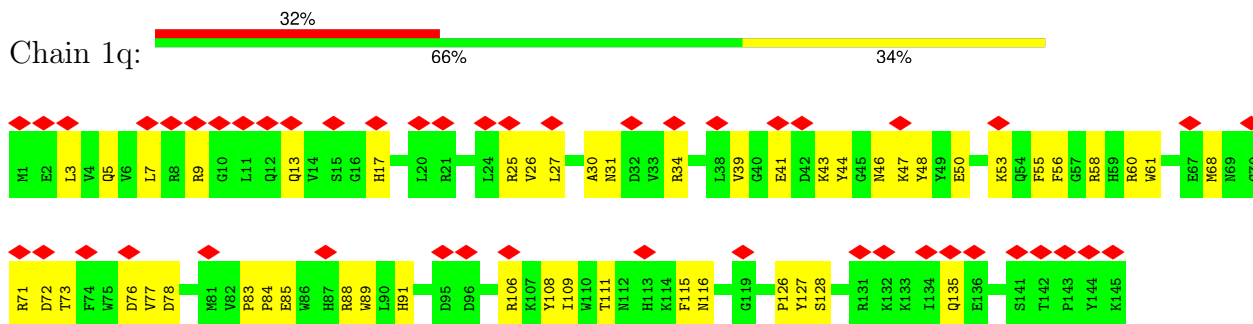
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



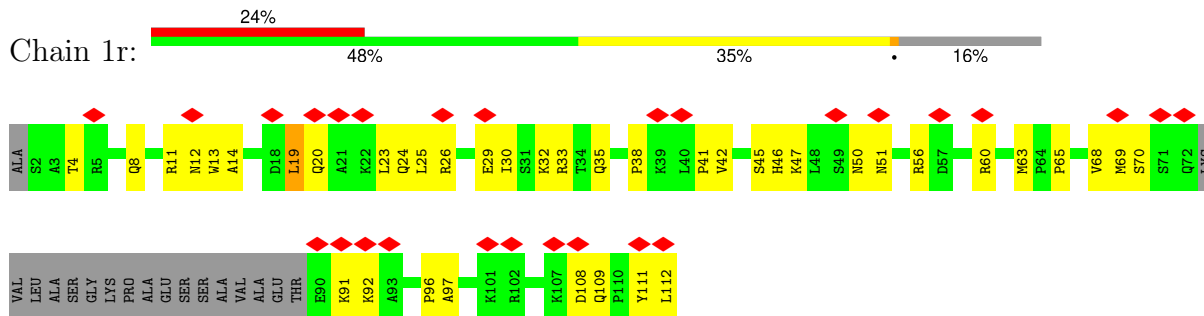
- Chain 1p:



- Chain 1q:



- Chain 1r:



- Chain 1s:



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	30000	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 ($e^-/\text{\AA}^2$)	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	0.782	Depositor
Minimum map value	-0.197	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	426.00003, 426.00003, 426.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.065, 1.065, 1.065	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/938	0.47	0/1281
2	1B	0.16	0/1273	0.39	0/1722
3	1C	0.15	0/1797	0.42	0/2447
4	1D	0.15	0/3545	0.41	0/4806
5	1E	0.16	0/1698	0.44	0/2311
6	1F	0.13	0/3401	0.37	0/4595
7	1G	0.12	0/5451	0.37	0/7387
8	1H	0.17	0/2566	0.45	0/3509
9	1I	0.18	0/1443	0.49	0/1952
10	1J	0.16	0/1357	0.44	0/1840
11	1K	0.19	0/751	0.56	0/1018
12	1L	0.16	0/4939	0.44	0/6718
13	1M	0.15	0/3713	0.40	0/5063
14	1N	0.17	0/2765	0.45	0/3758
15	1O	0.12	0/2650	0.33	0/3588
16	1P	0.12	0/2828	0.33	0/3834
17	1Q	0.17	0/1070	0.44	1/1446 (0.1%)
18	1R	0.15	0/755	0.40	0/1018
19	1S	0.18	0/711	0.50	0/956
20	1T	0.17	0/701	0.51	0/946
20	1U	0.18	0/706	0.53	1/954 (0.1%)
21	1V	0.17	0/946	0.48	0/1281
22	1W	0.27	0/995	0.52	0/1340
23	1X	0.14	0/1436	0.44	0/1938
24	1Y	0.09	0/1037	0.28	0/1404
25	1Z	0.16	0/1199	0.39	0/1617
26	1a	0.15	0/577	0.48	1/777 (0.1%)
27	1b	0.15	0/664	0.40	0/912
28	1c	0.17	0/430	0.55	0/581
29	1d	0.22	0/1016	0.43	0/1374
30	1e	0.17	0/836	0.50	0/1118
31	1f	0.17	0/499	0.55	1/673 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.17	0/858	0.50	0/1165
33	1h	0.27	0/1184	0.54	0/1603
34	1i	0.24	0/1138	0.54	1/1551 (0.1%)
35	1j	0.18	0/627	0.49	0/858
36	1k	0.15	0/668	0.42	0/903
37	1l	0.12	0/1365	0.41	0/1867
38	1m	0.14	0/1092	0.37	0/1481
39	1n	0.14	0/1549	0.39	0/2098
40	1o	0.15	0/1069	0.39	0/1430
41	1p	0.11	0/1481	0.34	0/1997
42	1q	0.14	0/1253	0.36	0/1704
43	1r	0.15	0/777	0.40	0/1051
44	1s	0.21	0/394	0.57	0/533
All	All	0.16	0/68148	0.43	5/92405 (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
7	1G	0	1
8	1H	0	1
21	1V	0	1
29	1d	0	1
33	1h	0	1
34	1i	0	1
All	All	0	6

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1a	57	VAL	N-CA-C	-7.34	106.16	113.20
17	1Q	113	PRO	CA-N-CD	-6.79	102.50	112.00
20	1U	46	ASP	N-CA-C	-5.92	107.29	114.75
34	1i	5	PRO	N-CA-CB	-5.42	97.55	103.25
31	1f	14	ILE	N-CA-C	-5.32	107.65	112.12

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	1G	649	SER	Peptide
8	1H	91	MET	Peptide
21	1V	113	TRP	Peptide
29	1d	86	ARG	Sidechain
33	1h	111	ARG	Sidechain
34	1i	10	ARG	Sidechain

5.2 Too-close contacts ⓘ

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	914	0	951	66	0
2	1B	1242	0	1249	89	0
3	1C	1746	0	1697	91	0
4	1D	3452	0	3389	204	0
5	1E	1658	0	1664	90	0
6	1F	3325	0	3288	168	0
7	1G	5362	0	5387	228	0
8	1H	2494	0	2591	203	0
9	1I	1412	0	1366	93	0
10	1J	1322	0	1319	96	0
11	1K	740	0	788	67	0
12	1L	4808	0	4945	269	0
13	1M	3622	0	3825	216	0
14	1N	2702	0	2862	162	0
15	1O	2590	0	2556	83	0
16	1P	2751	0	2776	109	0
17	1Q	1047	0	1042	55	0
18	1R	741	0	704	29	0
19	1S	700	0	719	44	0
20	1T	689	0	687	28	0
20	1U	694	0	691	41	0
21	1V	927	0	972	38	0
22	1W	971	0	975	64	0
23	1X	1398	0	1378	53	0
24	1Y	1016	0	1020	36	0
25	1Z	1168	0	1161	49	0
26	1a	562	0	557	29	0
27	1b	643	0	645	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	1c	417	0	425	17	0
29	1d	985	0	978	44	0
30	1e	816	0	823	50	0
31	1f	487	0	497	35	0
32	1g	835	0	795	45	0
33	1h	1151	0	1164	53	0
34	1i	1100	0	1107	54	0
35	1j	601	0	546	33	0
36	1k	649	0	626	28	0
37	1l	1310	0	1204	64	0
38	1m	1062	0	1075	54	0
39	1n	1495	0	1434	70	0
40	1o	1045	0	1018	55	0
41	1p	1449	0	1416	66	0
42	1q	1212	0	1174	50	0
43	1r	759	0	783	42	0
44	1s	382	0	351	30	0
45	1A	31	0	36	2	0
45	1D	46	0	66	4	0
45	1L	88	0	127	3	0
45	1M	76	0	100	4	0
45	1Y	106	0	137	11	0
45	1f	51	0	82	2	0
46	1A	27	0	28	1	0
46	1B	82	0	112	2	0
46	1H	54	0	88	3	0
46	1I	44	0	62	6	0
46	1J	32	0	38	2	0
46	1L	38	0	53	4	0
46	1M	35	0	44	1	0
46	1Y	46	0	66	2	0
46	1Z	34	0	42	5	0
46	1d	39	0	52	9	0
46	1f	34	0	40	3	0
46	1h	47	0	71	2	0
47	1B	8	0	0	1	0
47	1F	8	0	0	1	0
47	1G	16	0	0	2	0
47	1I	16	0	0	3	0
48	1E	4	0	0	2	0
48	1G	4	0	0	3	0
49	1F	31	0	19	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
50	1G	1	0	0	0	0
51	1H	51	0	46	4	0
51	1L	76	0	99	3	0
51	1N	132	0	155	8	0
51	1X	86	0	125	12	0
51	1a	61	0	66	4	0
52	1O	32	0	12	2	0
53	1O	1	0	0	0	0
54	1P	48	0	26	8	0
55	1R	1	0	0	0	0
56	1W	37	0	0	0	0
56	1n	37	0	0	2	0
57	1l	15	0	27	2	0
All	All	68026	0	68439	2958	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 22.

All (2958) 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)
13:1M:424:ASN:HD21	38:1m:56:LEU:HA	1.32	0.93
12:1L:151:SER:HB2	12:1L:252:MET:HE1	1.51	0.92
40:1o:113:ARG:HA	40:1o:116:GLN:HE21	1.37	0.89
10:1J:119:PHE:HB2	11:1K:6:MET:HE2	1.53	0.89
20:1T:52:MET:HE1	22:1W:37:ARG:HA	1.55	0.88
7:1G:98:LEU:HD21	7:1G:116:LEU:HD11	1.56	0.88
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.58	0.86
14:1N:30:TRP:HD1	14:1N:70:LEU:HD23	1.40	0.85
11:1K:37:MET:HB3	14:1N:68:MET:HE1	1.58	0.84
14:1N:217:MET:HG3	14:1N:323:MET:HE2	1.60	0.83
2:1B:62:MET:HB2	2:1B:153:ALA:HB1	1.59	0.83
12:1L:282:ALA:HB1	12:1L:411:MET:HE3	1.61	0.83
12:1L:411:MET:HE2	12:1L:411:MET:H	1.43	0.82
39:1n:126:ARG:HH12	39:1n:129:ARG:HD2	1.45	0.82
16:1P:90:VAL:HG12	16:1P:128:LYS:HB2	1.61	0.81
7:1G:143:GLY:HA2	7:1G:190:MET:HE1	1.63	0.81
12:1L:55:MET:HE3	12:1L:471:ASN:HD22	1.44	0.81
4:1D:346:ILE:HD11	7:1G:117:GLN:HA	1.63	0.81
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.61	0.81
19:1S:81:PHE:HD1	19:1S:85:GLN:HG3	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:252:PRO:HG2	17:1Q:44:ASN:HD22	1.47	0.80
29:1d:46:ASN:HB3	29:1d:51:ARG:HB2	1.64	0.80
20:1T:54:MET:HG3	20:1T:76:ILE:HD11	1.64	0.80
20:1T:51:ILE:HA	20:1T:54:MET:HG2	1.65	0.79
14:1N:267:ILE:HG22	14:1N:279:PRO:HB3	1.62	0.79
1:1A:67:LEU:HD21	11:1K:65:VAL:HA	1.64	0.79
10:1J:60:TYR:OH	11:1K:37:MET:SD	2.39	0.79
12:1L:546:GLN:HB2	13:1M:278:ARG:HG2	1.65	0.78
54:1P:501:NDP:H8A	54:1P:501:NDP:H51A	1.65	0.78
4:1D:64:LEU:HD22	4:1D:66:MET:HE2	1.63	0.78
13:1M:364:LEU:HD11	13:1M:369:LEU:HD13	1.65	0.78
32:1g:113:PHE:H	41:1p:158:GLN:HE22	1.32	0.77
6:1F:321:ALA:O	6:1F:324:GLN:NE2	2.18	0.77
3:1C:81:VAL:HG22	4:1D:388:ARG:HG2	1.67	0.77
12:1L:571:MET:HE2	12:1L:571:MET:HA	1.65	0.77
34:1i:10:ARG:HB2	39:1n:155:PRO:HB3	1.65	0.76
43:1r:109:GLN:HE22	43:1r:112:LEU:HA	1.50	0.76
9:1I:155:LEU:HB3	18:1R:36:ASN:HD22	1.50	0.76
13:1M:36:LEU:HB3	46:1f:101:PC1:H342	1.68	0.76
14:1N:108:LEU:HD21	14:1N:191:THR:HG21	1.67	0.76
18:1R:52:VAL:HG21	18:1R:57:ILE:HG13	1.67	0.76
16:1P:235:ARG:HB2	16:1P:341:ASN:HA	1.67	0.76
16:1P:203:GLN:HG2	16:1P:231:VAL:HG22	1.68	0.75
9:1I:150:ASN:ND2	42:1q:127:TYR:O	2.20	0.75
14:1N:261:MET:HE1	14:1N:340:THR:HA	1.69	0.75
35:1j:12:ARG:HB3	36:1k:21:TRP:HH2	1.52	0.75
5:1E:27:ASN:HB3	5:1E:53:LEU:HD11	1.68	0.74
15:1O:104:ARG:NH2	52:1O:401:GTP:N7	2.34	0.74
10:1J:146:LEU:HA	11:1K:58:MET:HE1	1.68	0.74
12:1L:286:LEU:HB2	12:1L:411:MET:HG3	1.68	0.74
23:1X:46:ARG:NH2	33:1h:142:ASP:OD2	2.20	0.74
5:1E:104:THR:HG23	6:1F:349:ARG:HH21	1.49	0.74
7:1G:146:VAL:HG12	7:1G:200:ILE:HD11	1.69	0.74
12:1L:375:ILE:HD11	12:1L:458:LEU:HD21	1.67	0.74
44:1s:40:ASN:O	44:1s:43:HIS:ND1	2.19	0.74
12:1L:254:VAL:HB	12:1L:329:ILE:HD11	1.67	0.74
45:1D:901:3PE:H3B2	12:1L:562:LEU:HG	1.69	0.74
5:1E:205:PRO:HA	44:1s:33:PHE:CE2	2.22	0.74
13:1M:325:MET:HE1	13:1M:441:ILE:HB	1.69	0.73
24:1Y:123:LEU:HB3	45:1Y:804:3PE:H292	1.70	0.73
16:1P:90:VAL:HG11	16:1P:218:ILE:HG23	1.69	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:1X:201:CDL:H521	31:1f:26:LEU:HD23	1.69	0.73
44:1s:33:PHE:HD1	44:1s:34:ASP:N	1.85	0.73
2:1B:122:GLY:HA2	2:1B:135:GLY:HA2	1.68	0.73
17:1Q:67:ASN:H	17:1Q:72:TRP:H	1.35	0.73
5:1E:205:PRO:HA	44:1s:33:PHE:HE2	1.54	0.73
15:1O:94:TYR:HB2	15:1O:144:ILE:HD11	1.70	0.73
15:1O:126:ARG:NH1	15:1O:206:TYR:OH	2.21	0.73
5:1E:183:LYS:O	5:1E:187:ARG:NH2	2.21	0.73
5:1E:184:PRO:HD2	44:1s:44:HIS:CD2	2.24	0.73
4:1D:180:PHE:HB3	4:1D:207:LEU:HD21	1.69	0.72
10:1J:110:GLU:O	30:1e:80:ARG:NH2	2.22	0.72
51:1L:702:CDL:H122	51:1L:702:CDL:H312	1.71	0.72
32:1g:94:GLU:HB3	41:1p:8:VAL:HG21	1.71	0.72
4:1D:425:PHE:HA	4:1D:428:VAL:HG12	1.72	0.72
10:1J:23:LYS:HD2	11:1K:23:ARG:HB3	1.72	0.72
38:1m:51:ASN:OD1	39:1n:168:HIS:ND1	2.15	0.72
4:1D:152:MET:O	4:1D:156:THR:OG1	2.06	0.72
8:1H:196:ALA:HB2	8:1H:274:ARG:HG2	1.70	0.72
12:1L:69:MET:HE1	13:1M:451:PRO:HD2	1.71	0.72
8:1H:39:VAL:HA	42:1q:31:ASN:HD21	1.53	0.72
12:1L:449:LEU:O	12:1L:453:SER:OG	2.08	0.72
9:1I:113:MET:HA	9:1I:116:CYS:HB3	1.72	0.72
7:1G:434:SER:OG	7:1G:436:ASN:ND2	2.23	0.71
7:1G:668:ILE:HB	7:1G:691:VAL:HG21	1.72	0.71
12:1L:324:LEU:HB3	12:1L:395:ILE:HD11	1.72	0.71
14:1N:59:TYR:HE1	14:1N:63:GLN:HE21	1.37	0.71
14:1N:239:VAL:HG21	29:1d:47:ALA:HB1	1.71	0.71
15:1O:301:GLY:HA2	15:1O:309:ASN:HD22	1.56	0.71
9:1I:104:ARG:O	9:1I:104:ARG:NH1	2.20	0.71
12:1L:69:MET:HB2	12:1L:76:LEU:HB2	1.72	0.71
51:1X:201:CDL:H321	29:1d:29:PRO:HB2	1.71	0.71
4:1D:80:ILE:HD11	4:1D:429:ASP:HB2	1.72	0.71
6:1F:31:TRP:NE1	44:1s:40:ASN:OD1	2.24	0.71
14:1N:154:MET:HE1	14:1N:191:THR:HB	1.71	0.71
5:1E:111:ARG:HB2	5:1E:152:PRO:HD3	1.72	0.71
7:1G:190:MET:HE2	7:1G:190:MET:HA	1.73	0.71
12:1L:407:TRP:CD1	12:1L:410:LEU:HB2	2.26	0.71
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.71	0.71
32:1g:85:MET:HB2	32:1g:88:TRP:HB3	1.73	0.71
2:1B:116:MET:SD	2:1B:156:LEU:HG	2.31	0.70
11:1K:62:ILE:HA	11:1K:65:VAL:HG23	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:240:ILE:HD11	29:1d:48:ILE:HG23	1.73	0.70
34:1i:76:ILE:HG13	34:1i:77:PRO:HD3	1.74	0.70
35:1j:53:TYR:OH	40:1o:98:MET:SD	2.47	0.70
17:1Q:69:LEU:HD23	17:1Q:70:MET:HG2	1.72	0.70
44:1s:34:ASP:OD1	44:1s:36:SER:N	2.23	0.70
3:1C:35:LYS:HA	21:1V:102:LEU:HA	1.74	0.70
1:1A:44:MET:HA	22:1W:96:VAL:HG11	1.73	0.70
12:1L:270:ASN:O	12:1L:274:GLN:NE2	2.23	0.70
32:1g:112:CYS:SG	41:1p:158:GLN:NE2	2.64	0.70
37:1l:134:PRO:HG3	40:1o:38:MET:HE3	1.74	0.70
17:1Q:42:ARG:HH21	17:1Q:44:ASN:HA	1.56	0.70
36:1k:18:TYR:HE1	36:1k:46:ARG:HD2	1.57	0.70
4:1D:163:ALA:H	8:1H:278:PRO:HA	1.55	0.70
3:1C:40:VAL:HG22	43:1r:69:MET:HE3	1.74	0.69
3:1C:205:ALA:O	43:1r:60:ARG:NH1	2.24	0.69
10:1J:167:VAL:HG22	14:1N:42:PRO:HG3	1.74	0.69
12:1L:253:VAL:HB	12:1L:310:LEU:HD11	1.74	0.69
14:1N:269:GLU:OE2	14:1N:269:GLU:N	2.19	0.69
3:1C:35:LYS:NZ	21:1V:97:LYS:O	2.25	0.69
37:1l:30:ARG:HH22	38:1m:35:ARG:HG3	1.54	0.69
5:1E:143:GLU:HG3	6:1F:349:ARG:HH22	1.57	0.69
38:1m:75:ILE:H	38:1m:75:ILE:HD12	1.57	0.69
4:1D:170:MET:HE2	4:1D:225:LEU:HD12	1.73	0.69
1:1A:8:LEU:O	1:1A:12:THR:OG1	2.09	0.69
18:1R:37:GLU:OE1	18:1R:37:GLU:N	2.24	0.69
37:1l:138:LEU:HB3	37:1l:141:GLU:HG2	1.75	0.69
6:1F:197:GLU:OE2	17:1Q:129:ARG:NH2	2.25	0.69
9:1I:174:LEU:HD13	43:1r:38:PRO:HD2	1.75	0.69
12:1L:407:TRP:HD1	12:1L:410:LEU:HB2	1.57	0.69
17:1Q:30:ILE:HG23	17:1Q:31:LYS:HD3	1.73	0.69
38:1m:1:SER:OG	38:1m:2:PHE:N	2.25	0.69
6:1F:370:ASP:OD2	7:1G:179:ASN:ND2	2.25	0.69
11:1K:36:MET:HG2	14:1N:68:MET:HE3	1.75	0.69
13:1M:32:LEU:O	13:1M:35:SER:OG	2.10	0.69
40:1o:113:ARG:HA	40:1o:116:GLN:NE2	2.07	0.69
4:1D:101:PRO:O	4:1D:105:ARG:NH1	2.25	0.68
14:1N:72:MET:HA	14:1N:75:ILE:HB	1.75	0.68
32:1g:101:GLU:OE1	32:1g:101:GLU:N	2.25	0.68
17:1Q:10:LEU:HB3	22:1W:16:SER:HB2	1.73	0.68
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.08	0.68
44:1s:42:GLN:N	44:1s:42:GLN:OE1	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:145:GLU:HB3	42:1q:126:PRO:HG3	1.76	0.68
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.26	0.68
8:1H:98:MET:HE1	46:1Z:201:PC1:H12	1.76	0.68
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.76	0.68
9:1I:14:MET:HE2	9:1I:14:MET:HA	1.75	0.68
12:1L:439:PRO:HD2	20:1U:57:GLU:HA	1.76	0.68
34:1i:116:ILE:HD12	34:1i:117:PRO:HD2	1.75	0.68
5:1E:146:GLY:N	48:1E:301:FES:S1	2.64	0.67
15:1O:126:ARG:NH2	52:1O:401:GTP:O2A	2.27	0.67
25:1Z:90:ASN:ND2	25:1Z:123:GLU:O	2.27	0.67
4:1D:161:ILE:HG23	4:1D:238:ARG:HD2	1.76	0.67
7:1G:221:GLU:HG3	7:1G:243:ARG:HG3	1.76	0.67
4:1D:18:VAL:HG12	4:1D:20:TYR:H	1.58	0.67
4:1D:412:ALA:HB3	8:1H:281:ARG:HD3	1.76	0.67
7:1G:644:GLN:NE2	19:1S:37:GLU:O	2.28	0.67
13:1M:68:LEU:HD22	13:1M:317:ILE:HG23	1.76	0.67
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.76	0.67
12:1L:183:VAL:HG21	13:1M:400:MET:HE1	1.76	0.67
2:1B:158:TYR:HE2	42:1q:78:ASP:HB2	1.60	0.67
34:1i:106:GLY:H	34:1i:116:ILE:HG23	1.60	0.67
13:1M:430:PHE:O	13:1M:434:ASN:ND2	2.26	0.67
2:1B:119:CYS:HA	2:1B:124:GLY:HA3	1.76	0.67
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.74	0.67
2:1B:46:TRP:H	2:1B:84:ASP:HB2	1.59	0.67
8:1H:98:MET:HE3	8:1H:100:LEU:H	1.58	0.67
12:1L:396:ILE:O	12:1L:400:ASN:ND2	2.26	0.67
20:1U:68:GLU:HG3	34:1i:0:ACE:H1	1.75	0.67
2:1B:86:MET:HB3	2:1B:113:VAL:HG22	1.75	0.67
12:1L:411:MET:O	12:1L:415:ALA:N	2.23	0.67
2:1B:89:ALA:HA	2:1B:116:MET:HB2	1.77	0.66
33:1h:23:LYS:HA	33:1h:23:LYS:HE2	1.77	0.66
6:1F:319:PHE:O	6:1F:323:VAL:HG23	1.95	0.66
12:1L:407:TRP:HA	12:1L:410:LEU:HD13	1.77	0.66
18:1R:20:ASP:O	18:1R:25:ARG:NH2	2.28	0.66
7:1G:437:HIS:HE1	7:1G:439:PHE:HB2	1.60	0.66
12:1L:131:LEU:HB2	12:1L:143:GLY:HA3	1.77	0.66
14:1N:135:LYS:NZ	14:1N:187:MET:SD	2.68	0.66
6:1F:368:GLY:HA3	6:1F:399:ILE:HD11	1.77	0.66
7:1G:579:ARG:HB2	7:1G:636:VAL:HG12	1.78	0.66
26:1a:23:THR:O	26:1a:27:HIS:ND1	2.27	0.66
6:1F:108:ARG:NH1	6:1F:145:GLU:OE2	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:36:GLN:NE2	17:1Q:47:SER:O	2.29	0.66
10:1J:173:ARG:HH12	15:1O:254:ARG:HE	1.43	0.66
7:1G:582:GLN:OE1	7:1G:620:ARG:NH2	2.29	0.66
12:1L:51:LEU:HD12	12:1L:91:PRO:HG2	1.77	0.66
17:1Q:107:GLU:OE1	17:1Q:107:GLU:N	2.29	0.66
25:1Z:80:ASP:OD1	25:1Z:81:ARG:N	2.29	0.66
7:1G:21:GLU:OE1	7:1G:21:GLU:N	2.29	0.66
30:1e:49:ILE:HD11	33:1h:118:GLY:HA3	1.77	0.66
30:1e:86:ILE:HG22	30:1e:91:TYR:HB3	1.77	0.66
40:1o:42:GLN:HA	40:1o:45:MET:HB3	1.78	0.66
5:1E:36:LYS:O	44:1s:65:GLN:NE2	2.29	0.66
6:1F:321:ALA:HA	6:1F:324:GLN:HE21	1.61	0.66
37:1l:128:VAL:HG12	40:1o:98:MET:HE1	1.78	0.66
7:1G:615:THR:OG1	7:1G:618:GLN:OE1	2.13	0.66
10:1J:82:VAL:HG13	10:1J:84:VAL:H	1.61	0.66
23:1X:134:ARG:O	27:1b:57:ARG:NH2	2.29	0.66
12:1L:276:MET:HA	12:1L:279:CYS:HB2	1.77	0.65
32:1g:62:PHE:HB3	33:1h:28:TYR:HD2	1.61	0.65
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.28	0.65
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	1.76	0.65
5:1E:87:TYR:HD2	6:1F:181:ALA:HB3	1.61	0.65
1:1A:80:GLN:HE22	8:1H:316:PRO:HA	1.61	0.65
3:1C:78:LEU:O	4:1D:390:LYS:NZ	2.30	0.65
3:1C:210:ARG:CZ	7:1G:35:MET:HE1	2.27	0.65
7:1G:331:LEU:HD22	7:1G:525:LEU:HD22	1.77	0.65
15:1O:288:GLN:NE2	32:1g:29:ASP:OD1	2.29	0.65
34:1i:6:ASP:HA	34:1i:9:LEU:HD23	1.79	0.65
39:1n:90:TYR:HD1	39:1n:91:GLU:HG2	1.61	0.65
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.78	0.65
12:1L:29:THR:O	12:1L:31:LEU:N	2.30	0.65
12:1L:222:GLY:HA2	12:1L:229:LEU:HD23	1.78	0.65
13:1M:7:PRO:HA	13:1M:10:MET:HB2	1.79	0.65
20:1U:45:LEU:N	56:1n:201:EHZ:O7	2.29	0.65
43:1r:32:LYS:O	43:1r:35:GLN:NE2	2.24	0.65
6:1F:120:GLU:HG3	6:1F:232:PRO:HG2	1.77	0.65
12:1L:584:ILE:HD11	14:1N:58:LYS:HG2	1.79	0.65
13:1M:59:ASP:OD1	13:1M:245:ARG:NH2	2.29	0.65
23:1X:46:ARG:NH1	25:1Z:76:GLN:OE1	2.30	0.65
10:1J:36:SER:HA	10:1J:39:VAL:HG22	1.79	0.65
10:1J:71:THR:HA	10:1J:75:ALA:HB3	1.79	0.65
13:1M:130:LEU:HD22	14:1N:294:MET:HE1	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:108:TYR:OH	15:1O:164:LEU:O	2.15	0.65
17:1Q:33:ARG:NH2	17:1Q:60:ASP:O	2.30	0.65
23:1X:110:VAL:HB	23:1X:116:TRP:HB2	1.79	0.65
51:1X:201:CDL:H571	51:1X:201:CDL:H112	1.78	0.65
31:1f:15:LEU:HA	31:1f:18:VAL:HG22	1.78	0.65
39:1n:50:HIS:ND1	39:1n:50:HIS:O	2.27	0.65
41:1p:8:VAL:HG23	41:1p:9:TYR:HD1	1.62	0.65
9:1I:69:ARG:HH12	18:1R:36:ASN:HD21	1.45	0.65
10:1J:138:GLU:N	10:1J:138:GLU:OE1	2.30	0.65
38:1m:32:GLN:HA	38:1m:35:ARG:HD3	1.79	0.65
12:1L:532:ILE:HD11	37:1l:101:MET:HB3	1.78	0.64
13:1M:130:LEU:O	13:1M:134:THR:OG1	2.13	0.64
14:1N:243:LEU:HD21	29:1d:44:ILE:HD11	1.79	0.64
39:1n:150:THR:HG22	39:1n:152:ALA:H	1.62	0.64
44:1s:72:SER:H	44:1s:75:HIS:HB2	1.62	0.64
16:1P:263:TYR:HD2	16:1P:284:VAL:HG13	1.62	0.64
1:1A:109:LYS:HA	1:1A:109:LYS:HE3	1.79	0.64
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.79	0.64
12:1L:387:THR:HG22	12:1L:465:GLY:H	1.62	0.64
4:1D:343:GLU:HG2	7:1G:128:SER:HB3	1.80	0.64
10:1J:100:GLU:OE1	10:1J:100:GLU:N	2.23	0.64
13:1M:14:MET:O	13:1M:18:SER:OG	2.15	0.64
33:1h:55:ILE:HG22	33:1h:57:GLU:H	1.62	0.64
2:1B:42:ARG:O	2:1B:164:GLN:NE2	2.29	0.64
6:1F:99:GLU:CD	6:1F:107:ASP:HB2	2.23	0.64
31:1f:49:ARG:HB2	31:1f:52:GLU:HG2	1.78	0.64
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.33	0.64
1:1A:60:ILE:HB	10:1J:168:ILE:HD12	1.80	0.64
38:1m:83:PRO:O	38:1m:86:SER:OG	2.16	0.64
5:1E:145:LEU:N	48:1E:301:FES:S1	2.71	0.64
51:1H:402:CDL:H722	51:1H:402:CDL:H521	1.80	0.64
2:1B:134:ARG:O	2:1B:138:ARG:NH1	2.30	0.64
5:1E:82:GLU:OE1	6:1F:200:GLN:NE2	2.31	0.64
15:1O:84:ASP:HA	15:1O:193:LYS:HD3	1.80	0.64
16:1P:135:LEU:HA	16:1P:167:LYS:HD3	1.79	0.64
5:1E:102:VAL:HG21	5:1E:117:LEU:HD23	1.79	0.63
51:1a:101:CDL:OB3	43:1r:4:THR:OG1	2.16	0.63
2:1B:146:VAL:HG11	2:1B:156:LEU:HD23	1.80	0.63
5:1E:202:LEU:HD23	6:1F:20:ARG:HD3	1.79	0.63
13:1M:423:ILE:HD12	13:1M:423:ILE:O	1.98	0.63
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.63	0.63
8:1H:269:THR:O	8:1H:273:ILE:HD12	1.97	0.63
13:1M:181:TYR:O	41:1p:152:ARG:NH2	2.30	0.63
20:1T:14:ARG:HH22	20:1T:17:TYR:HD2	1.46	0.63
20:1U:69:LYS:HA	34:1i:2:GLY:HA2	1.80	0.63
23:1X:92:GLY:N	26:1a:35:GLU:OE2	2.29	0.63
2:1B:108:PRO:HG3	8:1H:61:LEU:HD22	1.81	0.63
2:1B:114:VAL:HG23	2:1B:144:ILE:HB	1.81	0.63
5:1E:102:VAL:HG12	5:1E:154:VAL:HG22	1.79	0.63
13:1M:12:LEU:HD11	13:1M:97:THR:HG23	1.78	0.63
20:1T:14:ARG:NH1	20:1T:14:ARG:HA	2.13	0.63
31:1f:25:TYR:O	31:1f:29:ARG:N	2.29	0.63
3:1C:182:ARG:HH12	3:1C:184:VAL:HB	1.64	0.63
5:1E:22:ASP:O	5:1E:57:GLN:NE2	2.32	0.63
8:1H:307:LEU:HA	8:1H:310:MET:HB2	1.81	0.63
51:1N:402:CDL:OA7	51:1N:402:CDL:O1	2.16	0.63
10:1J:77:GLU:N	10:1J:77:GLU:OE1	2.32	0.63
13:1M:9:THR:HG21	51:1X:201:CDL:H632	1.80	0.63
14:1N:261:MET:HE2	46:1d:201:PC1:H3E2	1.80	0.63
13:1M:141:GLU:OE1	13:1M:141:GLU:N	2.32	0.63
13:1M:183:SER:H	41:1p:152:ARG:HH22	1.47	0.63
22:1W:66:MET:HE1	22:1W:106:PHE:HD1	1.64	0.63
11:1K:77:LEU:HD11	14:1N:41:ILE:HG21	1.81	0.63
16:1P:177:ARG:NH2	54:1P:501:NDP:O1A	2.31	0.63
31:1f:39:ASN:ND2	31:1f:46:ARG:O	2.31	0.63
45:1D:901:3PE:H382	13:1M:151:PHE:HB3	1.81	0.63
7:1G:231:MET:N	7:1G:231:MET:SD	2.72	0.63
12:1L:576:MET:HA	12:1L:579:ASN:HB2	1.81	0.63
37:1l:8:MET:HA	37:1l:26:LYS:HG3	1.81	0.63
4:1D:66:MET:HB3	4:1D:68:LEU:HD23	1.81	0.62
6:1F:50:LEU:HG	6:1F:169:SER:HB3	1.80	0.62
7:1G:135:ARG:NH1	7:1G:179:ASN:OD1	2.32	0.62
7:1G:596:ASP:OD1	7:1G:597:TRP:N	2.32	0.62
12:1L:578:SER:OG	14:1N:171:ASN:ND2	2.31	0.62
37:1l:5:THR:OG1	37:1l:7:ASP:OD1	2.17	0.62
39:1n:43:MET:HE3	39:1n:46:ARG:HH21	1.64	0.62
2:1B:34:ASP:HA	2:1B:173:LEU:HD21	1.81	0.62
2:1B:86:MET:HB2	2:1B:107:MET:HE1	1.82	0.62
3:1C:8:ARG:H	3:1C:8:ARG:HD2	1.64	0.62
9:1I:49:ASN:O	9:1I:53:GLU:N	2.32	0.62
13:1M:243:MET:O	13:1M:247:THR:OG1	2.17	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:115:GLU:OE2	29:1d:117:HIS:NE2	2.32	0.62
34:1i:26:GLU:OE2	34:1i:26:GLU:N	2.29	0.62
4:1D:80:ILE:HD12	4:1D:81:GLY:H	1.64	0.62
4:1D:410:MET:HE1	8:1H:282:TYR:HE1	1.64	0.62
8:1H:92:PRO:HG3	8:1H:255:TYR:HB3	1.82	0.62
9:1I:65:HIS:NE2	47:1I:201:SF4:S1	2.72	0.62
15:1O:37:ARG:HH12	15:1O:40:ARG:HH21	1.47	0.62
23:1X:17:VAL:HG11	25:1Z:74:LEU:HD11	1.80	0.62
29:1d:78:ARG:HH12	46:1d:201:PC1:H221	1.64	0.62
2:1B:82:GLN:HE22	8:1H:220:PHE:HE2	1.46	0.62
7:1G:232:ASP:OD1	7:1G:233:ALA:N	2.32	0.62
9:1I:45:PRO:HB2	9:1I:47:THR:HG23	1.82	0.62
14:1N:250:SER:O	14:1N:259:GLY:HA3	1.99	0.62
30:1e:60:ASP:HA	30:1e:63:VAL:HG12	1.81	0.62
42:1q:53:LYS:HA	42:1q:53:LYS:HE3	1.82	0.62
9:1I:39:SER:HB3	43:1r:14:ALA:HB3	1.81	0.62
23:1X:112:ASP:OD1	23:1X:113:LYS:N	2.32	0.62
42:1q:50:GLU:HG2	42:1q:60:ARG:HG2	1.80	0.62
6:1F:278:GLU:N	6:1F:278:GLU:OE1	2.30	0.62
8:1H:296:LEU:HA	27:1b:21:SER:HB3	1.80	0.62
13:1M:139:GLN:HG3	13:1M:340:ARG:HH22	1.64	0.62
14:1N:9:LEU:HB3	14:1N:39:ALA:HB1	1.81	0.62
32:1g:92:GLU:HB3	41:1p:64:HIS:HE2	1.65	0.62
37:1l:109:VAL:HA	37:1l:112:MET:HG2	1.82	0.62
4:1D:282:GLU:O	4:1D:313:GLN:NE2	2.25	0.62
5:1E:116:ILE:HD12	5:1E:152:PRO:HB2	1.82	0.62
6:1F:105:CYS:H	6:1F:257:ASN:HD22	1.46	0.62
8:1H:214:GLU:OE1	8:1H:214:GLU:N	2.31	0.62
12:1L:153:LEU:HD21	13:1M:360:LEU:HD21	1.82	0.62
16:1P:73:TRP:CZ2	54:1P:501:NDP:H2A	2.35	0.62
6:1F:157:TYR:HB2	6:1F:162:ILE:HG23	1.82	0.62
14:1N:332:LEU:HD21	51:1N:401:CDL:H432	1.82	0.62
9:1I:44:GLU:OE2	9:1I:44:GLU:N	2.30	0.62
17:1Q:129:ARG:HD3	44:1s:73:PRO:HB3	1.82	0.62
18:1R:51:GLU:HG3	18:1R:94:PRO:HA	1.82	0.62
43:1r:29:GLU:OE2	43:1r:29:GLU:N	2.27	0.62
3:1C:88:ASN:HD21	21:1V:110:GLN:HE21	1.48	0.62
6:1F:342:ASP:OD2	6:1F:429:ARG:NH2	2.33	0.62
12:1L:415:ALA:O	12:1L:419:THR:N	2.30	0.62
28:1c:39:VAL:O	28:1c:43:LYS:HG3	2.00	0.62
6:1F:15:LEU:HD13	6:1F:271:GLU:HB2	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:27:LEU:HD13	7:1G:37:ILE:HB	1.82	0.61
8:1H:63:PRO:O	8:1H:66:SER:OG	2.17	0.61
51:1N:401:CDL:HB62	51:1N:401:CDL:H322	1.82	0.61
27:1b:24:ILE:H	27:1b:24:ILE:HD12	1.65	0.61
39:1n:167:TRP:O	39:1n:171:THR:OG1	2.17	0.61
41:1p:116:GLU:OE1	41:1p:123:ASN:ND2	2.28	0.61
4:1D:201:GLN:HA	4:1D:323:ILE:HD12	1.82	0.61
7:1G:43:HIS:NE2	7:1G:261:GLU:OE2	2.32	0.61
7:1G:216:THR:O	7:1G:243:ARG:NH2	2.33	0.61
7:1G:380:VAL:HB	7:1G:453:LEU:HG	1.81	0.61
13:1M:37:ILE:H	13:1M:37:ILE:HD12	1.65	0.61
15:1O:265:ASN:HD22	15:1O:268:GLU:H	1.48	0.61
34:1i:43:GLU:O	34:1i:47:ASN:ND2	2.33	0.61
3:1C:211:GLN:NE2	21:1V:114:PRO:O	2.32	0.61
6:1F:101:GLU:O	6:1F:104:THR:OG1	2.15	0.61
14:1N:81:SER:O	14:1N:83:GLN:NE2	2.33	0.61
19:1S:12:LYS:HD2	19:1S:13:LEU:H	1.65	0.61
19:1S:73:GLU:C	19:1S:74:LYS:HE2	2.25	0.61
39:1n:107:HIS:HB3	39:1n:110:GLU:HG3	1.82	0.61
6:1F:348:ALA:HA	6:1F:376:MET:HE1	1.83	0.61
11:1K:78:LEU:HD21	11:1K:88:ASP:HB2	1.81	0.61
12:1L:346:ILE:HD11	12:1L:359:MET:HG2	1.83	0.61
13:1M:325:MET:HE3	13:1M:440:HIS:HB3	1.82	0.61
14:1N:55:ALA:HB1	14:1N:118:VAL:HG23	1.82	0.61
36:1k:24:GLU:N	36:1k:24:GLU:OE2	2.34	0.61
2:1B:173:LEU:HD23	2:1B:173:LEU:H	1.65	0.61
3:1C:35:LYS:HE2	21:1V:100:GLU:HB2	1.82	0.61
13:1M:278:ARG:NH1	37:1l:80:ASP:OD1	2.31	0.61
23:1X:110:VAL:O	23:1X:116:TRP:N	2.26	0.61
37:1l:69:LEU:HD23	37:1l:81:LEU:HD11	1.82	0.61
3:1C:193:GLU:OE2	3:1C:193:GLU:N	2.29	0.61
17:1Q:57:MET:HE2	17:1Q:84:LEU:HD12	1.81	0.61
23:1X:43:MET:HA	23:1X:46:ARG:HB2	1.81	0.61
2:1B:57:VAL:HG13	4:1D:189:MET:HE1	1.81	0.61
8:1H:98:MET:CE	8:1H:100:LEU:H	2.13	0.61
9:1l:64:GLU:HB3	9:1l:139:PHE:CD1	2.36	0.61
13:1M:237:LYS:HD2	13:1M:316:MET:HG3	1.83	0.61
8:1H:90:PRO:HD3	8:1H:162:LEU:HD13	1.83	0.61
15:1O:3:TYR:HD1	15:1O:7:ALA:HB3	1.66	0.61
32:1g:77:VAL:HA	32:1g:80:LEU:HG	1.82	0.61
8:1H:207:LEU:O	8:1H:209:SER:N	2.34	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:34:LEU:O	21:1V:44:ARG:NH1	2.34	0.61
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.83	0.61
9:1I:148:LEU:HD11	42:1q:126:PRO:HB3	1.82	0.61
10:1J:130:THR:HG22	25:1Z:121:MET:HB3	1.83	0.61
11:1K:26:LEU:HD22	11:1K:78:LEU:HD23	1.83	0.61
16:1P:202:LYS:HA	16:1P:291:ASP:HB2	1.82	0.61
1:1A:88:LEU:HD23	8:1H:309:ILE:HD12	1.81	0.60
7:1G:237:ASN:HD21	7:1G:255:HIS:HB2	1.64	0.60
8:1H:75:PRO:HG3	8:1H:215:TYR:HE2	1.66	0.60
12:1L:433:GLY:O	36:1k:59:ASN:ND2	2.34	0.60
15:1O:8:PHE:O	15:1O:13:ARG:NH1	2.33	0.60
25:1Z:141:ILE:HG22	46:1Z:201:PC1:H221	1.83	0.60
4:1D:180:PHE:O	4:1D:184:VAL:HG12	2.01	0.60
4:1D:325:VAL:HG22	4:1D:327:ASP:H	1.66	0.60
7:1G:157:THR:HA	7:1G:160:ILE:HD13	1.82	0.60
13:1M:101:LEU:HD23	13:1M:128:PRO:HG3	1.83	0.60
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.84	0.60
13:1M:286:ILE:HG12	13:1M:326:LEU:HB3	1.83	0.60
14:1N:294:MET:O	14:1N:298:TYR:N	2.31	0.60
32:1g:117:LYS:NZ	41:1p:74:THR:OG1	2.34	0.60
5:1E:120:ILE:HD12	5:1E:169:ILE:HD13	1.82	0.60
6:1F:99:GLU:HG3	6:1F:107:ASP:HB2	1.82	0.60
1:1A:61:THR:HG22	10:1J:168:ILE:HD11	1.83	0.60
2:1B:55:CYS:HB3	2:1B:116:MET:HE3	1.84	0.60
3:1C:116:PRO:HG3	22:1W:20:ILE:HG12	1.84	0.60
4:1D:413:ASP:OD2	8:1H:281:ARG:NH2	2.34	0.60
8:1H:149:ILE:HG23	8:1H:181:LEU:HD12	1.83	0.60
24:1Y:10:ASP:OD1	24:1Y:10:ASP:N	2.34	0.60
40:1o:47:ASP:OD2	41:1p:15:ARG:NH2	2.33	0.60
41:1p:55:HIS:O	41:1p:59:ARG:NH1	2.34	0.60
7:1G:174:THR:HA	7:1G:183:VAL:HA	1.83	0.60
7:1G:341:ASP:O	7:1G:508:LYS:NZ	2.34	0.60
8:1H:28:LEU:O	8:1H:32:GLN:HB2	2.01	0.60
13:1M:355:MET:HE1	13:1M:437:MET:HE2	1.82	0.60
14:1N:5:ILE:O	14:1N:8:THR:OG1	2.18	0.60
24:1Y:127:GLY:HA3	45:1Y:804:3PE:H231	1.84	0.60
35:1j:11:TYR:HD2	36:1k:16:PRO:HD2	1.65	0.60
40:1o:114:ARG:HD3	40:1o:117:ARG:HH12	1.67	0.60
1:1A:25:PRO:HG2	8:1H:60:PRO:HD3	1.83	0.60
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.34	0.60
7:1G:243:ARG:HB3	7:1G:248:MET:HE1	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:41:PHE:O	11:1K:45:THR:OG1	2.14	0.60
12:1L:561:ILE:HG13	46:1Y:803:PC1:H2A2	1.82	0.60
28:1c:32:ILE:HD12	28:1c:32:ILE:H	1.64	0.60
41:1p:148:HIS:O	41:1p:153:LYS:NZ	2.31	0.60
4:1D:43:LEU:HD13	11:1K:86:GLY:HA3	1.82	0.60
4:1D:105:ARG:NE	9:1I:117:ILE:HD11	2.17	0.60
13:1M:124:ALA:HB1	14:1N:256:PRO:HD3	1.83	0.60
16:1P:319:ARG:HA	16:1P:322:ARG:HD2	1.84	0.60
22:1W:61:ASP:HA	22:1W:64:ARG:HB2	1.83	0.60
24:1Y:140:VAL:HG23	33:1h:111:ARG:HG2	1.83	0.60
34:1i:119:MET:HE1	40:1o:63:ILE:HG21	1.84	0.60
39:1n:106:TRP:HB3	39:1n:110:GLU:HB2	1.83	0.60
3:1C:86:ARG:NH1	3:1C:91:GLU:OE1	2.34	0.60
12:1L:303:ALA:O	12:1L:306:THR:OG1	2.19	0.60
22:1W:19:PRO:HG2	22:1W:23:ARG:HE	1.65	0.60
26:1a:3:PHE:HA	26:1a:6:LEU:HD23	1.83	0.60
51:1a:101:CDL:O1	42:1q:9:ARG:NH2	2.33	0.60
5:1E:13:PRO:O	5:1E:16:ASN:ND2	2.35	0.60
6:1F:100:GLY:HA3	6:1F:184:TYR:HB2	1.83	0.60
7:1G:514:ILE:HD12	7:1G:519:PRO:HG3	1.84	0.60
8:1H:23:VAL:O	8:1H:27:VAL:HG12	2.02	0.60
9:1I:73:GLY:HA3	18:1R:43:LEU:HD12	1.83	0.60
26:1a:27:HIS:O	26:1a:31:ASN:ND2	2.35	0.60
4:1D:91:ILE:HG21	4:1D:389:CYS:HB3	1.83	0.60
7:1G:572:THR:HA	7:1G:582:GLN:HA	1.84	0.60
17:1Q:126:LYS:HB3	17:1Q:128:THR:HG22	1.82	0.60
39:1n:155:PRO:HG2	39:1n:157:ARG:HH12	1.67	0.60
6:1F:193:ILE:HD11	6:1F:215:VAL:H	1.67	0.59
13:1M:281:ASP:OD1	13:1M:284:SER:N	2.34	0.59
38:1m:36:LEU:HD13	39:1n:7:ALA:HB2	1.84	0.59
3:1C:198:ASP:OD2	7:1G:224:LYS:NZ	2.35	0.59
6:1F:365:CYS:HB2	47:1F:502:SF4:S2	2.42	0.59
8:1H:183:MET:HE1	46:1I:203:PC1:H282	1.84	0.59
20:1T:14:ARG:HA	20:1T:14:ARG:CZ	2.32	0.59
23:1X:95:LEU:HD13	23:1X:97:ARG:HD3	1.83	0.59
36:1k:13:MET:HA	36:1k:13:MET:HE3	1.83	0.59
39:1n:13:GLN:HA	39:1n:16:LEU:HD12	1.83	0.59
1:1A:70:ALA:HA	1:1A:73:LEU:HD23	1.84	0.59
8:1H:90:PRO:HG2	8:1H:240:ILE:HG12	1.84	0.59
12:1L:18:PRO:O	12:1L:22:SER:OG	2.18	0.59
1:1A:30:TYR:OH	2:1B:111:ARG:NH2	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:195:LEU:O	7:1G:198:ASN:ND2	2.34	0.59
12:1L:407:TRP:HD1	12:1L:407:TRP:O	1.85	0.59
13:1M:286:ILE:HD12	13:1M:286:ILE:H	1.67	0.59
13:1M:336:ARG:HB3	13:1M:426:ILE:HG13	1.84	0.59
25:1Z:94:GLU:HA	25:1Z:97:ILE:HG22	1.84	0.59
36:1k:38:ARG:NH1	39:1n:38:TYR:OH	2.36	0.59
1:1A:22:PHE:HA	8:1H:60:PRO:HG3	1.83	0.59
5:1E:12:THR:HB	5:1E:15:ASN:HB3	1.85	0.59
7:1G:330:ALA:HB1	7:1G:600:ILE:HG21	1.85	0.59
10:1J:44:VAL:HG22	10:1J:49:GLY:HA3	1.84	0.59
11:1K:5:TYR:O	11:1K:9:ILE:HG12	2.02	0.59
12:1L:161:ARG:NH1	39:1n:90:TYR:O	2.34	0.59
12:1L:383:MET:HE2	12:1L:383:MET:HA	1.85	0.59
17:1Q:37:ILE:HD11	17:1Q:105:VAL:HG22	1.84	0.59
19:1S:36:ILE:HG22	19:1S:40:TYR:HD2	1.67	0.59
25:1Z:137:THR:HG22	25:1Z:138:TYR:CD1	2.38	0.59
32:1g:62:PHE:HB3	33:1h:28:TYR:CD2	2.38	0.59
3:1C:164:LYS:NZ	4:1D:92:GLU:OE2	2.32	0.59
4:1D:152:MET:SD	4:1D:174:ARG:NH2	2.76	0.59
9:1I:95:GLU:O	9:1I:107:THR:N	2.34	0.59
11:1K:47:ILE:H	11:1K:47:ILE:HD12	1.68	0.59
31:1f:15:LEU:HD23	31:1f:15:LEU:H	1.66	0.59
37:1l:5:THR:OG1	37:1l:8:MET:SD	2.54	0.59
1:1A:37:TYR:OH	4:1D:54:GLN:OE1	2.21	0.59
14:1N:314:LYS:HE2	15:1O:271:ASN:HA	1.85	0.59
21:1V:3:LEU:HD22	21:1V:4:LEU:H	1.66	0.59
4:1D:354:GLU:O	4:1D:384:SER:OG	2.17	0.59
9:1I:28:THR:HG23	46:1I:203:PC1:H232	1.84	0.59
22:1W:83:VAL:O	22:1W:87:LYS:NZ	2.36	0.59
30:1e:29:PRO:HB3	33:1h:143:ASN:HD22	1.67	0.59
5:1E:34:ILE:HD12	5:1E:49:PRO:HB2	1.85	0.59
8:1H:5:ASN:HD21	26:1a:23:THR:HG22	1.68	0.59
12:1L:407:TRP:NE1	12:1L:411:MET:SD	2.76	0.59
12:1L:577:VAL:HG13	14:1N:164:ILE:HG23	1.85	0.59
13:1M:114:GLU:HG2	23:1X:168:PHE:HB3	1.83	0.59
23:1X:94:GLN:HE21	26:1a:37:ARG:HE	1.50	0.59
39:1n:122:GLU:HA	39:1n:125:LYS:HZ3	1.68	0.59
40:1o:26:PRO:HB2	40:1o:33:ARG:HH12	1.66	0.59
7:1G:575:ASN:HD21	7:1G:579:ARG:HB3	1.67	0.59
14:1N:194:LEU:HD23	14:1N:201:THR:HG21	1.85	0.59
22:1W:31:ARG:HB3	22:1W:83:VAL:HG21	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:35:VAL:HG12	45:1Y:801:3PE:H251	1.85	0.59
38:1m:5:TYR:HE2	38:1m:14:PRO:HD3	1.66	0.59
41:1p:106:GLN:HE21	41:1p:110:LYS:HZ3	1.50	0.59
3:1C:175:ARG:NH1	3:1C:177:ASP:OD2	2.35	0.58
4:1D:222:ILE:H	4:1D:222:ILE:HD12	1.68	0.58
15:1O:133:VAL:HG22	15:1O:202:ILE:HD12	1.85	0.58
1:1A:75:LEU:HD12	8:1H:151:LEU:HD21	1.85	0.58
6:1F:102:PRO:O	6:1F:302:SER:OG	2.22	0.58
8:1H:102:VAL:HG12	8:1H:237:PHE:HZ	1.69	0.58
12:1L:154:LEU:HD13	12:1L:243:VAL:HG13	1.85	0.58
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	1.84	0.58
41:1p:31:TYR:O	41:1p:35:ILE:HG22	2.03	0.58
2:1B:158:TYR:CE2	42:1q:78:ASP:HB2	2.38	0.58
3:1C:65:ARG:HH21	3:1C:123:VAL:HA	1.68	0.58
4:1D:350:LYS:HA	4:1D:353:THR:HG22	1.85	0.58
12:1L:73:THR:OG1	41:1p:106:GLN:OE1	2.21	0.58
12:1L:576:MET:O	12:1L:580:GLN:NE2	2.35	0.58
37:1l:29:MET:HE2	37:1l:76:PRO:HG3	1.84	0.58
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.27	0.58
13:1M:108:MET:HE1	51:1X:201:CDL:H221	1.85	0.58
16:1P:32:ARG:HD3	16:1P:58:HIS:CD2	2.39	0.58
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.68	0.58
17:1Q:54:LYS:HZ1	21:1V:115:ILE:HG22	1.68	0.58
17:1Q:70:MET:O	42:1q:128:SER:OG	2.17	0.58
19:1S:74:LYS:HE2	19:1S:74:LYS:N	2.19	0.58
20:1U:72:CYS:O	20:1U:76:ILE:N	2.37	0.58
23:1X:163:GLY:HA3	23:1X:171:MET:HA	1.85	0.58
24:1Y:140:VAL:O	33:1h:115:ARG:NH1	2.37	0.58
40:1o:61:TYR:HD2	40:1o:89:CYS:HB2	1.67	0.58
2:1B:81:ARG:HG3	8:1H:61:LEU:HD23	1.84	0.58
2:1B:130:TYR:HH	4:1D:84:HIS:HE2	1.51	0.58
12:1L:141:PHE:HB2	12:1L:186:MET:HE1	1.86	0.58
21:1V:21:GLU:CD	21:1V:21:GLU:H	2.11	0.58
27:1b:51:ASN:HB3	33:1h:139:THR:HG22	1.84	0.58
41:1p:8:VAL:HG23	41:1p:9:TYR:CD1	2.37	0.58
6:1F:103:GLY:O	6:1F:257:ASN:ND2	2.36	0.58
7:1G:193:SER:HB3	7:1G:196:SER:HB3	1.84	0.58
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.86	0.58
12:1L:539:TYR:OH	38:1m:9:ARG:NH2	2.33	0.58
15:1O:45:LYS:HG2	15:1O:235:VAL:HG21	1.84	0.58
15:1O:233:LYS:HA	15:1O:236:GLU:OE2	2.04	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:70:LYS:HE3	30:1e:71:THR:HG22	1.85	0.58
7:1G:453:LEU:HD12	7:1G:470:VAL:HG21	1.86	0.58
7:1G:470:VAL:HA	7:1G:473:ILE:HG12	1.86	0.58
19:1S:37:GLU:OE1	19:1S:38:LYS:NZ	2.36	0.58
35:1j:68:PRO:O	40:1o:114:ARG:NH2	2.37	0.58
4:1D:410:MET:HE1	8:1H:282:TYR:CE1	2.39	0.58
6:1F:110:ILE:O	6:1F:114:ASP:N	2.22	0.58
10:1J:172:THR:HA	11:1K:80:MET:HE3	1.85	0.58
13:1M:329:LEU:HG	13:1M:437:MET:HE3	1.85	0.58
29:1d:2:MET:N	29:1d:2:MET:SD	2.77	0.58
43:1r:25:LEU:H	43:1r:25:LEU:HD12	1.69	0.58
2:1B:122:GLY:N	9:1I:114:THR:OG1	2.37	0.58
7:1G:45:ARG:NE	7:1G:261:GLU:OE1	2.35	0.58
15:1O:275:ILE:HG22	15:1O:277:VAL:H	1.68	0.58
22:1W:66:MET:HA	22:1W:69:LYS:HB3	1.85	0.58
3:1C:42:VAL:HB	3:1C:48:LEU:HD23	1.86	0.57
5:1E:84:ALA:HA	5:1E:90:TYR:HD2	1.69	0.57
6:1F:272:MET:HE3	6:1F:318:ASP:HA	1.86	0.57
11:1K:20:LEU:HD13	12:1L:592:LEU:HB2	1.86	0.57
27:1b:59:ASP:OD1	27:1b:59:ASP:N	2.35	0.57
32:1g:80:LEU:HD22	32:1g:81:PRO:HD2	1.86	0.57
37:1l:80:ASP:HB3	37:1l:83:MET:HB2	1.86	0.57
7:1G:242:THR:HG21	7:1G:586:ALA:HB1	1.84	0.57
7:1G:285:ARG:NH1	7:1G:557:ALA:O	2.37	0.57
7:1G:364:LEU:HD22	7:1G:491:ASN:HB3	1.86	0.57
7:1G:437:HIS:CE1	7:1G:439:PHE:HB2	2.38	0.57
12:1L:511:LEU:HD11	39:1n:38:TYR:HD2	1.69	0.57
13:1M:277:LEU:HD21	13:1M:405:LEU:HB3	1.85	0.57
15:1O:171:TYR:OH	15:1O:207:LYS:NZ	2.37	0.57
34:1i:46:TRP:HZ2	34:1i:64:TYR:HD2	1.50	0.57
34:1i:85:LEU:HA	34:1i:89:VAL:HB	1.85	0.57
10:1J:9:LEU:HD22	10:1J:39:VAL:HB	1.86	0.57
12:1L:233:LEU:HD23	12:1L:307:SER:HB3	1.85	0.57
16:1P:293:THR:HG22	16:1P:295:PRO:HD3	1.86	0.57
31:1f:18:VAL:HA	31:1f:21:VAL:HG12	1.85	0.57
3:1C:77:ASP:OD1	3:1C:78:LEU:N	2.37	0.57
8:1H:133:LEU:HA	8:1H:136:VAL:HG23	1.84	0.57
9:1I:108:ARG:NH2	17:1Q:70:MET:O	2.37	0.57
12:1L:545:SER:OG	13:1M:274:SER:O	2.19	0.57
14:1N:235:ASN:HB3	14:1N:311:MET:HE2	1.87	0.57
17:1Q:29:HIS:HA	17:1Q:33:ARG:HG3	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:129:GLY:H	40:1o:97:ARG:HG3	1.69	0.57
7:1G:30:CYS:HB3	7:1G:35:MET:HB3	1.85	0.57
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.85	0.57
13:1M:24:TRP:CD1	13:1M:81:GLN:HE22	2.22	0.57
22:1W:50:PHE:HE2	22:1W:100:ARG:HA	1.68	0.57
1:1A:111:LEU:HD13	8:1H:290:TRP:HB3	1.86	0.57
7:1G:226:GLU:HG2	7:1G:253:ARG:HD2	1.86	0.57
13:1M:114:GLU:HB3	13:1M:117:LEU:HB3	1.85	0.57
18:1R:20:ASP:OD1	18:1R:21:GLY:N	2.38	0.57
20:1U:68:GLU:HG3	34:1i:0:ACE:CH3	2.34	0.57
26:1a:59:ARG:HB2	26:1a:62:VAL:HG12	1.85	0.57
29:1d:5:ARG:HB2	29:1d:8:ARG:HH12	1.68	0.57
37:1l:73:TRP:NE1	38:1m:61:ASP:OD1	2.38	0.57
46:1A:202:PC1:H341	8:1H:72:ILE:HG21	1.85	0.57
3:1C:202:PRO:HB2	17:1Q:48:GLY:HA3	1.85	0.57
5:1E:52:ASP:OD1	5:1E:56:ARG:NH1	2.36	0.57
8:1H:281:ARG:HG2	8:1H:283:ASP:HB3	1.87	0.57
18:1R:19:ASP:O	18:1R:25:ARG:NH1	2.29	0.57
2:1B:71:ARG:NH2	9:1I:49:ASN:OD1	2.38	0.57
4:1D:171:PHE:HA	4:1D:174:ARG:HB3	1.87	0.57
4:1D:332:PRO:HB3	4:1D:352:TYR:HE1	1.68	0.57
5:1E:154:VAL:O	5:1E:161:TYR:HB2	2.05	0.57
13:1M:127:VAL:HG13	14:1N:249:LEU:HD23	1.85	0.57
4:1D:75:LYS:HE2	4:1D:75:LYS:HA	1.87	0.57
38:1m:122:GLN:OE1	38:1m:125:ASN:ND2	2.38	0.57
7:1G:673:MET:HE1	7:1G:679:ARG:HA	1.86	0.57
13:1M:243:MET:HA	13:1M:246:ILE:HG22	1.86	0.57
29:1d:5:ARG:HB2	29:1d:8:ARG:NH1	2.20	0.57
12:1L:287:PHE:CE1	12:1L:527:GLY:HA3	2.40	0.56
20:1T:72:CYS:HB2	20:1T:75:GLU:HG3	1.86	0.56
40:1o:41:THR:OG1	40:1o:44:GLU:OE1	2.23	0.56
4:1D:22:THR:HG22	4:1D:25:THR:HG22	1.87	0.56
5:1E:101:GLN:HG2	5:1E:142:VAL:HG21	1.86	0.56
7:1G:201:ASP:HA	17:1Q:45:MET:HG3	1.86	0.56
10:1J:115:ILE:HG13	10:1J:116:ILE:HG12	1.87	0.56
10:1J:152:TRP:HB2	46:1J:201:PC1:H242	1.87	0.56
12:1L:203:MET:HB2	41:1p:113:GLN:HG3	1.86	0.56
14:1N:193:VAL:HG21	14:1N:200:MET:HB2	1.88	0.56
30:1e:15:ARG:O	30:1e:18:THR:OG1	2.22	0.56
30:1e:64:GLU:O	30:1e:68:ARG:N	2.37	0.56
6:1F:250:ASN:HB2	6:1F:318:ASP:HB2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:275:PRO:HB2	6:1F:278:GLU:OE1	2.04	0.56
7:1G:60:GLU:HB3	7:1G:78:ASN:HB3	1.86	0.56
7:1G:333:ASP:HB3	7:1G:611:LEU:HD11	1.86	0.56
8:1H:9:LEU:HG	8:1H:95:LEU:HD12	1.86	0.56
9:1I:112:ASP:O	9:1I:116:CYS:N	2.37	0.56
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.86	0.56
15:1O:65:ASP:HB3	15:1O:67:LYS:HD2	1.88	0.56
16:1P:73:TRP:HZ2	54:1P:501:NDP:H2A	1.70	0.56
20:1U:47:GLN:NE2	20:1U:70:LEU:O	2.38	0.56
51:1X:201:CDL:H192	51:1X:201:CDL:H231	1.87	0.56
37:1I:54:SER:N	37:1I:57:GLU:OE1	2.38	0.56
42:1q:73:THR:OG1	42:1q:76:ASP:O	2.22	0.56
12:1L:100:ILE:HD13	12:1L:246:LEU:HB2	1.87	0.56
12:1L:378:LEU:HD21	36:1k:66:LEU:HD11	1.86	0.56
12:1L:587:TYR:O	12:1L:590:SER:OG	2.23	0.56
13:1M:45:LEU:HD12	13:1M:46:GLY:H	1.69	0.56
13:1M:135:ARG:HB2	14:1N:302:LEU:HD13	1.88	0.56
16:1P:81:ILE:H	16:1P:81:ILE:HD12	1.71	0.56
16:1P:270:PHE:HD2	16:1P:279:THR:HB	1.71	0.56
20:1U:24:LYS:HZ1	36:1k:41:ARG:HH22	1.52	0.56
27:1b:15:GLU:HG2	27:1b:18:LEU:HB2	1.87	0.56
29:1d:14:LEU:HD11	29:1d:77:LYS:HB3	1.87	0.56
7:1G:147:LYS:N	7:1G:209:THR:O	2.38	0.56
39:1n:25:HIS:HE1	39:1n:78:PRO:HB3	1.70	0.56
2:1B:171:LYS:HB3	2:1B:174:ARG:HB3	1.88	0.56
7:1G:632:ARG:NH1	19:1S:57:CYS:SG	2.79	0.56
9:1I:132:VAL:HG21	9:1I:165:ILE:HG21	1.85	0.56
12:1L:443:ILE:HD11	35:1j:15:PRO:HG3	1.86	0.56
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.85	0.56
23:1X:143:SER:OG	23:1X:146:ARG:NH1	2.39	0.56
37:1I:97:SER:HB2	38:1m:6:LYS:HG2	1.87	0.56
6:1F:36:ALA:HB3	6:1F:116:HIS:HB3	1.88	0.56
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD12	1.88	0.56
16:1P:114:PRO:HA	16:1P:117:ILE:HG22	1.87	0.56
20:1U:23:ASP:OD2	36:1k:41:ARG:NH1	2.38	0.56
22:1W:38:ALA:HB3	22:1W:90:LEU:HD11	1.87	0.56
34:1i:103:ILE:H	34:1i:103:ILE:HD12	1.70	0.56
35:1j:70:ASP:OD1	35:1j:70:ASP:N	2.37	0.56
6:1F:184:TYR:HB3	6:1F:357:GLU:HG3	1.88	0.56
10:1J:113:VAL:HG22	10:1J:115:ILE:HG22	1.87	0.56
23:1X:13:LYS:HA	23:1X:13:LYS:HE3	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:459:TYR:O	32:1g:84:ARG:NH1	2.39	0.56
15:1O:78:SER:H	15:1O:92:ASN:HD21	1.52	0.56
19:1S:30:GLN:NE2	19:1S:34:ASP:OD1	2.39	0.56
25:1Z:21:TYR:OH	43:1r:108:ASP:OD2	2.20	0.56
34:1i:32:PRO:HB2	39:1n:113:MET:HE2	1.87	0.56
37:1l:115:MET:HE2	37:1l:115:MET:O	2.06	0.56
39:1n:61:GLN:O	39:1n:65:GLN:NE2	2.38	0.56
12:1L:464:ALA:O	12:1L:468:ILE:HD12	2.06	0.56
13:1M:102:LEU:HD13	13:1M:128:PRO:HB2	1.87	0.56
19:1S:81:PHE:CD1	19:1S:85:GLN:HG3	2.34	0.56
4:1D:63:ARG:NH1	22:1W:97:TRP:O	2.36	0.55
4:1D:143:GLU:HG2	4:1D:310:ILE:HB	1.88	0.55
8:1H:272:TRP:HZ2	9:1I:38:LEU:HB2	1.71	0.55
15:1O:38:LEU:HD11	15:1O:234:VAL:HG21	1.88	0.55
19:1S:42:GLU:HA	19:1S:45:LYS:HG2	1.89	0.55
38:1m:121:ASP:OD1	38:1m:123:THR:OG1	2.23	0.55
44:1s:37:THR:OG1	44:1s:38:TYR:N	2.38	0.55
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.88	0.55
10:1J:152:TRP:HA	10:1J:155:ILE:HD12	1.88	0.55
12:1L:511:LEU:HD11	39:1n:38:TYR:CD2	2.41	0.55
20:1U:6:LEU:HD23	20:1U:6:LEU:H	1.70	0.55
29:1d:48:ILE:HD12	29:1d:48:ILE:H	1.71	0.55
9:1I:13:ASP:OD1	9:1I:14:MET:N	2.39	0.55
10:1J:56:VAL:O	10:1J:60:TYR:HB2	2.06	0.55
12:1L:496:MET:HA	12:1L:499:MET:HB3	1.87	0.55
13:1M:255:ASN:OD1	13:1M:256:TYR:N	2.40	0.55
42:1q:71:ARG:HG3	42:1q:71:ARG:O	2.05	0.55
43:1r:26:ARG:HE	43:1r:30:ILE:HG21	1.70	0.55
6:1F:129:MET:SD	6:1F:221:THR:OG1	2.58	0.55
6:1F:298:ILE:HG23	6:1F:337:MET:HE1	1.87	0.55
11:1K:40:LEU:HD11	14:1N:71:MET:HB3	1.88	0.55
29:1d:113:LEU:HD21	41:1p:163:LEU:HD11	1.87	0.55
3:1C:62:THR:HG21	21:1V:92:LYS:HE2	1.86	0.55
5:1E:114:ASP:N	5:1E:114:ASP:OD1	2.36	0.55
7:1G:159:CYS:HB2	7:1G:199:ILE:HD11	1.89	0.55
8:1H:81:LEU:HA	8:1H:84:THR:HG22	1.89	0.55
8:1H:121:TRP:HZ3	10:1J:27:ILE:HG12	1.71	0.55
8:1H:292:SER:HB2	27:1b:17:VAL:HG11	1.87	0.55
12:1L:199:GLN:HE22	41:1p:110:LYS:HA	1.72	0.55
13:1M:49:SER:OG	13:1M:58:SER:O	2.24	0.55
16:1P:101:THR:HG23	16:1P:104:PHE:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:267:GLY:HA2	16:1P:279:THR:HG22	1.89	0.55
19:1S:17:GLU:OE1	19:1S:17:GLU:N	2.39	0.55
32:1g:39:GLU:OE2	32:1g:40:LYS:HD2	2.07	0.55
33:1h:69:HIS:CD2	33:1h:71:ILE:H	2.24	0.55
12:1L:17:ILE:H	12:1L:17:ILE:HD12	1.72	0.55
16:1P:328:THR:OG1	22:1W:48:HIS:O	2.23	0.55
20:1T:54:MET:N	20:1T:54:MET:HE2	2.22	0.55
35:1j:12:ARG:HB3	36:1k:21:TRP:CH2	2.37	0.55
2:1B:123:GLY:HA3	2:1B:127:HIS:ND1	2.22	0.55
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.87	0.55
7:1G:41:CYS:H	7:1G:52:CYS:HB3	1.70	0.55
7:1G:116:LEU:HD12	47:1G:801:SF4:S2	2.47	0.55
11:1K:22:TYR:HB3	11:1K:90:VAL:HG21	1.88	0.55
12:1L:464:ALA:HA	12:1L:467:ILE:HG22	1.88	0.55
26:1a:22:ALA:O	26:1a:26:ILE:HG12	2.05	0.55
13:1M:130:LEU:HD21	13:1M:150:LEU:HB2	1.89	0.55
27:1b:64:ASP:N	27:1b:64:ASP:OD1	2.36	0.55
28:1c:39:VAL:HG12	28:1c:43:LYS:HD2	1.87	0.55
34:1i:24:ASP:OD2	39:1n:124:TRP:NE1	2.38	0.55
34:1i:30:ARG:HH21	39:1n:115:PRO:HG2	1.72	0.55
7:1G:385:ARG:NH1	7:1G:414:ASP:OD1	2.39	0.55
9:1I:164:GLU:OE2	42:1q:88:ARG:N	2.40	0.55
12:1L:481:THR:OG1	40:1o:91:HIS:ND1	2.28	0.55
12:1L:504:LEU:O	12:1L:507:THR:OG1	2.19	0.55
38:1m:34:GLU:HA	38:1m:37:ALA:HB3	1.89	0.55
4:1D:165:THR:HG22	8:1H:32:GLN:HG3	1.89	0.55
4:1D:236:ARG:O	4:1D:240:VAL:HG12	2.07	0.55
7:1G:318:ILE:HD13	7:1G:522:LEU:HD11	1.88	0.55
8:1H:311:THR:O	25:1Z:55:ARG:NH2	2.40	0.55
14:1N:73:ALA:HB2	14:1N:97:MET:HG3	1.89	0.55
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.88	0.55
17:1Q:123:SER:O	17:1Q:129:ARG:NH1	2.40	0.55
19:1S:19:ARG:HB2	19:1S:65:TRP:HB2	1.89	0.55
29:1d:15:PRO:HB2	29:1d:17:GLU:OE1	2.07	0.55
34:1i:71:VAL:HA	34:1i:75:LEU:HB2	1.86	0.55
41:1p:29:VAL:O	41:1p:33:THR:HG23	2.07	0.55
2:1B:49:THR:O	2:1B:49:THR:OG1	2.25	0.54
4:1D:178:PHE:CE2	4:1D:189:MET:HG3	2.42	0.54
51:1H:402:CDL:HA62	51:1H:402:CDL:H1	1.89	0.54
14:1N:34:GLU:O	14:1N:38:LEU:N	2.24	0.54
18:1R:54:SER:HB2	18:1R:57:ILE:HD11	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:157:GLU:OE2	40:1o:34:LYS:NZ	2.39	0.54
2:1B:154:GLU:HB3	9:1I:50:TYR:HE2	1.72	0.54
5:1E:55:GLN:NE2	5:1E:91:ASN:OD1	2.40	0.54
7:1G:704:CYS:SG	9:1I:102:GLY:HA2	2.47	0.54
13:1M:250:LEU:O	13:1M:254:THR:OG1	2.25	0.54
14:1N:338:PRO:HA	23:1X:169:TRP:HZ2	1.72	0.54
14:1N:341:PRO:C	29:1d:79:GLN:HE22	2.15	0.54
37:1l:3:HIS:HD2	38:1m:60:GLU:HG3	1.72	0.54
1:1A:41:PHE:HB2	4:1D:50:ASN:ND2	2.22	0.54
1:1A:104:TYR:HE2	10:1J:166:VAL:HA	1.73	0.54
6:1F:17:ASP:HA	6:1F:20:ARG:HD2	1.88	0.54
6:1F:362:CYS:SG	6:1F:364:PRO:HD2	2.48	0.54
12:1L:355:ASP:OD2	12:1L:357:ARG:NH2	2.38	0.54
12:1L:512:LYS:HD3	12:1L:513:PHE:N	2.23	0.54
12:1L:594:THR:O	12:1L:598:SER:OG	2.20	0.54
15:1O:132:PHE:HA	15:1O:152:TYR:HE2	1.73	0.54
28:1c:32:ILE:O	28:1c:36:LYS:HG2	2.07	0.54
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.24	0.54
1:1A:42:ASP:N	22:1W:99:GLN:OE1	2.36	0.54
3:1C:59:PRO:HB3	21:1V:96:TRP:CE3	2.43	0.54
4:1D:34:ASN:HB3	4:1D:36:VAL:HG12	1.88	0.54
4:1D:109:VAL:HG12	4:1D:152:MET:HE2	1.90	0.54
8:1H:96:ILE:HG23	25:1Z:144:THR:HB	1.88	0.54
10:1J:36:SER:O	10:1J:40:GLY:N	2.38	0.54
12:1L:8:THR:O	12:1L:11:THR:OG1	2.22	0.54
20:1T:49:GLU:N	20:1T:49:GLU:OE2	2.37	0.54
22:1W:80:ASP:O	22:1W:83:VAL:HG12	2.08	0.54
32:1g:49:LYS:HE2	32:1g:49:LYS:HA	1.90	0.54
46:1L:703:PC1:H232	13:1M:449:LEU:HB2	1.88	0.54
15:1O:128:ILE:O	15:1O:156:LYS:NZ	2.41	0.54
15:1O:298:GLU:OE2	15:1O:298:GLU:N	2.31	0.54
20:1U:87:TYR:CE2	34:1i:19:ARG:HA	2.43	0.54
28:1c:23:THR:O	28:1c:27:LEU:N	2.37	0.54
30:1e:40:ILE:HD13	33:1h:128:ILE:HG21	1.89	0.54
7:1G:554:ALA:HA	7:1G:560:ILE:HD11	1.89	0.54
10:1J:164:GLY:O	10:1J:168:ILE:HG23	2.07	0.54
13:1M:42:LEU:HD12	13:1M:42:LEU:H	1.73	0.54
13:1M:324:SER:HB2	13:1M:440:HIS:HE1	1.72	0.54
15:1O:145:ARG:HH22	15:1O:280:PRO:HD2	1.72	0.54
20:1T:18:VAL:HA	20:1T:21:LEU:HD23	1.88	0.54
26:1a:50:ARG:O	26:1a:54:ILE:HG22	2.07	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:37:TYR:CZ	1:1A:39:CYS:HA	2.43	0.54
5:1E:202:LEU:HD22	6:1F:23:THR:HA	1.90	0.54
13:1M:258:ALA:HB1	13:1M:262:LEU:HD23	1.90	0.54
13:1M:382:ILE:HD13	13:1M:396:MET:HE2	1.89	0.54
15:1O:238:ILE:HA	15:1O:241:LEU:HD22	1.89	0.54
29:1d:2:MET:C	29:1d:4:GLY:H	2.15	0.54
30:1e:27:LYS:HB3	33:1h:138:LYS:HD2	1.90	0.54
37:1l:60:PRO:HB2	39:1n:85:PRO:HG3	1.89	0.54
40:1o:74:PRO:HD2	41:1p:25:LEU:HD11	1.90	0.54
4:1D:352:TYR:HD2	9:1I:86:VAL:HG21	1.72	0.54
6:1F:99:GLU:CG	6:1F:107:ASP:HB2	2.38	0.54
6:1F:193:ILE:HD11	6:1F:215:VAL:HG12	1.90	0.54
7:1G:54:MET:HA	7:1G:93:VAL:HG21	1.89	0.54
7:1G:637:GLU:HG2	19:1S:57:CYS:HA	1.90	0.54
8:1H:121:TRP:CZ3	10:1J:27:ILE:HG12	2.43	0.54
8:1H:174:MET:HB3	8:1H:242:PHE:HA	1.90	0.54
8:1H:195:ARG:HH11	8:1H:195:ARG:HA	1.72	0.54
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.42	0.54
10:1J:3:MET:O	10:1J:5:ILE:N	2.41	0.54
13:1M:66:LEU:HD21	13:1M:111:THR:HG23	1.90	0.54
13:1M:216:LEU:HD13	13:1M:220:HIS:CE1	2.43	0.54
13:1M:447:LEU:HD21	13:1M:454:ILE:HG13	1.90	0.54
45:1M:503:3PE:H3C1	45:1M:503:3PE:H251	1.89	0.54
14:1N:40:MET:SD	14:1N:134:GLN:NE2	2.79	0.54
14:1N:199:THR:HG21	14:1N:347:ASN:HB2	1.90	0.54
15:1O:43:ALA:HA	15:1O:48:LEU:HB2	1.90	0.54
19:1S:18:ILE:HG22	19:1S:52:ILE:HA	1.89	0.54
20:1U:58:PHE:HE2	20:1U:80:ILE:HD13	1.73	0.54
41:1p:31:TYR:O	41:1p:34:LYS:HG3	2.07	0.54
2:1B:82:GLN:NE2	8:1H:220:PHE:HE2	2.05	0.54
3:1C:68:THR:HG22	21:1V:82:GLN:HE21	1.71	0.54
3:1C:162:PHE:CE2	4:1D:88:GLU:HB2	2.43	0.54
7:1G:544:ILE:HG22	7:1G:559:VAL:HB	1.89	0.54
46:1H:401:PC1:H3E1	27:1b:24:ILE:HG12	1.90	0.54
9:1I:52:PHE:CE2	42:1q:30:ALA:HA	2.42	0.54
10:1J:162:LEU:O	10:1J:166:VAL:HG23	2.08	0.54
16:1P:25:GLY:O	54:1P:501:NDP:O3B	2.26	0.54
22:1W:73:VAL:HG21	22:1W:78:VAL:HB	1.90	0.54
23:1X:45:CYS:HA	23:1X:134:ARG:NH2	2.23	0.54
45:1Y:802:3PE:O14	45:1Y:802:3PE:N	2.30	0.54
25:1Z:127:LEU:HD23	25:1Z:127:LEU:H	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:90:ARG:NE	41:1p:100:GLU:OE1	2.36	0.54
45:1A:201:3PE:H271	8:1H:295:PRO:HB3	1.89	0.54
4:1D:123:GLU:HA	4:1D:126:LEU:HB2	1.90	0.54
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.89	0.54
6:1F:326:GLN:NE2	6:1F:420:ARG:HD3	2.22	0.54
12:1L:447:ASN:HD21	12:1L:449:LEU:HB2	1.72	0.54
13:1M:263:MET:HE1	38:1m:101:TYR:HB2	1.90	0.54
16:1P:23:VAL:O	16:1P:48:PRO:HD2	2.08	0.54
20:1U:36:PHE:HA	20:1U:40:LEU:HD23	1.90	0.54
51:1a:101:CDL:H162	51:1a:101:CDL:H331	1.90	0.54
6:1F:62:THR:HB	6:1F:239:GLY:HA3	1.88	0.53
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.90	0.53
10:1J:126:VAL:HB	25:1Z:120:MET:HE1	1.89	0.53
16:1P:319:ARG:HD2	22:1W:51:GLN:HE22	1.73	0.53
35:1j:12:ARG:NH2	36:1k:47:ASN:O	2.41	0.53
4:1D:218:PHE:HB3	4:1D:308:LEU:HD11	1.89	0.53
4:1D:303:GLU:O	4:1D:307:SER:OG	2.21	0.53
7:1G:365:ASN:ND2	7:1G:490:MET:O	2.41	0.53
7:1G:432:ILE:HG22	7:1G:473:ILE:HD12	1.89	0.53
8:1H:253:GLU:OE1	8:1H:253:GLU:N	2.27	0.53
10:1J:17:PHE:HA	10:1J:20:PHE:CE1	2.44	0.53
13:1M:290:SER:HA	13:1M:319:HIS:HE2	1.73	0.53
13:1M:313:THR:HA	13:1M:316:MET:HE2	1.89	0.53
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.90	0.53
22:1W:90:LEU:HD23	22:1W:94:ILE:HD11	1.89	0.53
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.41	0.53
39:1n:65:GLN:HA	39:1n:68:GLU:OE2	2.09	0.53
1:1A:24:LEU:HD23	46:1B:202:PC1:H351	1.89	0.53
1:1A:92:LEU:O	1:1A:96:ILE:HG13	2.07	0.53
3:1C:101:PHE:O	3:1C:103:SER:OG	2.25	0.53
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.43	0.53
5:1E:123:LYS:HZ2	5:1E:170:GLU:HG2	1.73	0.53
6:1F:66:ARG:HD3	6:1F:250:ASN:HD22	1.74	0.53
7:1G:335:LEU:HD12	7:1G:343:LEU:HB3	1.90	0.53
8:1H:98:MET:HE3	8:1H:99:ASN:N	2.24	0.53
10:1J:3:MET:SD	10:1J:3:MET:N	2.81	0.53
11:1K:44:SER:HB3	14:1N:75:ILE:HD12	1.89	0.53
12:1L:534:HIS:HD1	45:1L:701:3PE:H32	1.73	0.53
13:1M:65:LEU:HD22	13:1M:317:ILE:HD11	1.90	0.53
17:1Q:90:GLU:H	17:1Q:90:GLU:CD	2.15	0.53
22:1W:83:VAL:HG22	22:1W:87:LYS:HZ1	1.73	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:120:MET:HG3	30:1e:68:ARG:HH11	1.73	0.53
33:1h:70:PRO:HA	33:1h:73:ARG:HB2	1.89	0.53
5:1E:191:PHE:H	5:1E:194:GLU:CD	2.16	0.53
6:1F:15:LEU:HB2	6:1F:271:GLU:H	1.73	0.53
7:1G:329:VAL:HG23	7:1G:505:LEU:HD21	1.90	0.53
8:1H:28:LEU:HD11	8:1H:274:ARG:HD2	1.90	0.53
12:1L:593:ILE:O	12:1L:597:ILE:HG12	2.09	0.53
13:1M:299:VAL:O	13:1M:303:ILE:HG12	2.08	0.53
14:1N:179:MET:HE1	14:1N:215:MET:HG2	1.88	0.53
40:1o:61:TYR:HB3	40:1o:86:TRP:HA	1.89	0.53
43:1r:29:GLU:H	43:1r:29:GLU:CD	2.15	0.53
7:1G:160:ILE:HG13	7:1G:173:GLY:HA2	1.90	0.53
7:1G:335:LEU:HB3	7:1G:340:SER:HB3	1.90	0.53
12:1L:588:PHE:HA	12:1L:591:PHE:CD2	2.43	0.53
14:1N:217:MET:CG	14:1N:323:MET:HE2	2.37	0.53
16:1P:97:ARG:HG3	16:1P:99:TRP:H	1.72	0.53
19:1S:47:ASN:HD21	19:1S:94:LEU:HD21	1.74	0.53
21:1V:21:GLU:O	21:1V:25:ILE:HG23	2.08	0.53
22:1W:52:LEU:HD13	22:1W:54:ILE:HG22	1.91	0.53
23:1X:12:LEU:HD12	23:1X:13:LYS:HD2	1.90	0.53
26:1a:67:GLU:OE1	26:1a:67:GLU:N	2.33	0.53
2:1B:68:ASP:HB3	2:1B:71:ARG:HD3	1.90	0.53
6:1F:228:VAL:O	6:1F:231:SER:OG	2.24	0.53
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.89	0.53
8:1H:139:THR:HA	8:1H:142:TYR:HD1	1.74	0.53
12:1L:129:MET:HA	12:1L:129:MET:HE2	1.89	0.53
12:1L:151:SER:O	12:1L:155:ILE:HG13	2.09	0.53
12:1L:245:ALA:O	12:1L:249:SER:OG	2.26	0.53
14:1N:40:MET:HG2	14:1N:59:TYR:HE2	1.72	0.53
14:1N:269:GLU:HA	14:1N:272:LYS:HD3	1.90	0.53
15:1O:285:GLY:O	15:1O:289:SER:OG	2.25	0.53
35:1j:29:SER:HB3	36:1k:69:GLY:HA3	1.91	0.53
39:1n:97:LYS:HG2	39:1n:177:PRO:HG3	1.90	0.53
42:1q:46:ASN:HB3	42:1q:48:TYR:HE1	1.72	0.53
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.27	0.53
7:1G:47:SER:O	7:1G:161:ARG:NH1	2.42	0.53
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.43	0.53
12:1L:198:LEU:HD22	12:1L:262:ARG:HG2	1.90	0.53
12:1L:359:MET:HB3	12:1L:430:ALA:HA	1.90	0.53
14:1N:180:ALA:O	14:1N:184:ILE:HG13	2.09	0.53
16:1P:26:ALA:HA	16:1P:31:GLY:HA3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1c:45:ARG:HH11	29:1d:20:SER:HB3	1.72	0.53
31:1f:28:ARG:HE	46:1f:101:PC1:H112	1.73	0.53
32:1g:120:LEU:HD22	32:1g:121:PRO:HD2	1.91	0.53
2:1B:117:GLY:O	2:1B:121:ASN:ND2	2.41	0.53
3:1C:145:HIS:HB3	3:1C:148:LEU:HB2	1.91	0.53
4:1D:123:GLU:HG2	4:1D:128:ILE:O	2.09	0.53
6:1F:89:ARG:NH1	6:1F:217:GLY:O	2.42	0.53
1:1A:47:ALA:H	8:1H:126:LYS:NZ	2.07	0.53
3:1C:154:ASP:HB3	3:1C:157:PHE:HB2	1.91	0.53
3:1C:175:ARG:NH2	3:1C:186:GLU:OE1	2.40	0.53
4:1D:141:PHE:CZ	4:1D:184:VAL:HG11	2.44	0.53
5:1E:119:ALA:HB1	5:1E:169:ILE:HD11	1.89	0.53
12:1L:40:VAL:HG21	12:1L:101:MET:HE3	1.91	0.53
12:1L:415:ALA:HA	12:1L:418:LEU:HD12	1.90	0.53
14:1N:342:ALA:HB3	46:1d:201:PC1:H3D2	1.91	0.53
1:1A:34:THR:HG22	8:1H:64:GLY:N	2.24	0.53
3:1C:38:GLN:HG2	21:1V:106:PRO:HD3	1.91	0.53
7:1G:150:MET:HE2	7:1G:150:MET:HA	1.89	0.53
7:1G:261:GLU:HB2	17:1Q:44:ASN:HD21	1.72	0.53
12:1L:407:TRP:CD1	12:1L:407:TRP:O	2.62	0.53
22:1W:35:LEU:HD11	22:1W:83:VAL:HG23	1.90	0.53
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.89	0.53
4:1D:22:THR:HG23	4:1D:24:GLU:H	1.74	0.52
4:1D:193:TYR:HE1	4:1D:201:GLN:H	1.57	0.52
6:1F:96:ASN:N	6:1F:223:ALA:O	2.36	0.52
8:1H:113:VAL:O	8:1H:117:LEU:N	2.41	0.52
37:1l:157:GLU:HG3	40:1o:36:ARG:HG2	1.91	0.52
41:1p:128:LEU:O	41:1p:132:THR:OG1	2.26	0.52
3:1C:42:VAL:HA	3:1C:48:LEU:HA	1.91	0.52
6:1F:257:ASN:OD1	6:1F:257:ASN:N	2.42	0.52
37:1l:30:ARG:HH12	38:1m:35:ARG:HE	1.57	0.52
2:1B:152:THR:HG23	2:1B:155:ALA:H	1.75	0.52
7:1G:534:ARG:NH2	7:1G:556:MET:O	2.42	0.52
7:1G:673:MET:HA	7:1G:673:MET:HE3	1.90	0.52
8:1H:107:ALA:HB1	10:1J:57:PHE:HD2	1.74	0.52
13:1M:257:MET:HE1	46:1M:502:PC1:H241	1.91	0.52
13:1M:277:LEU:O	37:1l:88:ARG:NH2	2.42	0.52
13:1M:452:LYS:HZ2	13:1M:453:MET:HE1	1.75	0.52
14:1N:215:MET:HE1	14:1N:248:LEU:HD22	1.91	0.52
20:1U:51:ILE:O	20:1U:55:GLU:N	2.38	0.52
20:1U:58:PHE:HB3	20:1U:60:PHE:CZ	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:35:GLU:O	37:1l:49:LYS:N	2.35	0.52
38:1m:36:LEU:HD21	39:1n:150:THR:HA	1.91	0.52
41:1p:39:LEU:HD13	41:1p:40:VAL:HG23	1.91	0.52
43:1r:63:MET:HA	43:1r:63:MET:HE3	1.90	0.52
6:1F:258:ILE:HD13	6:1F:284:ALA:HB2	1.90	0.52
7:1G:55:CYS:SG	7:1G:68:ALA:N	2.83	0.52
7:1G:341:ASP:OD2	19:1S:16:ARG:NE	2.42	0.52
8:1H:93:TYR:CE2	26:1a:35:GLU:HB2	2.44	0.52
10:1J:17:PHE:HA	10:1J:20:PHE:HE1	1.74	0.52
12:1L:458:LEU:HD11	35:1j:28:PHE:HB3	1.91	0.52
23:1X:144:ARG:HH12	30:1e:57:ILE:HB	1.73	0.52
24:1Y:23:ALA:O	24:1Y:26:SER:OG	2.25	0.52
34:1i:59:VAL:O	34:1i:63:THR:OG1	2.27	0.52
40:1o:87:ASP:N	40:1o:87:ASP:OD1	2.38	0.52
4:1D:83:LEU:O	4:1D:83:LEU:HD13	2.09	0.52
5:1E:44:ALA:HB1	5:1E:75:VAL:HG22	1.92	0.52
5:1E:124:LEU:HB3	5:1E:126:ILE:HG22	1.90	0.52
7:1G:681:SER:OG	7:1G:684:MET:HB2	2.10	0.52
8:1H:100:LEU:HB3	8:1H:103:LEU:HB2	1.90	0.52
9:1I:116:CYS:SG	9:1I:117:ILE:N	2.82	0.52
10:1J:4:TYR:HD1	10:1J:5:ILE:HG12	1.75	0.52
12:1L:407:TRP:HE3	37:1l:115:MET:HE1	1.75	0.52
15:1O:141:GLN:NE2	15:1O:201:ASP:OD2	2.42	0.52
26:1a:2:TRP:O	26:1a:5:ILE:HB	2.10	0.52
34:1i:47:ASN:HA	34:1i:50:LEU:HB3	1.92	0.52
43:1r:11:ARG:NH2	43:1r:20:GLN:OE1	2.42	0.52
6:1F:107:ASP:OD1	6:1F:225:VAL:HG22	2.09	0.52
6:1F:140:GLY:HA2	6:1F:179:ARG:HE	1.75	0.52
7:1G:378:LEU:HD12	7:1G:409:ILE:HD11	1.91	0.52
10:1J:153:LEU:HD13	14:1N:28:LEU:HD21	1.91	0.52
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.45	0.52
15:1O:209:THR:O	15:1O:213:GLU:HG3	2.10	0.52
15:1O:307:GLY:O	15:1O:320:LYS:NZ	2.42	0.52
19:1S:61:GLN:OE1	19:1S:61:GLN:N	2.43	0.52
27:1b:15:GLU:N	27:1b:15:GLU:OE1	2.42	0.52
2:1B:98:PRO:HG2	22:1W:102:HIS:CE1	2.45	0.52
7:1G:215:PHE:HD2	9:1I:98:PRO:HG3	1.74	0.52
7:1G:391:PHE:O	7:1G:395:ILE:HD12	2.09	0.52
9:1I:117:ILE:HG22	47:1I:201:SF4:S2	2.50	0.52
12:1L:200:GLN:HG3	41:1p:110:LYS:HD2	1.92	0.52
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.24	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.92	0.52
16:1P:249:ALA:HB2	16:1P:318:LEU:HD12	1.90	0.52
22:1W:91:GLU:HA	22:1W:94:ILE:HG12	1.91	0.52
27:1b:20:ALA:O	27:1b:24:ILE:HD12	2.09	0.52
30:1e:60:ASP:OD1	30:1e:60:ASP:N	2.43	0.52
2:1B:143:ASP:HA	16:1P:57:MET:HE1	1.90	0.52
3:1C:50:ILE:O	3:1C:107:VAL:HA	2.10	0.52
4:1D:399:LEU:HD22	4:1D:423:ILE:HG21	1.92	0.52
6:1F:57:LEU:HD13	6:1F:80:SER:HB2	1.90	0.52
7:1G:349:PHE:CE2	7:1G:362:TYR:HB3	2.45	0.52
8:1H:81:LEU:HD22	8:1H:108:MET:HB3	1.92	0.52
16:1P:319:ARG:NH2	22:1W:52:LEU:O	2.42	0.52
23:1X:52:PRO:HB3	25:1Z:80:ASP:HB2	1.92	0.52
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.24	0.52
37:1l:60:PRO:HG3	37:1l:70:ARG:HH21	1.74	0.52
38:1m:49:GLN:O	38:1m:55:ARG:NH1	2.43	0.52
2:1B:101:ARG:HE	2:1B:105:ASP:CG	2.18	0.52
2:1B:150:PRO:HD3	4:1D:190:HIS:ND1	2.25	0.52
7:1G:336:ASN:HD21	19:1S:67:ARG:HD2	1.73	0.52
7:1G:384:PRO:HG2	7:1G:415:LEU:HD11	1.90	0.52
7:1G:439:PHE:O	7:1G:443:LEU:HD12	2.10	0.52
10:1J:27:ILE:O	10:1J:31:LEU:N	2.38	0.52
12:1L:290:LEU:O	12:1L:523:SER:OG	2.28	0.52
13:1M:14:MET:HE3	31:1f:16:VAL:HG23	1.91	0.52
13:1M:72:LEU:HA	13:1M:75:LEU:HD23	1.92	0.52
18:1R:49:VAL:HG23	18:1R:90:GLN:HB3	1.91	0.52
23:1X:142:HIS:HB2	25:1Z:115:ARG:HB2	1.91	0.52
28:1c:17:VAL:O	28:1c:21:LEU:HD12	2.10	0.52
2:1B:131:SER:O	2:1B:131:SER:OG	2.25	0.52
6:1F:232:PRO:HA	6:1F:235:CYS:HB2	1.91	0.52
7:1G:254:MET:HE1	7:1G:256:GLU:HG2	1.92	0.52
11:1K:5:TYR:HD1	11:1K:43:MET:HE1	1.74	0.52
13:1M:105:PHE:HB3	13:1M:125:THR:HG22	1.92	0.52
15:1O:167:HIS:HD2	15:1O:248:TRP:CD1	2.27	0.52
22:1W:32:VAL:HA	22:1W:35:LEU:HD12	1.92	0.52
38:1m:50:TYR:HA	38:1m:55:ARG:HH12	1.75	0.52
39:1n:30:CYS:O	39:1n:32:HIS:N	2.43	0.52
39:1n:139:LEU:O	39:1n:143:THR:HG23	2.10	0.52
4:1D:111:MET:HE2	4:1D:111:MET:N	2.25	0.51
4:1D:184:VAL:HG23	4:1D:203:LEU:HA	1.92	0.51
4:1D:394:PRO:HD2	4:1D:427:GLU:OE2	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1D:901:3PE:H251	12:1L:567:SER:HA	1.92	0.51
6:1F:68:ARG:O	6:1F:106:LYS:NZ	2.43	0.51
6:1F:242:PHE:CZ	6:1F:252:GLY:HA3	2.45	0.51
7:1G:382:THR:HB	7:1G:454:GLY:HA3	1.92	0.51
7:1G:670:ASP:OD1	7:1G:670:ASP:N	2.43	0.51
8:1H:200:LEU:HG	8:1H:282:TYR:HB3	1.92	0.51
14:1N:241:THR:O	14:1N:244:MET:HB2	2.10	0.51
14:1N:263:LYS:O	14:1N:267:ILE:HG13	2.10	0.51
17:1Q:7:ASP:HA	17:1Q:10:LEU:HG	1.91	0.51
17:1Q:54:LYS:NZ	21:1V:115:ILE:HG22	2.25	0.51
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.43	0.51
30:1e:36:GLU:HB2	30:1e:62:PHE:CE1	2.45	0.51
6:1F:259:SER:OG	6:1F:260:GLY:N	2.41	0.51
7:1G:80:LEU:HB3	7:1G:83:SER:HB2	1.91	0.51
7:1G:343:LEU:HD23	7:1G:343:LEU:H	1.75	0.51
7:1G:623:LEU:HA	7:1G:626:VAL:HG22	1.92	0.51
12:1L:119:LYS:NZ	51:1L:702:CDL:OB5	2.43	0.51
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	1.92	0.51
13:1M:168:GLN:HB2	13:1M:174:LEU:HD11	1.92	0.51
14:1N:325:LEU:N	51:1N:401:CDL:OB3	2.38	0.51
15:1O:92:ASN:OD1	15:1O:95:ARG:NH2	2.43	0.51
4:1D:302:GLU:OE2	9:1I:3:LYS:NZ	2.37	0.51
6:1F:91:LYS:O	6:1F:132:ARG:N	2.26	0.51
12:1L:276:MET:SD	12:1L:276:MET:N	2.78	0.51
46:1L:703:PC1:H291	13:1M:446:LEU:HD11	1.91	0.51
14:1N:175:LEU:HD12	14:1N:175:LEU:H	1.74	0.51
15:1O:67:LYS:HD3	15:1O:67:LYS:H	1.75	0.51
16:1P:240:ASP:HB3	16:1P:337:ALA:HB1	1.92	0.51
20:1U:72:CYS:HB3	20:1U:75:GLU:HB3	1.93	0.51
22:1W:17:VAL:HG11	22:1W:77:ARG:HH21	1.75	0.51
25:1Z:6:VAL:HG11	43:1r:41:PRO:HB3	1.91	0.51
34:1i:22:LEU:HD23	34:1i:22:LEU:H	1.75	0.51
39:1n:157:ARG:HH11	39:1n:157:ARG:HA	1.76	0.51
40:1o:36:ARG:HE	40:1o:96:LYS:HE2	1.75	0.51
7:1G:236:SER:HB2	7:1G:259:ASN:HD22	1.76	0.51
9:1I:69:ARG:HD3	42:1q:108:TYR:CG	2.45	0.51
12:1L:203:MET:HE2	41:1p:120:TYR:HD2	1.75	0.51
13:1M:35:SER:O	13:1M:39:LEU:HB2	2.11	0.51
18:1R:58:SER:HB3	18:1R:72:TYR:CE1	2.46	0.51
23:1X:8:THR:HG23	23:1X:10:GLU:H	1.75	0.51
23:1X:124:LEU:HD12	23:1X:124:LEU:H	1.76	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:125:TYR:HE2	25:1Z:136:ALA:HB3	1.74	0.51
37:1L:14:PRO:HD3	37:1L:46:ASP:HB3	1.92	0.51
3:1C:43:SER:HA	43:1r:65:PRO:HA	1.93	0.51
3:1C:162:PHE:HE2	4:1D:88:GLU:HB2	1.74	0.51
4:1D:72:MET:SD	4:1D:410:MET:HG2	2.51	0.51
4:1D:369:ALA:HB2	4:1D:374:PHE:HB3	1.91	0.51
5:1E:149:VAL:HG21	5:1E:193:CYS:SG	2.50	0.51
8:1H:85:MET:HG3	8:1H:105:MET:HE1	1.91	0.51
11:1K:59:MET:HG3	11:1K:60:PRO:HD3	1.92	0.51
12:1L:35:TYR:OH	34:1i:73:HIS:NE2	2.39	0.51
12:1L:480:THR:HG21	40:1o:90:GLU:HB2	1.91	0.51
12:1L:534:HIS:HB3	45:1L:701:3PE:H32	1.93	0.51
17:1Q:11:ILE:HG23	17:1Q:13:VAL:HG23	1.92	0.51
21:1V:78:GLU:HA	21:1V:81:LEU:HB3	1.93	0.51
39:1n:146:GLY:O	39:1n:149:ARG:NH1	2.44	0.51
44:1s:52:LEU:O	44:1s:56:VAL:HG13	2.11	0.51
9:1I:52:PHE:CE1	42:1q:77:VAL:HG21	2.45	0.51
12:1L:559:GLU:HB2	13:1M:214:LEU:HG	1.93	0.51
16:1P:32:ARG:NH2	16:1P:175:GLU:OE2	2.43	0.51
16:1P:172:PHE:CZ	16:1P:206:TYR:HB2	2.46	0.51
16:1P:210:VAL:HG23	16:1P:230:PHE:HD2	1.76	0.51
4:1D:193:TYR:OH	4:1D:201:GLN:O	2.15	0.51
5:1E:209:PRO:HB2	6:1F:43:TYR:CD2	2.45	0.51
13:1M:225:ILE:HG12	13:1M:331:ASN:HB2	1.92	0.51
14:1N:41:ILE:O	14:1N:45:MET:HG2	2.11	0.51
14:1N:241:THR:O	14:1N:301:SER:OG	2.16	0.51
20:1T:50:ILE:HD12	20:1T:50:ILE:H	1.75	0.51
23:1X:168:PHE:HE2	51:1X:201:CDL:H152	1.76	0.51
29:1d:17:GLU:OE1	29:1d:17:GLU:N	2.40	0.51
34:1i:42:MET:HA	34:1i:45:PHE:CZ	2.46	0.51
34:1i:89:VAL:O	34:1i:95:THR:OG1	2.29	0.51
38:1m:48:LEU:HD23	39:1n:165:LEU:HD21	1.93	0.51
4:1D:29:LYS:HD3	4:1D:30:PRO:O	2.11	0.51
6:1F:272:MET:CE	6:1F:318:ASP:HA	2.40	0.51
12:1L:17:ILE:HG23	12:1L:21:MET:HE3	1.92	0.51
14:1N:109:SER:HB2	14:1N:157:MET:SD	2.51	0.51
35:1j:12:ARG:HE	36:1k:50:TRP:CG	2.29	0.51
1:1A:80:GLN:NE2	8:1H:315:PRO:O	2.43	0.51
7:1G:263:ILE:HA	7:1G:390:LEU:HD11	1.93	0.51
9:1I:53:GLU:OE2	42:1q:58:ARG:HA	2.11	0.51
13:1M:24:TRP:CG	13:1M:81:GLN:HE22	2.28	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:210:THR:HG22	51:1N:402:CDL:H801	1.92	0.51
16:1P:167:LYS:HB2	16:1P:229:ALA:HA	1.91	0.51
21:1V:76:ILE:O	21:1V:80:ILE:HG12	2.10	0.51
24:1Y:68:ILE:HG12	24:1Y:99:THR:HG21	1.93	0.51
31:1f:11:TRP:O	31:1f:14:ILE:HG22	2.10	0.51
38:1m:18:ASP:OD1	38:1m:21:GLU:N	2.41	0.51
42:1q:34:ARG:NH1	42:1q:58:ARG:HH21	2.09	0.51
1:1A:88:LEU:HD21	8:1H:306:SER:HB3	1.93	0.51
6:1F:106:LYS:O	6:1F:110:ILE:HG22	2.11	0.51
6:1F:378:ARG:O	6:1F:382:GLY:N	2.43	0.51
7:1G:518:PRO:HB3	7:1G:538:PRO:HD3	1.93	0.51
10:1J:143:ILE:HD12	11:1K:61:ILE:HD12	1.93	0.51
13:1M:17:MET:HE1	31:1f:11:TRP:CZ2	2.46	0.51
16:1P:92:ILE:HG22	16:1P:130:ILE:HB	1.92	0.51
22:1W:57:LYS:NZ	22:1W:61:ASP:OD2	2.43	0.51
29:1d:2:MET:O	29:1d:4:GLY:N	2.44	0.51
40:1o:91:HIS:O	40:1o:95:VAL:HG23	2.10	0.51
40:1o:117:ARG:O	40:1o:121:MET:HB3	2.11	0.51
2:1B:131:SER:OG	4:1D:84:HIS:O	2.29	0.50
8:1H:187:ILE:HA	8:1H:190:LEU:HB2	1.93	0.50
9:1I:53:GLU:HG3	42:1q:61:TRP:HB3	1.93	0.50
9:1I:153:LYS:O	9:1I:157:ASN:N	2.30	0.50
9:1I:169:ILE:HD12	9:1I:176:ARG:HH12	1.74	0.50
12:1L:568:PHE:O	12:1L:572:LYS:N	2.42	0.50
13:1M:326:LEU:HA	13:1M:329:LEU:HD12	1.93	0.50
14:1N:128:LEU:HD21	14:1N:213:LEU:HD13	1.92	0.50
15:1O:236:GLU:OE1	21:1V:25:ILE:HB	2.11	0.50
16:1P:134:HIS:H	16:1P:149:LYS:HZ3	1.60	0.50
23:1X:34:GLN:HE22	23:1X:116:TRP:CG	2.28	0.50
25:1Z:59:ARG:NH1	27:1b:83:LEU:O	2.44	0.50
32:1g:63:PHE:O	32:1g:67:SER:OG	2.17	0.50
35:1j:26:GLU:HA	35:1j:29:SER:HB2	1.92	0.50
38:1m:27:GLU:OE1	38:1m:27:GLU:N	2.40	0.50
42:1q:56:PHE:HZ	43:1r:33:ARG:HE	1.59	0.50
1:1A:81:THR:O	27:1b:45:ASN:ND2	2.36	0.50
2:1B:44:SER:OG	8:1H:51:ASP:OD1	2.15	0.50
3:1C:177:ASP:OD1	16:1P:36:ASN:ND2	2.40	0.50
4:1D:4:TRP:O	13:1M:142:ARG:NH1	2.42	0.50
12:1L:466:PHE:O	12:1L:470:ASN:ND2	2.44	0.50
13:1M:105:PHE:O	13:1M:109:THR:HG23	2.11	0.50
13:1M:190:TRP:CE3	24:1Y:126:MET:HE1	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:66:GLU:HA	17:1Q:72:TRP:O	2.11	0.50
31:1f:10:HIS:CE1	45:1f:102:3PE:H231	2.46	0.50
32:1g:91:ARG:HH21	41:1p:65:ARG:H	1.58	0.50
44:1s:55:ASN:HA	44:1s:58:LEU:HB3	1.92	0.50
4:1D:148:LEU:O	4:1D:174:ARG:NH2	2.44	0.50
7:1G:348:VAL:HA	7:1G:510:GLY:HA2	1.93	0.50
7:1G:410:GLY:O	7:1G:421:HIS:NE2	2.45	0.50
9:1I:77:CYS:O	9:1I:105:ARG:HD3	2.11	0.50
21:1V:53:GLU:OE1	21:1V:53:GLU:N	2.45	0.50
21:1V:97:LYS:H	21:1V:97:LYS:HZ3	1.60	0.50
22:1W:20:ILE:HB	22:1W:80:ASP:OD2	2.11	0.50
23:1X:25:LYS:HA	23:1X:28:ALA:HB2	1.93	0.50
37:1l:55:GLN:HA	37:1l:58:ARG:HD2	1.93	0.50
39:1n:26:LEU:HD21	39:1n:39:PHE:HB3	1.93	0.50
43:1r:47:LYS:O	43:1r:51:ASN:ND2	2.44	0.50
1:1A:87:MET:HA	10:1J:147:TYR:HB3	1.94	0.50
3:1C:50:ILE:HB	3:1C:107:VAL:HG12	1.93	0.50
5:1E:160:TYR:C	5:1E:161:TYR:HD1	2.19	0.50
5:1E:203:THR:N	6:1F:17:ASP:OD2	2.44	0.50
7:1G:655:GLN:OE1	7:1G:655:GLN:N	2.42	0.50
12:1L:144:TRP:O	12:1L:223:LYS:NZ	2.43	0.50
23:1X:44:LEU:O	23:1X:48:GLU:HB2	2.11	0.50
28:1c:21:LEU:O	28:1c:25:VAL:HG23	2.11	0.50
35:1j:63:GLU:HG2	35:1j:64:LEU:HD12	1.94	0.50
38:1m:38:ILE:HG23	38:1m:41:ARG:HH21	1.75	0.50
4:1D:103:PHE:HA	4:1D:106:LEU:HD23	1.94	0.50
4:1D:190:HIS:O	9:1I:62:ARG:NH2	2.45	0.50
4:1D:259:MET:HA	4:1D:259:MET:HE3	1.92	0.50
5:1E:23:PHE:HA	5:1E:57:GLN:HE22	1.77	0.50
7:1G:163:ALA:HA	7:1G:167:ALA:HB3	1.94	0.50
12:1L:482:MET:SD	12:1L:482:MET:N	2.85	0.50
16:1P:322:ARG:HD3	16:1P:327:LEU:HA	1.93	0.50
19:1S:49:ASP:N	19:1S:49:ASP:OD1	2.41	0.50
22:1W:108:HIS:HB3	22:1W:111:GLU:OE2	2.11	0.50
29:1d:8:ARG:HE	46:1d:201:PC1:H242	1.77	0.50
33:1h:143:ASN:N	33:1h:143:ASN:OD1	2.44	0.50
37:1l:77:ILE:HD11	38:1m:67:TRP:CD2	2.46	0.50
2:1B:179:ARG:NH1	46:1B:202:PC1:O14	2.44	0.50
3:1C:50:ILE:N	3:1C:106:ARG:O	2.39	0.50
4:1D:339:LYS:HA	18:1R:69:PRO:HB3	1.94	0.50
7:1G:524:LEU:HB3	7:1G:545:TYR:HD1	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:33:LEU:HA	10:1J:36:SER:OG	2.10	0.50
11:1K:43:MET:HG2	14:1N:72:MET:HE2	1.93	0.50
12:1L:66:TRP:NE1	46:1L:703:PC1:O14	2.44	0.50
12:1L:542:LEU:HD13	37:1L:83:MET:HE1	1.92	0.50
13:1M:98:MET:HE2	13:1M:98:MET:HA	1.94	0.50
18:1R:41:ILE:HG22	18:1R:42:ASP:OD1	2.12	0.50
2:1B:95:LYS:HD2	3:1C:155:TYR:CD1	2.47	0.50
8:1H:117:LEU:HD11	10:1J:68:PHE:CD1	2.45	0.50
10:1J:134:GLY:N	26:1a:42:SER:OG	2.44	0.50
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.77	0.50
14:1N:164:ILE:H	14:1N:164:ILE:HD12	1.75	0.50
29:1d:28:ASP:OD2	29:1d:30:ARG:NH1	2.45	0.50
34:1i:15:ARG:HH22	34:1i:19:ARG:HH11	1.60	0.50
1:1A:32:GLU:H	1:1A:32:GLU:CD	2.20	0.50
3:1C:66:ASP:HB3	21:1V:89:LEU:HB2	1.94	0.50
7:1G:329:VAL:HG21	7:1G:623:LEU:HG	1.92	0.50
8:1H:24:GLU:OE1	8:1H:274:ARG:NH1	2.44	0.50
12:1L:471:ASN:OD1	12:1L:471:ASN:N	2.35	0.50
13:1M:15:THR:O	13:1M:93:LYS:HD3	2.12	0.50
13:1M:306:PRO:O	13:1M:310:MET:HG3	2.11	0.50
14:1N:187:MET:HA	14:1N:187:MET:HE3	1.93	0.50
15:1O:261:MET:SD	15:1O:264:GLN:NE2	2.84	0.50
29:1d:40:CYS:O	29:1d:44:ILE:HG22	2.12	0.50
40:1o:112:LYS:O	40:1o:116:GLN:HG3	2.12	0.50
2:1B:72:PHE:CE2	2:1B:161:LEU:HD21	2.46	0.50
8:1H:75:PRO:HG3	8:1H:215:TYR:CE2	2.46	0.50
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.18	0.50
13:1M:14:MET:HE1	31:1f:12:VAL:O	2.11	0.50
14:1N:71:MET:O	14:1N:74:ILE:N	2.45	0.50
16:1P:197:GLY:HA3	16:1P:238:LEU:HD12	1.94	0.50
17:1Q:56:LYS:HB3	17:1Q:58:GLU:OE2	2.12	0.50
25:1Z:121:MET:HA	25:1Z:124:LEU:HG	1.94	0.50
39:1n:83:GLU:OE2	39:1n:89:SER:OG	2.23	0.50
4:1D:211:ILE:HG22	4:1D:315:LEU:HD11	1.94	0.49
6:1F:184:TYR:CE1	49:1F:501:FMN:H6	2.47	0.49
6:1F:374:LYS:HB3	7:1G:132:GLU:HG2	1.93	0.49
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.46	0.49
15:1O:46:LEU:HD11	15:1O:235:VAL:HB	1.94	0.49
16:1P:171:ILE:HD11	16:1P:207:ILE:HA	1.93	0.49
20:1U:42:LEU:HD13	20:1U:46:ASP:HB3	1.94	0.49
22:1W:91:GLU:OE2	22:1W:95:ASN:ND2	2.45	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:120:ARG:O	38:1m:108:ARG:NH1	2.36	0.49
39:1n:50:HIS:O	39:1n:53:GLU:HG2	2.11	0.49
44:1s:45:GLU:OE1	44:1s:45:GLU:N	2.44	0.49
1:1A:46:SER:OG	1:1A:47:ALA:N	2.40	0.49
4:1D:2:ARG:NH1	32:1g:29:ASP:O	2.44	0.49
4:1D:137:ILE:HG12	4:1D:203:LEU:HD11	1.94	0.49
6:1F:13:GLY:HA2	6:1F:271:GLU:HB3	1.94	0.49
6:1F:289:GLY:HA3	6:1F:293:ASN:HD22	1.77	0.49
7:1G:39:ARG:HB2	48:1G:803:FES:S2	2.52	0.49
7:1G:201:ASP:OD2	7:1G:268:ARG:NH2	2.45	0.49
7:1G:318:ILE:HD11	7:1G:514:ILE:HG13	1.93	0.49
9:1I:31:VAL:HG11	46:1I:203:PC1:H241	1.93	0.49
12:1L:64:SER:HA	12:1L:79:SER:HA	1.94	0.49
12:1L:317:ILE:HD13	12:1L:322:PRO:HB3	1.94	0.49
13:1M:126:LEU:O	13:1M:130:LEU:HD12	2.12	0.49
16:1P:200:THR:O	16:1P:238:LEU:N	2.43	0.49
17:1Q:32:THR:O	17:1Q:62:ARG:NH2	2.45	0.49
31:1f:18:VAL:O	31:1f:22:PHE:HB2	2.12	0.49
31:1f:43:LEU:HD11	41:1p:67:PHE:CD1	2.47	0.49
39:1n:176:ARG:HG3	39:1n:178:MET:SD	2.51	0.49
42:1q:17:HIS:ND1	42:1q:26:VAL:HG21	2.27	0.49
1:1A:84:LEU:HA	1:1A:87:MET:HB3	1.94	0.49
45:1A:201:3PE:O12	45:1A:201:3PE:N	2.35	0.49
4:1D:206:GLY:N	25:1Z:9:ASP:OD2	2.45	0.49
7:1G:148:THR:HG23	7:1G:150:MET:HE3	1.95	0.49
10:1J:146:LEU:CA	11:1K:58:MET:HE1	2.41	0.49
12:1L:14:ILE:HA	12:1L:17:ILE:HD13	1.94	0.49
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	1.93	0.49
13:1M:12:LEU:HB3	13:1M:13:PRO:HD3	1.95	0.49
13:1M:47:GLU:HG2	41:1p:89:MET:HE1	1.94	0.49
13:1M:62:SER:O	13:1M:66:LEU:HD12	2.13	0.49
13:1M:115:LEU:HB3	13:1M:164:LEU:HD13	1.95	0.49
13:1M:237:LYS:NZ	13:1M:316:MET:O	2.36	0.49
14:1N:248:LEU:HD12	14:1N:293:TYR:HA	1.94	0.49
34:1i:108:THR:O	41:1p:18:ALA:N	2.44	0.49
38:1m:60:GLU:OE1	38:1m:60:GLU:N	2.28	0.49
1:1A:29:ALA:O	16:1P:320:ARG:NH1	2.42	0.49
3:1C:56:GLY:C	3:1C:59:PRO:HD2	2.38	0.49
3:1C:89:ARG:HG3	3:1C:90:PHE:CD2	2.47	0.49
4:1D:259:MET:HG3	4:1D:398:HIS:CD2	2.47	0.49
6:1F:230:VAL:O	6:1F:234:ILE:HG12	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:703:ILE:HG13	18:1R:83:THR:HG21	1.95	0.49
8:1H:20:LEU:HD13	26:1a:12:MET:HE1	1.94	0.49
8:1H:26:LYS:NZ	8:1H:35:LYS:O	2.45	0.49
12:1L:90:ILE:HB	12:1L:91:PRO:HD3	1.94	0.49
12:1L:173:LEU:HD12	13:1M:405:LEU:HD21	1.95	0.49
12:1L:269:THR:O	12:1L:271:LYS:NZ	2.33	0.49
12:1L:314:MET:HA	12:1L:317:ILE:HG22	1.94	0.49
14:1N:102:LEU:HD21	14:1N:141:VAL:HB	1.94	0.49
14:1N:178:ILE:O	14:1N:182:SER:N	2.37	0.49
21:1V:111:TRP:O	21:1V:112:LYS:HG2	2.12	0.49
36:1k:31:VAL:O	36:1k:35:LEU:N	2.36	0.49
37:1l:126:GLN:HB2	37:1l:128:VAL:HG13	1.93	0.49
2:1B:108:PRO:O	8:1H:58:LYS:NZ	2.43	0.49
4:1D:219:SER:OG	25:1Z:20:ASP:OD1	2.24	0.49
6:1F:287:VAL:HG11	6:1F:294:LEU:HB2	1.95	0.49
7:1G:665:GLN:HG2	7:1G:671:PHE:HA	1.93	0.49
8:1H:89:LEU:HD12	8:1H:89:LEU:H	1.77	0.49
9:1l:5:VAL:HG23	43:1r:112:LEU:HD23	1.95	0.49
12:1L:313:MET:HE1	12:1L:329:ILE:HD12	1.93	0.49
12:1L:412:THR:O	12:1L:416:THR:OG1	2.20	0.49
13:1M:269:MET:HE2	13:1M:399:ASN:CG	2.37	0.49
13:1M:285:LEU:HD22	13:1M:342:MET:HE1	1.93	0.49
13:1M:401:MET:HE2	13:1M:401:MET:HA	1.94	0.49
16:1P:172:PHE:HB2	16:1P:179:LEU:HD23	1.93	0.49
25:1Z:134:LEU:HD13	25:1Z:138:TYR:HB2	1.94	0.49
37:1l:98:TRP:HA	37:1l:101:MET:HB2	1.93	0.49
37:1l:112:MET:HA	37:1l:112:MET:HE3	1.94	0.49
2:1B:43:SER:HB3	8:1H:40:VAL:HG21	1.93	0.49
4:1D:165:THR:HB	4:1D:169:TRP:CZ2	2.48	0.49
6:1F:338:ASP:OD1	6:1F:341:THR:OG1	2.28	0.49
10:1J:71:THR:HG22	11:1K:27:MET:HG2	1.93	0.49
10:1J:125:TRP:HH2	25:1Z:126:GLY:HA2	1.77	0.49
10:1J:163:ILE:HG13	14:1N:12:THR:HG21	1.95	0.49
13:1M:42:LEU:HD11	13:1M:67:VAL:HG11	1.93	0.49
14:1N:255:PRO:HG3	14:1N:260:PHE:CG	2.47	0.49
15:1O:43:ALA:O	15:1O:48:LEU:N	2.40	0.49
16:1P:133:SER:O	16:1P:167:LYS:HA	2.12	0.49
20:1U:32:VAL:HG13	20:1U:33:ASN:OD1	2.13	0.49
23:1X:7:PRO:HD2	25:1Z:84:LEU:HD11	1.95	0.49
30:1e:6:GLN:HE22	30:1e:14:ASP:H	1.61	0.49
33:1h:115:ARG:HG3	33:1h:123:TYR:CD1	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:12:ARG:HG2	36:1k:50:TRP:CD2	2.47	0.49
35:1j:36:ILE:HD12	35:1j:37:LEU:HB3	1.95	0.49
41:1p:28:PRO:O	41:1p:32:LEU:HD22	2.13	0.49
5:1E:109:MET:HA	5:1E:113:SER:H	1.77	0.49
12:1L:279:CYS:O	12:1L:283:ILE:HG22	2.12	0.49
12:1L:304:PHE:HZ	12:1L:526:LEU:HD23	1.77	0.49
14:1N:122:ILE:HD11	14:1N:127:GLY:HA2	1.94	0.49
51:1N:401:CDL:H473	46:1d:201:PC1:H392	1.94	0.49
15:1O:161:CYS:SG	15:1O:162:GLU:N	2.85	0.49
20:1U:48:VAL:O	20:1U:52:MET:HG2	2.12	0.49
40:1o:108:LEU:O	40:1o:112:LYS:HG3	2.13	0.49
4:1D:248:GLU:HA	4:1D:248:GLU:OE1	2.11	0.49
5:1E:60:TRP:HA	5:1E:91:ASN:HB2	1.95	0.49
7:1G:276:ARG:HB2	7:1G:680:ALA:HB1	1.93	0.49
7:1G:366:THR:HG21	7:1G:450:MET:SD	2.53	0.49
8:1H:63:PRO:HG3	8:1H:214:GLU:HB3	1.95	0.49
8:1H:65:THR:O	8:1H:124:ASN:ND2	2.30	0.49
8:1H:263:THR:O	8:1H:267:THR:OG1	2.21	0.49
16:1P:214:ILE:O	16:1P:218:ILE:HG12	2.13	0.49
18:1R:20:ASP:C	18:1R:25:ARG:HH22	2.21	0.49
20:1U:47:GLN:HE21	20:1U:71:MET:HB3	1.77	0.49
22:1W:111:GLU:H	22:1W:111:GLU:CD	2.21	0.49
32:1g:88:TRP:CD1	32:1g:91:ARG:HH22	2.30	0.49
57:1l:201:MYR:O1	40:1o:1:GLY:N	2.44	0.49
42:1q:46:ASN:HB3	42:1q:48:TYR:CE1	2.48	0.49
2:1B:94:ASN:HD21	2:1B:131:SER:HA	1.77	0.49
6:1F:24:ASN:HB3	6:1F:114:ASP:OD1	2.13	0.49
7:1G:336:ASN:HB3	19:1S:71:GLY:HA2	1.95	0.49
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	1.94	0.49
8:1H:91:MET:O	8:1H:93:TYR:N	2.46	0.49
9:1I:78:ILE:O	9:1I:104:ARG:NH2	2.34	0.49
12:1L:76:LEU:HD21	12:1L:196:TRP:CE3	2.48	0.49
13:1M:208:PRO:HB2	13:1M:291:VAL:HG13	1.94	0.49
20:1U:54:MET:HA	20:1U:54:MET:HE3	1.93	0.49
23:1X:44:LEU:HD12	23:1X:130:VAL:HG13	1.95	0.49
25:1Z:68:ARG:CZ	25:1Z:72:MET:HE1	2.43	0.49
38:1m:120:LEU:HB3	38:1m:122:GLN:NE2	2.28	0.49
39:1n:178:MET:SD	39:1n:178:MET:N	2.86	0.49
2:1B:52:LEU:HG	4:1D:61:VAL:HG11	1.94	0.49
5:1E:30:ARG:HG2	44:1s:52:LEU:HB3	1.94	0.49
6:1F:302:SER:HB3	6:1F:350:LEU:HD11	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:23:LYS:NZ	11:1K:24:SER:HB2	2.28	0.49
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.94	0.49
30:1e:37:LYS:O	30:1e:41:GLU:HG3	2.13	0.49
34:1i:109:ILE:HG22	34:1i:112:THR:H	1.78	0.49
4:1D:234:ILE:HG12	8:1H:280:PHE:HE1	1.77	0.48
7:1G:232:ASP:OD1	7:1G:234:VAL:HG23	2.13	0.48
7:1G:278:ARG:HD2	7:1G:278:ARG:HA	1.67	0.48
7:1G:403:ASP:OD1	17:1Q:127:ARG:NH1	2.46	0.48
9:1I:64:GLU:HB3	9:1I:139:PHE:CE1	2.48	0.48
12:1L:21:MET:N	12:1L:21:MET:HE2	2.28	0.48
14:1N:5:ILE:O	14:1N:9:LEU:HD12	2.12	0.48
31:1f:49:ARG:HH21	31:1f:52:GLU:CD	2.21	0.48
32:1g:41:ASN:OD1	32:1g:41:ASN:N	2.45	0.48
39:1n:90:TYR:CD1	39:1n:91:GLU:HG2	2.45	0.48
39:1n:100:GLU:O	39:1n:121:ARG:NH2	2.42	0.48
42:1q:44:TYR:HE2	42:1q:83:PRO:HB3	1.77	0.48
1:1A:106:TRP:CG	8:1H:291:LYS:HZ1	2.31	0.48
4:1D:161:ILE:HD12	4:1D:238:ARG:HD3	1.94	0.48
4:1D:173:GLU:HA	4:1D:176:LYS:HG2	1.95	0.48
5:1E:27:ASN:HA	5:1E:30:ARG:HD2	1.94	0.48
5:1E:134:ASP:OD1	5:1E:136:LEU:HB2	2.13	0.48
6:1F:117:LYS:HG2	6:1F:229:ALA:HB1	1.95	0.48
6:1F:344:VAL:HG12	6:1F:380:VAL:HG22	1.95	0.48
8:1H:184:MET:HE1	8:1H:293:PHE:CG	2.48	0.48
12:1L:538:THR:HG23	37:1l:89:VAL:HG22	1.93	0.48
14:1N:30:TRP:CD1	14:1N:70:LEU:HD23	2.33	0.48
20:1U:22:TYR:CZ	20:1U:24:LYS:HD3	2.47	0.48
20:1U:61:GLU:HB2	39:1n:84:SER:HB2	1.94	0.48
21:1V:63:ASP:OD1	21:1V:65:LYS:N	2.45	0.48
24:1Y:68:ILE:HD11	24:1Y:96:GLY:HA2	1.94	0.48
30:1e:91:TYR:HD1	30:1e:92:THR:N	2.12	0.48
35:1j:34:PHE:O	35:1j:38:TRP:HB3	2.14	0.48
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.13	0.48
40:1o:18:PRO:HA	40:1o:21:MET:HE1	1.94	0.48
2:1B:71:ARG:HG2	2:1B:72:PHE:HD1	1.78	0.48
4:1D:105:ARG:HE	9:1I:117:ILE:HD11	1.78	0.48
4:1D:158:ALA:HA	4:1D:161:ILE:HB	1.96	0.48
4:1D:261:ARG:NE	4:1D:303:GLU:OE2	2.46	0.48
4:1D:395:GLY:C	4:1D:428:VAL:HG23	2.38	0.48
7:1G:286:ASN:OD1	7:1G:290:LEU:N	2.35	0.48
12:1L:147:VAL:CG2	12:1L:252:MET:HG3	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:470:ASN:O	40:1o:69:LYS:NZ	2.25	0.48
13:1M:75:LEU:HD12	13:1M:436:LEU:HD12	1.95	0.48
16:1P:331:MET:N	16:1P:331:MET:HE3	2.28	0.48
21:1V:53:GLU:O	21:1V:57:MET:HB2	2.13	0.48
21:1V:68:GLU:HG2	21:1V:75:GLN:HA	1.95	0.48
31:1f:3:VAL:HA	31:1f:6:ILE:HG22	1.95	0.48
32:1g:37:LEU:HD13	32:1g:49:LYS:HZ3	1.78	0.48
37:1l:91:THR:O	37:1l:91:THR:OG1	2.32	0.48
4:1D:156:THR:HA	4:1D:159:LEU:HB2	1.94	0.48
5:1E:86:PHE:CD1	7:1G:177:ARG:HB3	2.47	0.48
5:1E:193:CYS:SG	6:1F:267:THR:HG22	2.53	0.48
6:1F:385:ARG:HG3	6:1F:386:PRO:HD2	1.95	0.48
7:1G:284:ILE:HG22	7:1G:559:VAL:HG22	1.96	0.48
8:1H:133:LEU:HD11	10:1J:72:THR:HG21	1.95	0.48
13:1M:30:HIS:HB3	31:1f:16:VAL:HG11	1.94	0.48
13:1M:119:TYR:HA	13:1M:122:PHE:HB3	1.95	0.48
13:1M:336:ARG:HH21	13:1M:429:SER:HA	1.78	0.48
14:1N:209:ILE:O	14:1N:213:LEU:HD22	2.13	0.48
14:1N:260:PHE:CE2	14:1N:264:TRP:HB2	2.48	0.48
15:1O:138:MET:O	15:1O:143:PHE:HB2	2.13	0.48
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	1.96	0.48
17:1Q:36:ARG:HD2	17:1Q:36:ARG:C	2.38	0.48
24:1Y:22:TYR:O	24:1Y:25:THR:OG1	2.27	0.48
25:1Z:86:MET:HE1	25:1Z:125:TYR:CE1	2.47	0.48
38:1m:27:GLU:O	38:1m:30:LYS:NZ	2.42	0.48
2:1B:79:SER:O	2:1B:82:GLN:HB2	2.14	0.48
5:1E:87:TYR:CD2	6:1F:181:ALA:HB3	2.46	0.48
6:1F:214:GLY:N	6:1F:218:CYS:O	2.47	0.48
7:1G:126:ASP:OD1	43:1r:56:ARG:NH2	2.45	0.48
8:1H:20:LEU:HD22	8:1H:232:ILE:HD11	1.94	0.48
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.49	0.48
8:1H:208:VAL:HG12	8:1H:209:SER:N	2.28	0.48
11:1K:37:MET:O	11:1K:41:PHE:N	2.36	0.48
12:1L:56:HIS:CG	41:1p:29:VAL:HG21	2.48	0.48
13:1M:207:MET:HE1	13:1M:240:GLY:N	2.28	0.48
16:1P:319:ARG:HD3	16:1P:322:ARG:HH11	1.79	0.48
32:1g:91:ARG:NH2	41:1p:65:ARG:H	2.11	0.48
33:1h:53:ALA:HB2	41:1p:61:TYR:HD2	1.78	0.48
37:1l:115:MET:O	37:1l:119:GLY:N	2.41	0.48
2:1B:66:ARG:HH12	9:1I:56:PRO:HD2	1.79	0.48
2:1B:68:ASP:CG	2:1B:71:ARG:HB3	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:31:GLU:OE1	21:1V:46:TYR:OH	2.27	0.48
5:1E:128:VAL:HA	5:1E:139:LEU:HG	1.95	0.48
7:1G:228:ILE:HA	7:1G:237:ASN:HA	1.96	0.48
8:1H:296:LEU:HD22	27:1b:17:VAL:HG23	1.94	0.48
13:1M:271:MET:O	13:1M:275:ILE:HG12	2.14	0.48
14:1N:76:ILE:HB	14:1N:94:ALA:HB2	1.96	0.48
14:1N:162:ILE:HG13	14:1N:188:GLY:HA3	1.95	0.48
33:1h:114:MET:HE2	33:1h:122:TRP:H	1.79	0.48
36:1k:15:LEU:HD23	36:1k:15:LEU:H	1.77	0.48
5:1E:51:LEU:HD21	5:1E:80:VAL:HG13	1.94	0.48
10:1J:4:TYR:HD1	10:1J:5:ILE:H	1.60	0.48
10:1J:68:PHE:O	10:1J:71:THR:OG1	2.24	0.48
12:1L:61:MET:HG3	12:1L:82:MET:HB2	1.95	0.48
12:1L:271:LYS:HD3	12:1L:271:LYS:N	2.28	0.48
13:1M:160:LEU:HD13	13:1M:164:LEU:HG	1.95	0.48
22:1W:102:HIS:HA	22:1W:105:ARG:HD2	1.95	0.48
30:1e:27:LYS:HD3	30:1e:27:LYS:N	2.29	0.48
39:1n:59:ALA:HA	39:1n:62:LEU:HD12	1.96	0.48
1:1A:38:GLU:HB2	1:1A:43:PRO:HG3	1.96	0.48
4:1D:86:GLY:O	4:1D:90:LEU:HD12	2.14	0.48
6:1F:12:PHE:HB2	6:1F:273:SER:O	2.14	0.48
6:1F:363:THR:HG23	6:1F:364:PRO:HD3	1.96	0.48
7:1G:488:LYS:HD3	7:1G:488:LYS:N	2.29	0.48
9:1I:97:GLU:O	9:1I:104:ARG:HB2	2.13	0.48
12:1L:48:LEU:O	12:1L:51:LEU:N	2.46	0.48
12:1L:108:MET:HE1	12:1L:117:PHE:CG	2.48	0.48
12:1L:171:ALA:HA	12:1L:232:TRP:HB2	1.94	0.48
14:1N:245:MET:HG2	14:1N:297:ALA:HB1	1.95	0.48
15:1O:251:GLN:HB3	15:1O:256:PHE:CE1	2.49	0.48
16:1P:265:TRP:O	16:1P:269:LEU:HD12	2.14	0.48
20:1T:56:ASP:OD1	20:1T:57:GLU:N	2.46	0.48
22:1W:44:PRO:HD3	22:1W:60:ARG:HH21	1.79	0.48
28:1c:35:HIS:O	28:1c:39:VAL:HG23	2.13	0.48
34:1i:102:ARG:HH21	40:1o:49:GLN:HB2	1.77	0.48
40:1o:112:LYS:O	40:1o:115:GLU:HG3	2.14	0.48
44:1s:50:THR:O	44:1s:54:LEU:HD22	2.14	0.48
1:1A:53:MET:HE3	10:1J:70:TYR:CD1	2.49	0.48
3:1C:23:SER:HB2	43:1r:68:VAL:HG11	1.96	0.48
4:1D:312:SER:HB2	25:1Z:19:ILE:HB	1.94	0.48
4:1D:393:ALA:HB3	4:1D:396:PHE:HB2	1.96	0.48
5:1E:52:ASP:OD2	6:1F:179:ARG:NH1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:195:ARG:HD2	8:1H:274:ARG:HG3	1.93	0.48
12:1L:357:ARG:NH1	39:1n:28:SER:HB2	2.29	0.48
12:1L:584:ILE:HD11	14:1N:58:LYS:HE3	1.94	0.48
13:1M:5:ILE:O	13:1M:9:THR:HG23	2.13	0.48
31:1f:45:LYS:H	41:1p:68:ARG:NH2	2.12	0.48
39:1n:122:GLU:O	39:1n:126:ARG:HG2	2.14	0.48
43:1r:92:LYS:HA	43:1r:92:LYS:HE3	1.96	0.48
2:1B:117:GLY:HA2	2:1B:148:GLY:O	2.14	0.48
3:1C:52:ILE:HD11	3:1C:57:VAL:HA	1.95	0.48
5:1E:186:PRO:HG2	5:1E:191:PHE:O	2.14	0.48
6:1F:37:GLN:NE2	6:1F:41:ASP:O	2.47	0.48
8:1H:85:MET:HE1	8:1H:108:MET:HB2	1.95	0.48
14:1N:183:SER:O	14:1N:187:MET:N	2.43	0.48
14:1N:270:MET:HE1	14:1N:282:MET:SD	2.54	0.48
14:1N:344:SER:O	29:1d:82:MET:HG3	2.14	0.48
16:1P:174:ARG:HA	16:1P:317:VAL:HG13	1.96	0.48
16:1P:248:VAL:HG22	16:1P:334:VAL:HG11	1.95	0.48
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.95	0.48
4:1D:149:ASN:HD22	4:1D:370:PRO:CB	2.26	0.47
8:1H:22:LEU:HB2	8:1H:48:PRO:HG3	1.96	0.47
8:1H:102:VAL:O	8:1H:106:LEU:N	2.45	0.47
51:1H:402:CDL:H512	51:1H:402:CDL:HB4	1.43	0.47
12:1L:147:VAL:HG22	12:1L:252:MET:HE2	1.96	0.47
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.96	0.47
12:1L:499:MET:HG3	12:1L:500:LEU:HD23	1.95	0.47
15:1O:53:GLU:HG2	15:1O:104:ARG:HH12	1.79	0.47
18:1R:27:ARG:O	18:1R:31:ARG:NH1	2.47	0.47
30:1e:44:HIS:HD2	33:1h:129:ASP:HA	1.79	0.47
30:1e:52:GLU:O	30:1e:56:LYS:HB2	2.14	0.47
1:1A:12:THR:O	1:1A:16:LEU:HD22	2.14	0.47
1:1A:25:PRO:HB3	8:1H:57:THR:HA	1.96	0.47
2:1B:101:ARG:HA	2:1B:101:ARG:HD2	1.63	0.47
5:1E:191:PHE:HB3	44:1s:38:TYR:CE1	2.48	0.47
6:1F:68:ARG:HG3	6:1F:226:GLU:HB3	1.96	0.47
7:1G:415:LEU:O	7:1G:417:TYR:N	2.47	0.47
9:1I:147:LEU:HD23	9:1I:147:LEU:HA	1.73	0.47
12:1L:10:THR:O	12:1L:14:ILE:HG23	2.14	0.47
12:1L:357:ARG:HH11	39:1n:28:SER:HB2	1.80	0.47
13:1M:252:PRO:HG3	29:1d:117:HIS:CE1	2.49	0.47
13:1M:265:SER:O	13:1M:269:MET:HB3	2.14	0.47
14:1N:179:MET:CE	14:1N:215:MET:HG2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:112:LYS:HE2	16:1P:112:LYS:HB2	1.75	0.47
21:1V:46:TYR:CZ	43:1r:91:LYS:HE3	2.48	0.47
1:1A:113:TRP:NE1	8:1H:286:MET:HE2	2.28	0.47
2:1B:62:MET:HA	2:1B:67:TYR:HD2	1.79	0.47
4:1D:166:PRO:HA	4:1D:169:TRP:CD1	2.49	0.47
9:1I:11:SER:O	9:1I:16:SER:OG	2.27	0.47
10:1J:25:SER:HB2	10:1J:81:GLU:O	2.13	0.47
12:1L:346:ILE:HG13	12:1L:350:LEU:HD23	1.96	0.47
14:1N:112:HIS:HB2	14:1N:184:ILE:HD13	1.95	0.47
15:1O:157:LYS:O	15:1O:161:CYS:HB3	2.15	0.47
23:1X:110:VAL:O	23:1X:115:GLY:N	2.46	0.47
24:1Y:104:THR:HG21	24:1Y:109:ILE:HD11	1.95	0.47
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.25	0.47
1:1A:74:PRO:HB3	10:1J:143:ILE:HG22	1.96	0.47
2:1B:94:ASN:ND2	2:1B:131:SER:HA	2.29	0.47
3:1C:80:ALA:HA	3:1C:92:ILE:HA	1.96	0.47
4:1D:281:VAL:HG21	4:1D:310:ILE:HG23	1.97	0.47
5:1E:105:THR:HG23	5:1E:107:PRO:HD2	1.96	0.47
8:1H:139:THR:HA	8:1H:142:TYR:CD1	2.49	0.47
9:1I:54:LYS:HD3	42:1q:91:HIS:NE2	2.29	0.47
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.14	0.47
17:1Q:17:LEU:H	17:1Q:17:LEU:HD12	1.79	0.47
20:1U:28:GLU:OE1	20:1U:28:GLU:N	2.45	0.47
32:1g:40:LYS:HA	32:1g:40:LYS:HE3	1.96	0.47
38:1m:102:TYR:O	38:1m:106:THR:OG1	2.19	0.47
44:1s:33:PHE:CD1	44:1s:34:ASP:N	2.74	0.47
1:1A:84:LEU:HD12	1:1A:84:LEU:H	1.80	0.47
7:1G:470:VAL:HG23	7:1G:490:MET:HE1	1.96	0.47
14:1N:312:LYS:HG2	14:1N:315:TRP:CH2	2.49	0.47
19:1S:17:GLU:OE2	19:1S:67:ARG:HD3	2.14	0.47
27:1b:62:MET:SD	27:1b:62:MET:N	2.87	0.47
4:1D:109:VAL:HG13	4:1D:424:VAL:HG11	1.96	0.47
5:1E:120:ILE:HG21	5:1E:139:LEU:HD13	1.95	0.47
7:1G:285:ARG:HE	7:1G:289:GLY:C	2.22	0.47
7:1G:381:GLY:HA3	7:1G:457:ALA:HB2	1.97	0.47
12:1L:326:PHE:O	12:1L:329:ILE:HG22	2.14	0.47
12:1L:350:LEU:HD21	12:1L:362:LEU:HD11	1.97	0.47
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.50	0.47
13:1M:224:PRO:O	13:1M:228:SER:OG	2.30	0.47
14:1N:215:MET:SD	14:1N:244:MET:HE1	2.55	0.47
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:19:ASP:OD1	18:1R:20:ASP:N	2.47	0.47
34:1i:22:LEU:HA	34:1i:25:GLN:HG2	1.97	0.47
1:1A:35:SER:O	2:1B:81:ARG:NH2	2.47	0.47
1:1A:113:TRP:HE1	8:1H:283:ASP:HA	1.80	0.47
2:1B:84:ASP:OD2	8:1H:54:LYS:HD2	2.15	0.47
2:1B:93:THR:HG21	4:1D:83:LEU:C	2.39	0.47
2:1B:126:TYR:OH	4:1D:85:ARG:NH2	2.47	0.47
3:1C:78:LEU:HB2	3:1C:130:TYR:HB3	1.96	0.47
4:1D:115:GLU:HA	4:1D:118:TYR:HB3	1.97	0.47
4:1D:205:LEU:HB2	43:1r:35:GLN:HG2	1.97	0.47
5:1E:98:TYR:N	5:1E:136:LEU:O	2.46	0.47
5:1E:122:LYS:HE3	5:1E:122:LYS:HB3	1.77	0.47
7:1G:144:PRO:HG3	7:1G:698:VAL:HB	1.96	0.47
7:1G:335:LEU:HA	7:1G:338:VAL:HG12	1.95	0.47
7:1G:522:LEU:HB3	7:1G:543:ILE:HD13	1.97	0.47
7:1G:568:GLU:HG2	7:1G:587:VAL:HG13	1.97	0.47
46:1l:203:PC1:H122	25:1Z:30:LEU:O	2.14	0.47
11:1K:81:VAL:O	11:1K:85:TYR:HB2	2.15	0.47
12:1L:132:VAL:HG23	12:1L:258:PHE:CZ	2.49	0.47
12:1L:309:GLN:O	12:1L:313:MET:HG2	2.15	0.47
12:1L:316:THR:O	12:1L:321:GLN:HB2	2.15	0.47
12:1L:561:ILE:HG23	12:1L:562:LEU:H	1.79	0.47
13:1M:94:LEU:HD23	45:1M:503:3PE:H351	1.97	0.47
13:1M:129:THR:O	13:1M:132:ILE:N	2.48	0.47
13:1M:150:LEU:HD23	14:1N:294:MET:SD	2.54	0.47
13:1M:220:HIS:CD2	13:1M:232:ALA:HB2	2.50	0.47
13:1M:438:ALA:HA	13:1M:441:ILE:HG22	1.97	0.47
14:1N:24:SER:OG	30:1e:14:ASP:OD1	2.32	0.47
15:1O:77:CYS:HB3	15:1O:95:ARG:HG2	1.97	0.47
16:1P:135:LEU:HD12	16:1P:229:ALA:HB1	1.96	0.47
16:1P:180:ASN:OD1	16:1P:320:ARG:NH2	2.45	0.47
18:1R:18:TYR:HE2	18:1R:24:ARG:HB2	1.79	0.47
20:1T:18:VAL:HG23	20:1T:54:MET:HE1	1.97	0.47
24:1Y:61:THR:O	24:1Y:65:ILE:HG13	2.15	0.47
24:1Y:139:LYS:HG2	24:1Y:140:VAL:HG12	1.97	0.47
45:1Y:801:3PE:H222	45:1Y:801:3PE:H32	1.97	0.47
31:1f:7:VAL:O	31:1f:11:TRP:HB3	2.15	0.47
31:1f:14:ILE:O	31:1f:18:VAL:HG13	2.14	0.47
34:1i:72:THR:HG23	34:1i:73:HIS:ND1	2.29	0.47
35:1j:50:HIS:ND1	35:1j:50:HIS:O	2.47	0.47
37:1l:127:PRO:HD3	40:1o:3:HIS:CE1	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:174:ARG:NH2	39:1n:176:ARG:O	2.48	0.47
3:1C:35:LYS:HB3	3:1C:36:TYR:CD1	2.50	0.47
3:1C:104:ARG:HH22	4:1D:373:GLU:CD	2.22	0.47
3:1C:132:ARG:HH21	3:1C:149:ARG:C	2.22	0.47
4:1D:234:ILE:HG12	8:1H:280:PHE:CE1	2.50	0.47
4:1D:291:GLY:O	4:1D:296:ARG:NH1	2.47	0.47
4:1D:335:ARG:HH21	4:1D:339:LYS:HZ3	1.63	0.47
6:1F:42:TRP:CD1	6:1F:161:LEU:HG	2.50	0.47
6:1F:166:ALA:N	6:1F:171:TYR:O	2.47	0.47
7:1G:126:ASP:OD2	43:1r:56:ARG:NH1	2.48	0.47
7:1G:349:PHE:HE2	7:1G:362:TYR:HB3	1.78	0.47
8:1H:19:PHE:CD1	8:1H:48:PRO:HG2	2.49	0.47
8:1H:197:PRO:O	8:1H:280:PHE:HB2	2.15	0.47
9:1I:165:ILE:O	9:1I:169:ILE:HG12	2.14	0.47
12:1L:482:MET:HB2	12:1L:486:MET:HE1	1.97	0.47
12:1L:605:HIS:ND1	14:1N:92:PRO:HB2	2.30	0.47
13:1M:237:LYS:HD2	13:1M:316:MET:CG	2.44	0.47
13:1M:446:LEU:HD21	32:1g:70:LEU:HD22	1.97	0.47
16:1P:244:TYR:O	16:1P:248:VAL:HG23	2.15	0.47
17:1Q:63:GLU:HG2	17:1Q:65:TRP:HE3	1.80	0.47
24:1Y:89:TYR:HB3	24:1Y:121:ALA:HB1	1.97	0.47
32:1g:91:ARG:NH1	32:1g:92:GLU:OE1	2.47	0.47
4:1D:342:MET:O	4:1D:346:ILE:HG22	2.15	0.47
5:1E:97:LYS:HB3	5:1E:136:LEU:HD13	1.97	0.47
6:1F:222:VAL:HG21	49:1F:501:FMN:H3'	1.97	0.47
7:1G:41:CYS:HA	7:1G:156:CYS:HB2	1.97	0.47
12:1L:4:PHE:O	12:1L:8:THR:HG23	2.15	0.47
12:1L:457:LEU:O	12:1L:461:SER:N	2.38	0.47
13:1M:183:SER:O	13:1M:184:HIS:ND1	2.47	0.47
14:1N:25:HIS:NE2	30:1e:17:MET:HB3	2.29	0.47
14:1N:258:SER:HB2	14:1N:336:VAL:HB	1.97	0.47
16:1P:248:VAL:O	16:1P:322:ARG:NH2	2.35	0.47
29:1d:8:ARG:NE	46:1d:201:PC1:H242	2.30	0.47
6:1F:59:GLU:O	6:1F:63:SER:N	2.44	0.47
9:1I:111:ILE:HG22	9:1I:113:MET:SD	2.55	0.47
9:1I:114:THR:HG21	9:1I:144:HIS:HE1	1.79	0.47
10:1J:67:VAL:HG21	11:1K:31:LEU:HD13	1.97	0.47
10:1J:67:VAL:O	10:1J:71:THR:HG23	2.14	0.47
12:1L:206:ASN:HB2	12:1L:266:LEU:HD11	1.96	0.47
12:1L:407:TRP:CD1	12:1L:411:MET:HE1	2.50	0.47
13:1M:33:LEU:O	13:1M:36:LEU:HB2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.14	0.47
13:1M:119:TYR:CD2	13:1M:160:LEU:HD12	2.50	0.47
13:1M:122:PHE:HD1	13:1M:238:LEU:HD13	1.80	0.47
14:1N:34:GLU:OE2	14:1N:34:GLU:N	2.48	0.47
14:1N:250:SER:OG	14:1N:333:SER:O	2.29	0.47
24:1Y:120:THR:O	24:1Y:124:VAL:HG13	2.15	0.47
25:1Z:38:VAL:O	25:1Z:42:THR:HG23	2.15	0.47
28:1c:5:ARG:HB2	28:1c:5:ARG:NH1	2.30	0.47
29:1d:13:PHE:HD1	29:1d:14:LEU:H	1.63	0.47
30:1e:44:HIS:CD2	33:1h:130:LYS:H	2.33	0.47
4:1D:152:MET:HA	4:1D:155:THR:OG1	2.15	0.46
4:1D:326:ASP:OD1	7:1G:127:ARG:NH2	2.49	0.46
6:1F:318:ASP:OD1	6:1F:321:ALA:N	2.47	0.46
7:1G:365:ASN:HB3	7:1G:488:LYS:HG3	1.97	0.46
7:1G:383:ASN:HD21	7:1G:413:VAL:HG21	1.80	0.46
8:1H:184:MET:HE1	8:1H:293:PHE:CD2	2.50	0.46
8:1H:296:LEU:O	8:1H:300:LEU:HD12	2.15	0.46
12:1L:375:ILE:HG21	35:1j:32:MET:HG2	1.96	0.46
20:1U:35:HIS:N	20:1U:39:ASP:OD2	2.44	0.46
45:1Y:804:3PE:H2	45:1Y:804:3PE:H221	1.52	0.46
26:1a:21:MET:O	26:1a:25:HIS:N	2.40	0.46
31:1f:1:MET:SD	31:1f:1:MET:N	2.69	0.46
34:1i:71:VAL:O	34:1i:76:ILE:HG23	2.15	0.46
37:1l:7:ASP:OD1	37:1l:7:ASP:N	2.43	0.46
3:1C:53:HIS:ND1	3:1C:55:ASP:OD1	2.49	0.46
4:1D:4:TRP:CG	13:1M:140:THR:HG1	2.32	0.46
4:1D:55:HIS:CE1	8:1H:208:VAL:H	2.33	0.46
4:1D:217:ASN:ND2	43:1r:23:LEU:O	2.49	0.46
7:1G:190:MET:O	7:1G:192:MET:HE3	2.15	0.46
7:1G:252:PRO:HG3	7:1G:268:ARG:HH22	1.79	0.46
7:1G:543:ILE:HG22	7:1G:557:ALA:HA	1.97	0.46
8:1H:273:ILE:HG23	8:1H:277:TYR:CD2	2.50	0.46
9:1I:64:GLU:OE1	9:1I:157:ASN:ND2	2.43	0.46
9:1I:137:PHE:CD1	9:1I:137:PHE:C	2.93	0.46
10:1J:26:PRO:HB2	10:1J:71:THR:HG21	1.96	0.46
12:1L:20:MET:HB2	12:1L:21:MET:HE2	1.97	0.46
13:1M:123:GLU:O	13:1M:123:GLU:HG2	2.16	0.46
15:1O:26:THR:HG22	15:1O:124:LEU:HD21	1.97	0.46
17:1Q:9:GLN:O	22:1W:23:ARG:NH2	2.47	0.46
24:1Y:128:GLN:HE22	45:1Y:804:3PE:H121	1.80	0.46
35:1j:38:TRP:HA	36:1k:77:PHE:HE1	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:83:MET:HA	37:1l:83:MET:HE3	1.95	0.46
4:1D:71:GLU:HB2	4:1D:410:MET:HE3	1.97	0.46
6:1F:134:ALA:HB2	6:1F:173:PHE:CZ	2.51	0.46
6:1F:161:LEU:H	6:1F:161:LEU:HD22	1.80	0.46
6:1F:215:VAL:HG12	6:1F:220:THR:HG21	1.97	0.46
7:1G:36:GLN:OE1	17:1Q:49:VAL:HG12	2.15	0.46
8:1H:205:SER:OG	8:1H:279:ARG:NH2	2.44	0.46
10:1J:23:LYS:O	10:1J:23:LYS:HG2	2.15	0.46
12:1L:55:MET:HG2	12:1L:471:ASN:HB2	1.96	0.46
45:1L:704:3PE:O12	45:1L:704:3PE:N	2.29	0.46
13:1M:160:LEU:HD23	13:1M:199:CYS:HA	1.96	0.46
14:1N:114:TRP:O	14:1N:118:VAL:HG12	2.14	0.46
14:1N:217:MET:HG2	14:1N:326:LEU:HD12	1.96	0.46
16:1P:215:ILE:HA	16:1P:218:ILE:HG12	1.97	0.46
19:1S:23:CYS:HB2	19:1S:60:VAL:H	1.80	0.46
25:1Z:120:MET:HG3	30:1e:68:ARG:HD3	1.96	0.46
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.15	0.46
33:1h:63:HIS:HE2	33:1h:80:TYR:HB3	1.81	0.46
35:1j:10:ARG:HD3	35:1j:13:GLN:HB2	1.97	0.46
37:1l:98:TRP:O	37:1l:101:MET:HB2	2.15	0.46
57:1l:201:MYR:H52	57:1l:201:MYR:H92	1.97	0.46
41:1p:106:GLN:O	41:1p:110:LYS:HD3	2.15	0.46
1:1A:67:LEU:HD21	11:1K:65:VAL:HG13	1.98	0.46
6:1F:250:ASN:CG	6:1F:319:PHE:HB2	2.41	0.46
8:1H:98:MET:CE	46:1Z:201:PC1:H12	2.45	0.46
8:1H:165:LEU:HD12	8:1H:240:ILE:HG13	1.97	0.46
12:1L:598:SER:HA	12:1L:604:TYR:HE1	1.80	0.46
54:1P:501:NDP:H51A	54:1P:501:NDP:C8A	2.42	0.46
20:1T:47:GLN:HA	20:1T:50:ILE:HD13	1.97	0.46
27:1b:20:ALA:O	27:1b:23:ALA:N	2.46	0.46
35:1j:71:GLU:N	35:1j:71:GLU:OE2	2.48	0.46
4:1D:300:ARG:NH2	4:1D:420:THR:O	2.48	0.46
8:1H:157:ASN:HD22	8:1H:159:SER:H	1.63	0.46
12:1L:14:ILE:HD11	12:1L:43:ALA:HA	1.96	0.46
12:1L:144:TRP:CH2	12:1L:256:GLY:HA2	2.50	0.46
13:1M:452:LYS:HZ3	32:1g:83:TYR:HD2	1.63	0.46
19:1S:78:LEU:HA	19:1S:81:PHE:CD2	2.51	0.46
19:1S:82:SER:O	19:1S:86:VAL:HG12	2.16	0.46
20:1T:81:ALA:HA	20:1T:86:VAL:HG12	1.97	0.46
24:1Y:17:CYS:HB2	24:1Y:74:CYS:HB2	1.91	0.46
24:1Y:28:GLY:O	24:1Y:62:SER:OG	2.25	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:39:SER:HB2	45:1Y:801:3PE:H31	1.96	0.46
33:1h:36:VAL:O	33:1h:40:ILE:HG13	2.16	0.46
34:1i:49:PHE:CD2	34:1i:57:LYS:HG3	2.50	0.46
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.48	0.46
41:1p:116:GLU:HG3	41:1p:123:ASN:HB2	1.97	0.46
44:1s:41:LEU:HD22	44:1s:41:LEU:H	1.80	0.46
3:1C:76:ALA:N	3:1C:95:ASN:O	2.47	0.46
4:1D:246:THR:HB	21:1V:12:GLY:HA3	1.97	0.46
4:1D:410:MET:HE2	4:1D:410:MET:HB3	1.74	0.46
7:1G:42:TYR:HB3	48:1G:803:FES:S2	2.56	0.46
8:1H:235:ASN:HD21	8:1H:266:LEU:C	2.24	0.46
10:1J:24:PRO:HG2	10:1J:29:GLY:N	2.30	0.46
17:1Q:114:LYS:HE2	17:1Q:114:LYS:HB2	1.75	0.46
20:1U:87:TYR:HE2	34:1i:19:ARG:HA	1.78	0.46
22:1W:52:LEU:HD23	22:1W:52:LEU:HA	1.82	0.46
23:1X:165:ARG:O	33:1h:104:ARG:NH1	2.44	0.46
25:1Z:28:ARG:HH12	43:1r:14:ALA:C	2.22	0.46
26:1a:7:PRO:HG3	51:1a:101:CDL:H152	1.98	0.46
1:1A:77:TRP:HH2	8:1H:100:LEU:HD11	1.81	0.46
2:1B:65:PRO:HD3	4:1D:168:PHE:HD2	1.80	0.46
2:1B:116:MET:O	2:1B:120:ALA:HB3	2.15	0.46
8:1H:173:TRP:CD1	8:1H:243:LEU:HA	2.51	0.46
15:1O:135:LEU:HD21	15:1O:149:VAL:HG22	1.97	0.46
15:1O:270:LEU:O	15:1O:273:THR:OG1	2.29	0.46
23:1X:23:VAL:HG13	23:1X:81:PHE:CZ	2.51	0.46
23:1X:81:PHE:CG	23:1X:106:PHE:HE2	2.34	0.46
25:1Z:40:ILE:HD12	25:1Z:40:ILE:H	1.81	0.46
29:1d:2:MET:O	29:1d:8:ARG:NH1	2.48	0.46
30:1e:85:LEU:O	30:1e:89:GLY:N	2.48	0.46
34:1i:107:ASP:OD1	40:1o:67:LYS:NZ	2.45	0.46
2:1B:53:ALA:HB2	4:1D:83:LEU:HD21	1.98	0.46
4:1D:76:CYS:SG	4:1D:406:SER:OG	2.61	0.46
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.15	0.46
4:1D:152:MET:HB2	4:1D:156:THR:HG23	1.97	0.46
4:1D:292:ASP:OD1	4:1D:294:TYR:N	2.49	0.46
4:1D:371:LYS:NZ	4:1D:422:ASP:OD2	2.49	0.46
5:1E:100:ILE:HD12	5:1E:156:ILE:HD12	1.97	0.46
5:1E:149:VAL:HA	6:1F:259:SER:HB2	1.98	0.46
7:1G:249:ARG:HD2	7:1G:251:LEU:HD13	1.97	0.46
9:1I:161:TRP:HB3	9:1I:165:ILE:HD11	1.97	0.46
10:1J:12:ILE:HA	10:1J:15:ILE:HD11	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:131:ILE:O	13:1M:135:ARG:HB3	2.16	0.46
14:1N:159:MET:O	14:1N:159:MET:HE3	2.16	0.46
15:1O:195:THR:HG22	15:1O:197:ALA:H	1.80	0.46
15:1O:316:TRP:HB3	28:1c:12:PRO:HG3	1.98	0.46
20:1U:36:PHE:HE1	20:1U:73:PRO:HG3	1.80	0.46
20:1U:68:GLU:OE1	20:1U:68:GLU:N	2.40	0.46
24:1Y:2:LYS:HE3	24:1Y:2:LYS:HB3	1.75	0.46
30:1e:60:ASP:O	30:1e:64:GLU:HB2	2.16	0.46
2:1B:89:ALA:HB2	2:1B:116:MET:HG3	1.98	0.46
3:1C:99:LEU:HD13	4:1D:251:LEU:HD12	1.97	0.46
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.51	0.46
4:1D:220:PHE:O	4:1D:221:ARG:NH1	2.47	0.46
6:1F:175:VAL:O	44:1s:62:ARG:NH1	2.46	0.46
14:1N:344:SER:HA	14:1N:347:ASN:HB3	1.97	0.46
19:1S:35:PHE:CE1	19:1S:39:ARG:HG2	2.51	0.46
25:1Z:28:ARG:NH2	43:1r:13:TRP:O	2.49	0.46
34:1i:56:TRP:CD1	34:1i:57:LYS:HZ3	2.34	0.46
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.98	0.46
2:1B:25:ARG:HG3	2:1B:28:TYR:H	1.81	0.46
3:1C:89:ARG:HG3	3:1C:90:PHE:H	1.81	0.46
4:1D:161:ILE:HD12	4:1D:238:ARG:CD	2.46	0.46
5:1E:86:PHE:CE1	7:1G:177:ARG:HB3	2.50	0.46
6:1F:194:GLU:OE2	6:1F:199:LYS:HD3	2.15	0.46
6:1F:299:PRO:HD3	6:1F:306:LEU:HA	1.98	0.46
8:1H:277:TYR:OH	9:1I:30:LEU:O	2.31	0.46
12:1L:126:ILE:O	12:1L:130:ILE:HG13	2.16	0.46
13:1M:73:LEU:HD13	13:1M:77:LEU:HG	1.97	0.46
13:1M:125:THR:O	13:1M:129:THR:HG23	2.16	0.46
14:1N:27:LEU:O	14:1N:31:ILE:HG12	2.16	0.46
19:1S:77:SER:C	19:1S:78:LEU:HD12	2.41	0.46
23:1X:126:LYS:NZ	27:1b:75:PRO:O	2.48	0.46
35:1j:47:VAL:O	35:1j:47:VAL:HG12	2.16	0.46
37:1l:101:MET:HA	37:1l:101:MET:HE3	1.97	0.46
43:1r:8:GLN:O	43:1r:12:ASN:ND2	2.28	0.46
4:1D:184:VAL:HG22	4:1D:193:TYR:CE2	2.50	0.45
5:1E:145:LEU:HD12	5:1E:153:MET:HG3	1.97	0.45
6:1F:188:GLU:OE1	6:1F:191:ALA:N	2.42	0.45
9:1I:149:TYR:CG	9:1I:153:LYS:HD2	2.51	0.45
14:1N:255:PRO:HG3	14:1N:260:PHE:CD2	2.51	0.45
19:1S:63:LYS:HB3	19:1S:65:TRP:HE1	1.81	0.45
23:1X:156:ASP:OD1	23:1X:156:ASP:N	2.48	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:79:TRP:CZ3	41:1p:40:VAL:HA	2.51	0.45
40:1o:11:ASP:OD2	40:1o:13:SER:OG	2.27	0.45
4:1D:120:LEU:O	4:1D:124:LYS:HB3	2.16	0.45
6:1F:111:ILE:HD11	6:1F:149:LEU:HG	1.98	0.45
7:1G:349:PHE:HB2	7:1G:509:PRO:HB2	1.98	0.45
8:1H:110:SER:HB2	8:1H:143:GLU:OE2	2.17	0.45
10:1J:103:MET:O	10:1J:107:ALA:N	2.42	0.45
13:1M:75:LEU:HG	13:1M:440:HIS:NE2	2.31	0.45
13:1M:126:LEU:HD23	13:1M:150:LEU:HD13	1.97	0.45
16:1P:105:ASP:OD1	16:1P:108:ASP:N	2.46	0.45
20:1U:69:LYS:HD2	34:1i:3:TYR:CD1	2.52	0.45
34:1i:15:ARG:O	34:1i:19:ARG:N	2.45	0.45
35:1j:56:PRO:HA	35:1j:59:TRP:CE3	2.51	0.45
37:1l:13:TYR:HD2	37:1l:15:LYS:HZ2	1.62	0.45
40:1o:53:GLN:H	40:1o:53:GLN:CD	2.22	0.45
4:1D:409:HIS:HB3	4:1D:413:ASP:HB2	1.97	0.45
5:1E:211:PHE:HB3	6:1F:237:ARG:HD3	1.98	0.45
6:1F:136:ILE:HD11	6:1F:177:VAL:HG22	1.98	0.45
9:1I:145:GLU:H	9:1I:145:GLU:CD	2.24	0.45
11:1K:37:MET:HE1	11:1K:41:PHE:HB2	1.97	0.45
12:1L:406:ALA:HB3	37:1l:119:GLY:HA2	1.98	0.45
13:1M:252:PRO:HG3	29:1d:117:HIS:NE2	2.32	0.45
45:1M:503:3PE:H372	45:1M:503:3PE:H331	1.98	0.45
18:1R:73:ILE:HD12	18:1R:73:ILE:C	2.42	0.45
39:1n:34:ASP:OD1	39:1n:34:ASP:N	2.49	0.45
6:1F:406:ALA:O	6:1F:410:GLY:N	2.44	0.45
7:1G:154:ILE:HD11	7:1G:205:VAL:HG11	1.98	0.45
8:1H:102:VAL:HG12	8:1H:237:PHE:CZ	2.50	0.45
9:1I:169:ILE:O	9:1I:173:TYR:HB3	2.16	0.45
11:1K:66:PHE:CE2	14:1N:31:ILE:HD12	2.51	0.45
12:1L:261:ILE:CD1	12:1L:326:PHE:HB2	2.46	0.45
13:1M:36:LEU:HD11	46:1f:101:PC1:H371	1.44	0.45
15:1O:285:GLY:HA3	32:1g:28:GLU:OE2	2.17	0.45
19:1S:63:LYS:HZ1	19:1S:76:VAL:C	2.24	0.45
22:1W:62:LYS:HZ3	22:1W:107:PHE:HA	1.82	0.45
24:1Y:61:THR:HG21	45:1Y:802:3PE:H221	1.99	0.45
45:1f:102:3PE:H2A1	45:1f:102:3PE:H3A2	1.98	0.45
35:1j:69:ASP:CG	40:1o:113:ARG:HB3	2.42	0.45
3:1C:39:GLN:O	3:1C:51:PHE:HB2	2.16	0.45
4:1D:105:ARG:CZ	9:1I:117:ILE:HD11	2.47	0.45
4:1D:176:LYS:NZ	43:1r:26:ARG:HG3	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:334:LYS:HE2	4:1D:334:LYS:HB3	1.76	0.45
6:1F:47:GLU:O	6:1F:51:LYS:N	2.49	0.45
6:1F:256:PHE:HD1	6:1F:332:ALA:HB1	1.82	0.45
7:1G:139:ASP:OD1	7:1G:139:ASP:N	2.49	0.45
7:1G:571:ALA:O	7:1G:583:THR:N	2.47	0.45
8:1H:173:TRP:HB3	8:1H:175:ILE:HG22	1.98	0.45
8:1H:178:SER:HB3	8:1H:181:LEU:HB2	1.98	0.45
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.15	0.45
12:1L:342:CYS:O	12:1L:346:ILE:HG22	2.16	0.45
12:1L:379:ALA:O	12:1L:388:GLY:HA3	2.17	0.45
13:1M:10:MET:CE	31:1f:15:LEU:HD12	2.46	0.45
13:1M:71:TRP:CH2	13:1M:439:LEU:HD22	2.52	0.45
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.47	0.45
15:1O:198:TYR:HD2	15:1O:199:LEU:HD22	1.81	0.45
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	1.99	0.45
20:1T:36:PHE:HA	20:1T:40:LEU:HB2	1.98	0.45
23:1X:100:ARG:HA	23:1X:100:ARG:HD3	1.67	0.45
29:1d:86:ARG:HG2	29:1d:86:ARG:HH11	1.80	0.45
30:1e:66:LEU:HB3	30:1e:67:LEU:HD22	1.98	0.45
37:1l:70:ARG:HD2	37:1l:86:ARG:HD2	1.99	0.45
38:1m:111:LYS:O	38:1m:115:ILE:HG22	2.17	0.45
40:1o:95:VAL:O	40:1o:99:LYS:HG2	2.17	0.45
2:1B:154:GLU:H	2:1B:154:GLU:HG2	1.61	0.45
3:1C:58:ILE:HG23	3:1C:59:PRO:HD3	1.99	0.45
4:1D:345:LEU:HD23	7:1G:103:LEU:HD12	1.99	0.45
6:1F:250:ASN:ND2	6:1F:319:PHE:HB2	2.31	0.45
7:1G:424:ASP:C	7:1G:424:ASP:OD1	2.60	0.45
9:1I:120:GLY:N	47:1I:201:SF4:S4	2.79	0.45
10:1J:86:ASN:OD1	10:1J:88:THR:N	2.50	0.45
10:1J:95:SER:O	10:1J:99:MET:HB2	2.17	0.45
12:1L:282:ALA:C	12:1L:411:MET:HG2	2.41	0.45
12:1L:526:LEU:HD22	12:1L:530:PRO:HG2	1.98	0.45
13:1M:418:LYS:HE2	39:1n:94:GLU:HB3	1.99	0.45
13:1M:450:ASN:OD1	13:1M:452:LYS:HG2	2.17	0.45
20:1T:34:SER:H	20:1T:73:PRO:HD2	1.81	0.45
23:1X:144:ARG:NH1	30:1e:58:GLU:OE1	2.49	0.45
51:1X:201:CDL:CB5	29:1d:29:PRO:HB3	2.47	0.45
27:1b:78:GLU:OE1	27:1b:78:GLU:N	2.49	0.45
30:1e:9:LEU:H	30:1e:9:LEU:HD12	1.81	0.45
31:1f:43:LEU:HD11	41:1p:67:PHE:HD1	1.81	0.45
2:1B:57:VAL:HG21	4:1D:152:MET:HE1	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:9:HIS:CD2	5:1E:11:ASP:H	2.34	0.45
7:1G:475:GLN:HE21	7:1G:646:ASN:ND2	2.14	0.45
8:1H:30:TYR:HE2	26:1a:1:MET:C	2.24	0.45
8:1H:102:VAL:HA	8:1H:105:MET:HB2	1.99	0.45
8:1H:110:SER:O	8:1H:113:VAL:HG22	2.16	0.45
11:1K:48:ILE:HD11	11:1K:56:ALA:HB3	1.99	0.45
13:1M:282:LEU:HD23	13:1M:342:MET:SD	2.57	0.45
14:1N:129:LEU:HB2	51:1N:402:CDL:H521	1.98	0.45
14:1N:199:THR:HA	14:1N:202:ILE:HD12	1.99	0.45
15:1O:53:GLU:HG2	15:1O:104:ARG:NH1	2.32	0.45
22:1W:17:VAL:HG11	22:1W:77:ARG:HE	1.81	0.45
23:1X:144:ARG:NH1	30:1e:57:ILE:HB	2.32	0.45
1:1A:26:GLN:HG3	1:1A:27:LEU:N	2.31	0.45
1:1A:37:TYR:HA	2:1B:106:GLN:HE22	1.81	0.45
1:1A:68:GLU:O	1:1A:71:LEU:HB2	2.17	0.45
4:1D:308:LEU:HA	4:1D:308:LEU:HD23	1.83	0.45
6:1F:34:LYS:HA	6:1F:37:GLN:HB3	1.97	0.45
6:1F:110:ILE:HG13	6:1F:114:ASP:HB2	1.98	0.45
7:1G:121:MET:HE2	7:1G:121:MET:HB3	1.91	0.45
9:1I:52:PHE:HE1	42:1q:77:VAL:HG21	1.81	0.45
12:1L:338:MET:HE3	12:1L:338:MET:HB2	1.83	0.45
12:1L:557:TRP:O	12:1L:561:ILE:HG22	2.17	0.45
13:1M:7:PRO:O	13:1M:11:LEU:HD12	2.17	0.45
13:1M:37:ILE:HG12	31:1f:20:PHE:CD1	2.52	0.45
15:1O:265:ASN:ND2	15:1O:268:GLU:H	2.14	0.45
21:1V:82:GLN:O	21:1V:86:GLU:N	2.39	0.45
22:1W:68:MET:N	22:1W:68:MET:SD	2.90	0.45
26:1a:21:MET:N	26:1a:21:MET:SD	2.80	0.45
31:1f:42:LEU:HA	31:1f:45:LYS:HD2	1.98	0.45
34:1i:54:ALA:HB3	34:1i:57:LYS:CE	2.47	0.45
37:1l:66:HIS:O	37:1l:70:ARG:N	2.49	0.45
37:1l:86:ARG:NH1	39:1n:91:GLU:OE2	2.36	0.45
38:1m:52:ASP:HB3	38:1m:55:ARG:HB2	1.98	0.45
3:1C:193:GLU:OE1	17:1Q:73:SER:HB2	2.17	0.45
4:1D:111:MET:SD	4:1D:189:MET:HG2	2.57	0.45
4:1D:414:VAL:O	4:1D:418:ILE:HG13	2.17	0.45
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.52	0.45
5:1E:41:GLY:HA2	44:1s:70:ARG:O	2.16	0.45
6:1F:61:LYS:HZ1	6:1F:77:LEU:H	1.65	0.45
7:1G:317:ALA:O	7:1G:344:CYS:N	2.50	0.45
7:1G:443:LEU:HD22	7:1G:477:ILE:HG21	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:153:LYS:HA	9:1I:156:ASN:HB2	1.99	0.45
12:1L:81:LYS:HD2	12:1L:262:ARG:HH12	1.82	0.45
12:1L:403:TYR:HE2	40:1o:18:PRO:HB2	1.82	0.45
13:1M:21:ASN:OD1	13:1M:22:MET:HE2	2.17	0.45
15:1O:188:ASN:O	15:1O:192:MET:HE2	2.16	0.45
23:1X:37:LYS:HE2	23:1X:37:LYS:HB2	1.87	0.45
34:1i:76:ILE:HA	34:1i:79:TRP:CD1	2.52	0.45
37:1l:13:TYR:O	37:1l:15:LYS:NZ	2.49	0.45
1:1A:42:ASP:HB2	22:1W:99:GLN:HE22	1.82	0.45
2:1B:52:LEU:HB2	2:1B:90:GLY:HA3	1.99	0.45
3:1C:175:ARG:HD3	16:1P:13:ARG:HD2	1.98	0.45
6:1F:202:LYS:NZ	7:1G:181:MET:HE1	2.32	0.45
7:1G:102:PRO:HG3	7:1G:151:THR:HG23	1.99	0.45
7:1G:141:ASN:OD1	7:1G:141:ASN:N	2.48	0.45
8:1H:233:MET:SD	8:1H:234:MET:N	2.90	0.45
8:1H:260:VAL:O	8:1H:264:LEU:HB2	2.16	0.45
8:1H:262:LYS:HD3	8:1H:262:LYS:HA	1.63	0.45
46:1H:401:PC1:H272	9:1I:30:LEU:HD21	1.99	0.45
12:1L:395:ILE:O	12:1L:399:VAL:HG12	2.17	0.45
12:1L:424:THR:HG21	12:1L:498:PHE:HA	1.98	0.45
13:1M:295:ALA:HA	13:1M:298:ILE:HD12	1.99	0.45
15:1O:295:LYS:O	15:1O:299:LEU:HD23	2.17	0.45
16:1P:145:TYR:O	16:1P:149:LYS:HG2	2.16	0.45
30:1e:91:TYR:HE1	30:1e:93:PRO:HA	1.82	0.45
39:1n:68:GLU:OE1	39:1n:68:GLU:N	2.50	0.45
43:1r:109:GLN:NE2	43:1r:111:TYR:O	2.51	0.45
4:1D:292:ASP:OD1	4:1D:292:ASP:C	2.61	0.44
7:1G:381:GLY:O	7:1G:456:SER:OG	2.32	0.44
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.17	0.44
10:1J:115:ILE:O	10:1J:117:PHE:N	2.51	0.44
12:1L:559:GLU:O	12:1L:563:PRO:HG2	2.17	0.44
13:1M:31:SER:HB2	13:1M:74:PRO:HD3	1.99	0.44
13:1M:47:GLU:HG3	41:1p:92:ARG:HB2	1.98	0.44
14:1N:309:ASN:O	14:1N:312:LYS:NZ	2.44	0.44
15:1O:188:ASN:O	15:1O:191:GLU:HG3	2.17	0.44
15:1O:262:LEU:HD12	15:1O:262:LEU:HA	1.79	0.44
22:1W:26:ASN:O	22:1W:30:ARG:HG2	2.17	0.44
25:1Z:86:MET:HE1	25:1Z:125:TYR:HE1	1.83	0.44
31:1f:29:ARG:HA	31:1f:32:GLU:OE1	2.17	0.44
7:1G:110:GLN:O	7:1G:114:CYS:N	2.50	0.44
8:1H:142:TYR:CE2	8:1H:146:LEU:HD22	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:12:PHE:CE1	11:1K:36:MET:HE2	2.53	0.44
11:1K:94:ASN:HD22	12:1L:583:LEU:HD21	1.82	0.44
12:1L:40:VAL:HG12	12:1L:98:TRP:HB2	1.98	0.44
13:1M:10:MET:HE1	31:1f:15:LEU:HD12	1.98	0.44
20:1T:7:THR:H	20:1T:10:ALA:HB3	1.82	0.44
22:1W:64:ARG:HD2	22:1W:68:MET:HE1	1.98	0.44
23:1X:95:LEU:HB3	23:1X:97:ARG:HG2	2.00	0.44
23:1X:146:ARG:HH21	30:1e:42:CYS:HB2	1.82	0.44
31:1f:24:CYS:HA	31:1f:27:ASP:HB3	1.98	0.44
32:1g:110:SER:O	41:1p:161:ARG:NH2	2.49	0.44
34:1i:93:PRO:HB3	41:1p:4:TRP:CE2	2.52	0.44
36:1k:75:ALA:O	36:1k:79:VAL:HG22	2.17	0.44
1:1A:69:ILE:O	1:1A:72:LEU:HD12	2.17	0.44
4:1D:8:VAL:O	4:1D:12:GLU:HG2	2.17	0.44
5:1E:150:ASN:HB3	5:1E:163:ASP:HB2	1.99	0.44
8:1H:187:ILE:HG22	8:1H:190:LEU:HD12	1.99	0.44
12:1L:83:ASP:C	12:1L:83:ASP:OD1	2.60	0.44
13:1M:257:MET:HE2	13:1M:257:MET:HA	2.00	0.44
14:1N:128:LEU:HD23	14:1N:216:PHE:HB2	1.99	0.44
20:1U:75:GLU:OE2	34:1i:3:TYR:HE2	1.99	0.44
30:1e:6:GLN:NE2	30:1e:13:LEU:HB2	2.32	0.44
41:1p:106:GLN:O	41:1p:110:LYS:N	2.40	0.44
1:1A:8:LEU:HD12	1:1A:8:LEU:HA	1.81	0.44
2:1B:25:ARG:HH11	2:1B:27:GLU:HB3	1.82	0.44
3:1C:36:TYR:HE2	3:1C:59:PRO:HG2	1.81	0.44
3:1C:169:SER:OG	3:1C:190:LEU:HD11	2.17	0.44
4:1D:99:ALA:HA	4:1D:102:TYR:HD2	1.81	0.44
7:1G:138:GLU:H	7:1G:138:GLU:CD	2.23	0.44
7:1G:360:SER:HB2	7:1G:639:ALA:HB1	1.99	0.44
7:1G:522:LEU:HD22	7:1G:537:LEU:HD21	1.99	0.44
8:1H:42:PRO:O	8:1H:45:LEU:HD23	2.17	0.44
8:1H:170:GLU:HB3	8:1H:171:HIS:H	1.70	0.44
10:1J:20:PHE:CD2	11:1K:32:CYS:HA	2.52	0.44
11:1K:34:GLU:O	11:1K:37:MET:HG3	2.17	0.44
12:1L:342:CYS:O	12:1L:345:SER:OG	2.28	0.44
12:1L:583:LEU:HB2	12:1L:586:LEU:HG	1.99	0.44
46:1L:703:PC1:H222	32:1g:78:ALA:HB2	1.98	0.44
13:1M:119:TYR:HD1	13:1M:120:ILE:HD13	1.82	0.44
14:1N:217:MET:HE1	14:1N:329:MET:HG3	1.98	0.44
14:1N:258:SER:O	14:1N:261:MET:HB2	2.17	0.44
15:1O:208:LYS:HE3	15:1O:208:LYS:HB3	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:88:THR:OG1	17:1Q:91:ASP:OD2	2.22	0.44
20:1T:17:TYR:HD1	20:1T:20:LYS:NZ	2.15	0.44
22:1W:43:VAL:N	22:1W:44:PRO:HD2	2.33	0.44
28:1c:27:LEU:HD23	28:1c:27:LEU:HA	1.81	0.44
46:1d:201:PC1:H222	46:1d:201:PC1:H2	1.45	0.44
33:1h:64:TRP:HE3	33:1h:64:TRP:O	2.00	0.44
36:1k:18:TYR:HD2	36:1k:19:LYS:HZ2	1.66	0.44
41:1p:77:GLU:OE2	41:1p:78:GLU:N	2.50	0.44
4:1D:149:ASN:ND2	4:1D:370:PRO:HB2	2.30	0.44
4:1D:176:LYS:HE3	43:1r:26:ARG:HH11	1.83	0.44
6:1F:278:GLU:HB3	6:1F:282:LYS:HE2	1.99	0.44
6:1F:293:ASN:O	6:1F:339:ARG:N	2.50	0.44
8:1H:98:MET:SD	46:1Z:201:PC1:H12	2.57	0.44
8:1H:168:THR:OG1	25:1Z:57:ARG:NH1	2.51	0.44
12:1L:159:HIS:HB3	13:1M:416:ARG:HG2	1.99	0.44
12:1L:295:GLN:O	12:1L:425:ARG:NH1	2.48	0.44
13:1M:152:TYR:O	13:1M:205:VAL:HG21	2.16	0.44
16:1P:7:PRO:HA	16:1P:16:VAL:HG12	1.98	0.44
16:1P:34:VAL:HG11	16:1P:92:ILE:HD11	1.99	0.44
16:1P:220:ASP:HB3	16:1P:223:ALA:HB2	1.99	0.44
54:1P:501:NDP:H2N	54:1P:501:NDP:H2D	1.75	0.44
29:1d:2:MET:C	29:1d:4:GLY:N	2.73	0.44
35:1j:37:LEU:HD12	36:1k:77:PHE:CE1	2.52	0.44
38:1m:114:LEU:HB3	38:1m:120:LEU:HD23	1.98	0.44
5:1E:147:ALA:HB3	5:1E:153:MET:SD	2.57	0.44
6:1F:32:ARG:NH1	44:1s:42:GLN:HG2	2.32	0.44
7:1G:227:SER:O	7:1G:253:ARG:NH1	2.51	0.44
7:1G:319:ALA:HA	7:1G:525:LEU:HB3	1.99	0.44
10:1J:23:LYS:HD2	11:1K:23:ARG:CB	2.44	0.44
12:1L:128:MET:HE3	12:1L:251:THR:HB	1.99	0.44
12:1L:209:PRO:HD2	12:1L:270:ASN:HB2	1.98	0.44
13:1M:94:LEU:HA	13:1M:97:THR:OG1	2.18	0.44
14:1N:160:LEU:O	14:1N:164:ILE:HD12	2.17	0.44
16:1P:182:PHE:O	16:1P:185:MET:HB2	2.16	0.44
22:1W:50:PHE:CE2	22:1W:100:ARG:HA	2.51	0.44
33:1h:64:TRP:CD1	33:1h:77:ARG:HA	2.52	0.44
38:1m:5:TYR:CE2	38:1m:14:PRO:HD3	2.50	0.44
5:1E:60:TRP:CE2	5:1E:94:PRO:HG3	2.53	0.44
6:1F:137:TYR:CG	6:1F:192:LEU:HD21	2.53	0.44
11:1K:8:ILE:HD13	11:1K:42:ILE:HG22	1.99	0.44
11:1K:41:PHE:HD1	11:1K:42:ILE:HD13	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:365:THR:O	13:1M:374:ASN:ND2	2.50	0.44
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.52	0.44
14:1N:219:LEU:HD23	14:1N:219:LEU:HA	1.75	0.44
20:1U:86:VAL:C	20:1U:87:TYR:HD1	2.26	0.44
22:1W:104:MET:HE3	22:1W:107:PHE:HB2	2.00	0.44
26:1a:2:TRP:H	26:1a:2:TRP:HE3	1.64	0.44
42:1q:34:ARG:HH11	42:1q:58:ARG:HH21	1.64	0.44
4:1D:414:VAL:HA	4:1D:417:ILE:HD12	2.00	0.44
7:1G:40:PHE:HB2	7:1G:52:CYS:HB2	2.00	0.44
7:1G:53:ARG:NH2	7:1G:56:LEU:HD21	2.33	0.44
8:1H:3:MET:N	8:1H:3:MET:SD	2.91	0.44
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.52	0.44
9:1I:79:ALA:HB2	9:1I:105:ARG:O	2.17	0.44
10:1J:139:GLU:HA	11:1K:57:ASN:ND2	2.32	0.44
11:1K:93:LEU:HD21	14:1N:57:THR:HG21	1.99	0.44
12:1L:152:PHE:CD1	12:1L:168:ALA:HB1	2.53	0.44
12:1L:425:ARG:HG3	12:1L:429:PHE:HD2	1.83	0.44
13:1M:44:GLN:HG3	13:1M:45:LEU:N	2.33	0.44
13:1M:329:LEU:HB3	13:1M:359:TRP:CE2	2.53	0.44
14:1N:115:VAL:HG13	14:1N:116:PRO:HD3	1.99	0.44
14:1N:269:GLU:HA	14:1N:272:LYS:HB2	2.00	0.44
18:1R:27:ARG:HH21	42:1q:127:TYR:HA	1.83	0.44
23:1X:45:CYS:HA	23:1X:134:ARG:HH22	1.82	0.44
32:1g:80:LEU:CD2	32:1g:81:PRO:HD2	2.47	0.44
39:1n:61:GLN:OE1	39:1n:65:GLN:NE2	2.49	0.44
2:1B:87:ILE:O	2:1B:87:ILE:HG23	2.18	0.44
4:1D:37:ASP:OD1	14:1N:51:ARG:NH1	2.51	0.44
4:1D:150:HIS:HA	4:1D:153:ALA:HB3	2.00	0.44
4:1D:161:ILE:HG21	4:1D:235:TRP:CZ3	2.53	0.44
5:1E:162:GLU:OE1	5:1E:186:PRO:HG3	2.18	0.44
7:1G:174:THR:OG1	7:1G:175:THR:N	2.50	0.44
9:1I:164:GLU:HG3	42:1q:88:ARG:HB3	2.00	0.44
10:1J:15:ILE:HD12	10:1J:16:GLY:N	2.33	0.44
12:1L:331:MET:N	12:1L:331:MET:SD	2.91	0.44
12:1L:370:THR:O	12:1L:374:ILE:HG13	2.18	0.44
13:1M:76:MET:HB3	13:1M:226:ALA:HB1	2.00	0.44
13:1M:265:SER:OG	13:1M:295:ALA:O	2.36	0.44
13:1M:395:LEU:HD21	38:1m:100:TRP:CZ2	2.52	0.44
14:1N:40:MET:O	14:1N:44:LEU:HD23	2.18	0.44
15:1O:97:GLN:HG2	15:1O:135:LEU:HB2	2.00	0.44
19:1S:18:ILE:HD11	19:1S:64:LEU:HG	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:71:LEU:HD12	24:1Y:72:THR:N	2.33	0.44
24:1Y:127:GLY:HA2	24:1Y:132:TRP:HB2	2.00	0.44
27:1b:43:ARG:HH21	27:1b:79:TRP:CD1	2.36	0.44
34:1i:16:GLU:HA	34:1i:19:ARG:HG2	1.99	0.44
42:1q:71:ARG:HG2	42:1q:115:PHE:CZ	2.53	0.44
2:1B:122:GLY:H	9:1I:114:THR:HG1	1.66	0.43
3:1C:164:LYS:HD3	3:1C:164:LYS:HA	1.73	0.43
5:1E:81:TYR:O	5:1E:85:THR:HG22	2.18	0.43
6:1F:199:LYS:NZ	17:1Q:131:SER:O	2.40	0.43
6:1F:202:LYS:HZ2	7:1G:181:MET:HE1	1.83	0.43
7:1G:343:LEU:HD12	7:1G:507:TYR:CZ	2.52	0.43
7:1G:498:SER:O	7:1G:500:VAL:N	2.51	0.43
8:1H:17:VAL:HG11	8:1H:225:MET:HA	2.00	0.43
8:1H:105:MET:HA	8:1H:105:MET:HE3	2.00	0.43
9:1I:67:LEU:HB2	9:1I:154:LEU:HB3	2.00	0.43
11:1K:53:PHE:CE1	11:1K:55:LEU:HB2	2.53	0.43
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.00	0.43
15:1O:53:GLU:OE2	15:1O:104:ARG:NH2	2.52	0.43
16:1P:37:HIS:CD2	16:1P:40:ARG:HH21	2.36	0.43
16:1P:134:HIS:HD2	16:1P:136:ASN:H	1.65	0.43
16:1P:174:ARG:HH21	16:1P:316:GLU:HB3	1.83	0.43
16:1P:203:GLN:NE2	16:1P:232:GLY:O	2.51	0.43
19:1S:70:PHE:O	19:1S:72:GLN:NE2	2.50	0.43
46:1Y:803:PC1:H143	38:1m:76:TYR:CE1	2.53	0.43
29:1d:45:ASP:O	29:1d:49:ARG:HG2	2.18	0.43
39:1n:103:LEU:HD23	39:1n:103:LEU:HA	1.83	0.43
2:1B:95:LYS:HD3	3:1C:154:ASP:HA	2.00	0.43
4:1D:83:LEU:HD12	4:1D:426:GLY:HA2	2.00	0.43
6:1F:51:LYS:HB3	6:1F:55:TRP:HD1	1.83	0.43
6:1F:164:LYS:HE3	6:1F:164:LYS:HB3	1.77	0.43
6:1F:349:ARG:O	6:1F:349:ARG:NH1	2.40	0.43
7:1G:100:ASN:HA	7:1G:134:LYS:HB3	2.00	0.43
10:1J:10:SER:O	10:1J:14:VAL:HG23	2.18	0.43
10:1J:52:LEU:HD12	11:1K:41:PHE:CZ	2.52	0.43
10:1J:150:GLY:HA2	30:1e:16:TRP:CH2	2.53	0.43
12:1L:553:LEU:O	12:1L:558:LEU:N	2.41	0.43
20:1T:60:PHE:CZ	20:1T:80:ILE:HG22	2.53	0.43
20:1U:77:VAL:HA	20:1U:80:ILE:HD12	2.00	0.43
33:1h:32:THR:C	33:1h:35:PRO:HD2	2.43	0.43
36:1k:48:GLU:HG2	39:1n:33:ARG:HB3	2.00	0.43
42:1q:41:GLU:OE1	42:1q:47:LYS:NZ	2.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:29:GLY:O	8:1H:34:ARG:N	2.52	0.43
8:1H:121:TRP:CD1	8:1H:121:TRP:C	2.96	0.43
10:1J:64:MET:HA	10:1J:67:VAL:HG12	2.00	0.43
12:1L:62:ILE:C	12:1L:63:ILE:HD13	2.44	0.43
12:1L:100:ILE:HD11	12:1L:242:PRO:HA	1.98	0.43
12:1L:287:PHE:CZ	12:1L:527:GLY:HA3	2.52	0.43
13:1M:5:ILE:HG22	51:1X:201:CDL:H631	1.99	0.43
16:1P:210:VAL:HG23	16:1P:230:PHE:CD2	2.53	0.43
17:1Q:26:PRO:O	17:1Q:30:ILE:HG22	2.18	0.43
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.54	0.43
34:1i:19:ARG:O	34:1i:23:LYS:HB2	2.18	0.43
3:1C:39:GLN:HB2	43:1r:70:SER:HA	2.00	0.43
3:1C:74:SER:O	3:1C:96:LEU:HA	2.18	0.43
3:1C:100:ARG:HH12	21:1V:73:GLY:C	2.26	0.43
3:1C:179:GLU:H	16:1P:36:ASN:ND2	2.17	0.43
4:1D:29:LYS:HE2	4:1D:29:LYS:HA	1.99	0.43
4:1D:146:ARG:HH12	4:1D:270:ARG:NH1	2.16	0.43
6:1F:25:LEU:O	6:1F:113:HIS:ND1	2.51	0.43
6:1F:273:SER:OG	6:1F:318:ASP:HB3	2.19	0.43
7:1G:113:GLU:CD	7:1G:219:PRO:HG3	2.43	0.43
7:1G:254:MET:HE3	7:1G:254:MET:C	2.43	0.43
7:1G:595:GLU:HB2	7:1G:598:LYS:HB2	2.01	0.43
8:1H:235:ASN:O	8:1H:238:THR:HG22	2.19	0.43
10:1J:173:ARG:NH1	15:1O:254:ARG:HE	2.12	0.43
11:1K:37:MET:CB	14:1N:68:MET:HE1	2.41	0.43
12:1L:51:LEU:HD23	12:1L:55:MET:SD	2.58	0.43
12:1L:341:MET:HG2	12:1L:454:ILE:HD11	2.00	0.43
12:1L:395:ILE:HD13	12:1L:395:ILE:HA	1.80	0.43
12:1L:447:ASN:ND2	12:1L:449:LEU:HB2	2.33	0.43
13:1M:6:ILE:HG13	51:1X:201:CDL:H642	1.99	0.43
13:1M:439:LEU:HD23	13:1M:439:LEU:HA	1.86	0.43
51:1N:401:CDL:H412	51:1N:401:CDL:H382	1.88	0.43
16:1P:153:GLU:HG2	16:1P:165:ILE:HG21	2.00	0.43
19:1S:20:ILE:O	19:1S:20:ILE:HG23	2.18	0.43
19:1S:63:LYS:HB3	19:1S:65:TRP:NE1	2.34	0.43
22:1W:66:MET:HE1	22:1W:106:PHE:CD1	2.48	0.43
23:1X:67:LEU:HD23	23:1X:67:LEU:HA	1.86	0.43
27:1b:42:ILE:O	27:1b:46:ARG:HG3	2.19	0.43
39:1n:10:THR:OG1	39:1n:11:HIS:N	2.50	0.43
3:1C:72:PHE:CD2	3:1C:98:SER:HB3	2.53	0.43
6:1F:189:GLU:OE1	6:1F:222:VAL:HB	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:207:PRO:HD2	7:1G:71:MET:HE1	1.99	0.43
8:1H:211:PHE:HD1	8:1H:211:PHE:H	1.66	0.43
8:1H:264:LEU:HD21	26:1a:9:ILE:HG23	2.00	0.43
9:1I:161:TRP:HZ3	42:1q:84:PRO:HA	1.84	0.43
12:1L:204:LEU:HD12	12:1L:206:ASN:OD1	2.18	0.43
12:1L:237:MET:HE1	12:1L:354:GLN:HE22	1.84	0.43
12:1L:598:SER:HA	12:1L:604:TYR:CE1	2.53	0.43
13:1M:194:PHE:HE2	24:1Y:126:MET:HE3	1.83	0.43
14:1N:320:THR:HG21	15:1O:265:ASN:HA	2.00	0.43
16:1P:117:ILE:O	16:1P:121:SER:OG	2.25	0.43
20:1T:53:ALA:C	20:1T:54:MET:HE2	2.43	0.43
45:1Y:801:3PE:N	45:1Y:802:3PE:O12	2.37	0.43
33:1h:69:HIS:HD2	33:1h:70:PRO:N	2.16	0.43
34:1i:12:GLN:HA	34:1i:15:ARG:HB2	1.99	0.43
1:1A:83:ASN:OD1	1:1A:86:THR:HG23	2.19	0.43
1:1A:92:LEU:HD13	8:1H:302:MET:HG2	2.00	0.43
4:1D:55:HIS:NE2	8:1H:206:GLU:O	2.52	0.43
5:1E:103:CYS:SG	5:1E:153:MET:HE3	2.58	0.43
6:1F:298:ILE:HD11	6:1F:335:ILE:HB	2.00	0.43
9:1I:173:TYR:CE1	9:1I:174:LEU:HG	2.54	0.43
10:1J:4:TYR:CD1	10:1J:5:ILE:HG12	2.53	0.43
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.18	0.43
12:1L:142:ILE:HD11	13:1M:371:PRO:HB3	2.01	0.43
12:1L:257:VAL:HG13	12:1L:314:MET:HB3	1.99	0.43
12:1L:408:ALA:HA	12:1L:411:MET:CE	2.48	0.43
12:1L:486:MET:HA	12:1L:489:THR:HB	2.00	0.43
15:1O:38:LEU:HD12	15:1O:38:LEU:HA	1.83	0.43
16:1P:181:TYR:CE2	16:1P:283:LYS:HG2	2.53	0.43
18:1R:75:LEU:HD21	18:1R:91:PHE:HB3	2.00	0.43
30:1e:29:PRO:HG3	33:1h:140:THR:HB	1.99	0.43
34:1i:76:ILE:HA	34:1i:79:TRP:HD1	1.84	0.43
39:1n:132:TRP:O	39:1n:136:VAL:HG12	2.19	0.43
2:1B:92:LEU:HD21	2:1B:100:LEU:HD23	1.99	0.43
3:1C:158:GLU:OE2	17:1Q:24:GLY:HA3	2.19	0.43
3:1C:184:VAL:HG11	22:1W:110:THR:HG21	2.00	0.43
3:1C:203:TRP:CZ3	7:1G:36:GLN:HG2	2.54	0.43
4:1D:163:ALA:HB2	8:1H:277:TYR:C	2.43	0.43
6:1F:256:PHE:HD2	6:1F:270:GLU:HB3	1.84	0.43
6:1F:270:GLU:OE2	6:1F:271:GLU:N	2.46	0.43
7:1G:147:LYS:HE3	7:1G:149:ILE:HD11	2.00	0.43
8:1H:97:ASN:OD1	46:1Z:201:PC1:H131	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:49:ASN:HB2	9:1I:53:GLU:OE1	2.19	0.43
12:1L:124:PHE:CE1	12:1L:147:VAL:HG23	2.53	0.43
12:1L:439:PRO:HB3	35:1j:12:ARG:HG3	1.99	0.43
12:1L:521:LYS:O	12:1L:525:MET:HG2	2.18	0.43
51:1L:702:CDL:H382	33:1h:26:ARG:HA	2.01	0.43
13:1M:283:LYS:HE2	13:1M:283:LYS:HB3	1.89	0.43
14:1N:4:ILE:O	14:1N:7:THR:OG1	2.31	0.43
18:1R:46:GLU:H	18:1R:46:GLU:CD	2.25	0.43
19:1S:40:TYR:CE2	19:1S:54:ILE:HD11	2.53	0.43
23:1X:74:LYS:HB2	26:1a:66:LEU:HD13	1.99	0.43
23:1X:84:TYR:HE1	23:1X:99:CYS:HB3	1.83	0.43
33:1h:49:GLU:OE1	33:1h:68:LYS:HE3	2.17	0.43
38:1m:25:SER:OG	38:1m:27:GLU:OE1	2.32	0.43
39:1n:100:GLU:OE1	39:1n:121:ARG:NH2	2.51	0.43
1:1A:28:ASN:N	8:1H:59:GLU:OE2	2.44	0.43
7:1G:66:VAL:HB	7:1G:71:MET:HG2	1.99	0.43
7:1G:650:LYS:HA	7:1G:650:LYS:HD2	1.79	0.43
8:1H:92:PRO:HG2	8:1H:256:THR:HG23	2.00	0.43
8:1H:169:GLN:HG2	8:1H:174:MET:HE2	2.00	0.43
10:1J:55:MET:HE2	10:1J:55:MET:HA	2.01	0.43
11:1K:85:TYR:CE2	11:1K:93:LEU:HA	2.53	0.43
12:1L:147:VAL:HG22	12:1L:252:MET:HG3	2.00	0.43
12:1L:190:LEU:HD22	13:1M:383:THR:HB	2.01	0.43
12:1L:362:LEU:HD12	12:1L:366:MET:SD	2.59	0.43
14:1N:269:GLU:H	14:1N:269:GLU:CD	2.16	0.43
16:1P:40:ARG:NH1	22:1W:110:THR:OG1	2.52	0.43
17:1Q:19:ILE:HD12	17:1Q:19:ILE:HA	1.86	0.43
21:1V:48:GLU:HA	21:1V:51:THR:HG22	2.01	0.43
23:1X:42:PHE:HD2	23:1X:43:MET:HG2	1.83	0.43
29:1d:105:ASP:OD1	29:1d:105:ASP:O	2.36	0.43
33:1h:40:ILE:HD12	33:1h:41:THR:N	2.34	0.43
33:1h:41:THR:O	33:1h:45:VAL:HG13	2.19	0.43
33:1h:61:PRO:HG2	33:1h:66:TYR:OH	2.18	0.43
39:1n:21:ARG:HD3	39:1n:70:PHE:CZ	2.54	0.43
2:1B:163:LEU:HG	2:1B:167:ILE:HD12	2.01	0.43
7:1G:276:ARG:HD2	42:1q:135:GLN:HE22	1.84	0.43
7:1G:521:VAL:HG22	7:1G:542:PHE:HB3	2.00	0.43
7:1G:689:LYS:HB3	7:1G:689:LYS:HE2	1.72	0.43
8:1H:98:MET:HE2	8:1H:100:LEU:HB2	2.01	0.43
10:1J:39:VAL:O	10:1J:43:ILE:HG12	2.18	0.43
12:1L:296:ASN:O	12:1L:356:ILE:HG12	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:407:TRP:CD1	12:1L:407:TRP:C	2.97	0.43
13:1M:14:MET:HG2	13:1M:30:HIS:HD1	1.84	0.43
13:1M:91:ARG:HD3	13:1M:135:ARG:HH22	1.83	0.43
13:1M:91:ARG:NH2	15:1O:290:ASP:OD1	2.52	0.43
22:1W:61:ASP:N	22:1W:61:ASP:OD1	2.50	0.43
22:1W:115:PRO:HB3	22:1W:120:SER:HB2	1.99	0.43
27:1b:30:ILE:HD12	27:1b:31:LEU:N	2.34	0.43
28:1c:28:TRP:O	28:1c:32:ILE:HD12	2.19	0.43
32:1g:48:ASP:N	32:1g:54:ASP:OD1	2.52	0.43
46:1h:201:PC1:H372	46:1h:201:PC1:H251	2.01	0.43
34:1i:10:ARG:NH2	39:1n:164:PRO:O	2.50	0.43
35:1j:47:VAL:O	35:1j:48:LEU:HD23	2.19	0.43
37:1l:43:GLY:HA3	38:1m:75:ILE:O	2.19	0.43
37:1l:97:SER:HA	38:1m:5:TYR:HD1	1.83	0.43
39:1n:69:GLU:O	39:1n:73:GLY:N	2.38	0.43
1:1A:65:PHE:O	1:1A:69:ILE:HG23	2.19	0.43
2:1B:171:LYS:HB3	2:1B:174:ARG:HE	1.82	0.43
4:1D:183:ARG:HD3	43:1r:33:ARG:HH12	1.84	0.43
8:1H:25:ARG:NH2	8:1H:47:GLN:HE21	2.17	0.43
10:1J:127:ILE:HD12	10:1J:127:ILE:HA	1.88	0.43
12:1L:246:LEU:O	12:1L:251:THR:OG1	2.28	0.43
12:1L:565:THR:O	12:1L:569:ILE:HG12	2.18	0.43
14:1N:215:MET:HE2	14:1N:215:MET:HB2	1.81	0.43
15:1O:23:LYS:HA	15:1O:167:HIS:ND1	2.34	0.43
18:1R:13:HIS:HD1	18:1R:13:HIS:H	1.67	0.43
21:1V:113:TRP:CG	21:1V:113:TRP:O	2.71	0.43
46:1d:201:PC1:H32	46:1d:201:PC1:H321	1.58	0.43
32:1g:100:ARG:HD3	32:1g:107:LEU:HA	2.01	0.43
4:1D:110:SER:HB3	4:1D:113:CYS:HB3	2.00	0.42
4:1D:335:ARG:HH21	4:1D:339:LYS:NZ	2.16	0.42
6:1F:126:GLY:O	6:1F:130:GLY:N	2.51	0.42
6:1F:409:ASP:OD1	6:1F:409:ASP:N	2.52	0.42
7:1G:55:CYS:HB3	48:1G:803:FES:S2	2.59	0.42
7:1G:237:ASN:OD1	7:1G:237:ASN:N	2.52	0.42
7:1G:453:LEU:HB3	7:1G:492:ILE:HD12	2.01	0.42
7:1G:462:ASP:HB3	7:1G:657:LEU:HG	2.00	0.42
46:1I:203:PC1:H133	25:1Z:28:ARG:O	2.18	0.42
12:1L:30:ASN:O	12:1L:33:PRO:HD2	2.19	0.42
13:1M:16:TRP:HH2	29:1d:53:VAL:HG21	1.84	0.42
13:1M:42:LEU:CD1	13:1M:67:VAL:HG11	2.49	0.42
13:1M:129:THR:O	13:1M:133:ILE:HD12	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:49:ASN:H	14:1N:52:ALA:HB3	1.84	0.42
15:1O:27:VAL:HG23	15:1O:35:LYS:HD3	2.01	0.42
15:1O:31:ILE:O	15:1O:179:ILE:HD12	2.19	0.42
22:1W:114:ARG:HG3	22:1W:115:PRO:HD2	2.01	0.42
25:1Z:123:GLU:HG3	30:1e:75:LEU:HD21	2.00	0.42
35:1j:67:LEU:HD11	40:1o:110:ARG:HH21	1.84	0.42
37:1l:117:TRP:O	37:1l:120:GLU:HG2	2.19	0.42
38:1m:2:PHE:CZ	39:1n:69:GLU:HB3	2.54	0.42
39:1n:25:HIS:CE1	39:1n:78:PRO:HB3	2.53	0.42
40:1o:21:MET:N	40:1o:21:MET:SD	2.92	0.42
42:1q:39:VAL:HG11	42:1q:89:TRP:CH2	2.53	0.42
3:1C:20:LYS:O	3:1C:20:LYS:HD3	2.19	0.42
3:1C:29:VAL:HG22	3:1C:63:PHE:HE2	1.84	0.42
3:1C:182:ARG:HH21	22:1W:104:MET:HG3	1.84	0.42
4:1D:287:ILE:O	9:1I:5:VAL:HG12	2.19	0.42
5:1E:23:PHE:HB2	5:1E:28:TYR:CZ	2.54	0.42
6:1F:248:GLU:O	6:1F:250:ASN:N	2.50	0.42
7:1G:363:LEU:HD12	7:1G:363:LEU:HA	1.74	0.42
7:1G:646:ASN:OD1	7:1G:647:GLU:N	2.49	0.42
8:1H:81:LEU:HA	8:1H:81:LEU:HD23	1.91	0.42
8:1H:158:GLY:HA2	8:1H:315:PRO:HG2	2.01	0.42
8:1H:291:LYS:HD2	8:1H:291:LYS:HA	1.69	0.42
51:1H:402:CDL:OA4	16:1P:251:ARG:NH1	2.51	0.42
10:1J:159:TRP:HE1	14:1N:12:THR:HG22	1.84	0.42
12:1L:61:MET:HA	41:1p:114:GLN:NE2	2.34	0.42
12:1L:154:LEU:HB3	12:1L:243:VAL:HG11	2.01	0.42
12:1L:323:HIS:CG	12:1L:475:MET:HE3	2.54	0.42
12:1L:384:PRO:HA	12:1L:389:PHE:CG	2.54	0.42
12:1L:529:TYR:CZ	12:1L:533:MET:HG3	2.54	0.42
12:1L:602:PHE:CD1	12:1L:602:PHE:C	2.97	0.42
13:1M:104:LEU:HD23	51:1X:201:CDL:H472	2.00	0.42
13:1M:175:ASN:O	13:1M:179:ILE:HG12	2.18	0.42
13:1M:186:LEU:HD23	13:1M:186:LEU:HA	1.85	0.42
13:1M:190:TRP:CD2	24:1Y:126:MET:HE1	2.54	0.42
13:1M:243:MET:HE2	13:1M:301:ILE:HD12	2.00	0.42
16:1P:93:ASN:HD21	16:1P:114:PRO:HG3	1.84	0.42
16:1P:331:MET:HE3	16:1P:331:MET:H	1.84	0.42
20:1U:15:VAL:HG12	20:1U:54:MET:HE1	2.01	0.42
22:1W:77:ARG:O	22:1W:81:LEU:N	2.37	0.42
46:1d:201:PC1:H153	30:1e:2:PHE:CE1	2.54	0.42
46:1h:201:PC1:O14	46:1h:201:PC1:H121	2.18	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:4:THR:O	34:1i:5:PRO:C	2.61	0.42
34:1i:70:ALA:O	34:1i:74:VAL:HG12	2.19	0.42
36:1k:27:PRO:HD2	36:1k:52:TYR:HD2	1.84	0.42
42:1q:47:LYS:HE2	42:1q:47:LYS:HB2	1.96	0.42
1:1A:90:MET:HA	1:1A:90:MET:HE2	2.00	0.42
4:1D:169:TRP:CZ3	8:1H:32:GLN:HA	2.54	0.42
5:1E:191:PHE:HB3	44:1s:38:TYR:HE1	1.83	0.42
8:1H:235:ASN:HD21	8:1H:267:THR:N	2.18	0.42
10:1J:139:GLU:HB2	11:1K:49:LEU:HD11	2.01	0.42
14:1N:159:MET:HG2	14:1N:278:MET:SD	2.59	0.42
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	2.00	0.42
16:1P:135:LEU:HB3	16:1P:169:SER:HA	2.00	0.42
23:1X:43:MET:HE3	23:1X:47:TRP:CZ3	2.55	0.42
29:1d:112:ILE:O	41:1p:159:LYS:NZ	2.41	0.42
32:1g:62:PHE:CE2	33:1h:24:LEU:HB3	2.54	0.42
33:1h:51:GLU:N	33:1h:51:GLU:OE1	2.53	0.42
37:1l:141:GLU:HA	41:1p:122:GLN:CD	2.43	0.42
38:1m:36:LEU:O	38:1m:40:SER:OG	2.28	0.42
40:1o:110:ARG:CZ	40:1o:114:ARG:HE	2.32	0.42
42:1q:5:GLN:OE1	42:1q:5:GLN:HA	2.19	0.42
42:1q:68:MET:HG2	42:1q:115:PHE:HE2	1.84	0.42
3:1C:54:PRO:HG3	3:1C:110:TYR:O	2.19	0.42
4:1D:112:MET:HA	4:1D:115:GLU:OE1	2.18	0.42
4:1D:126:LEU:HD23	4:1D:359:PRO:HD3	2.00	0.42
4:1D:307:SER:O	4:1D:311:ILE:HG12	2.19	0.42
4:1D:417:ILE:O	4:1D:420:THR:HG22	2.19	0.42
6:1F:322:LEU:HG	6:1F:329:LEU:HA	2.01	0.42
8:1H:247:HIS:HB2	8:1H:255:TYR:CD1	2.54	0.42
9:1I:165:ILE:HA	9:1I:168:ASN:HB2	2.01	0.42
10:1J:79:TYR:CD2	16:1P:325:ARG:HD2	2.55	0.42
10:1J:146:LEU:HA	10:1J:146:LEU:HD23	1.90	0.42
11:1K:48:ILE:HG23	11:1K:49:LEU:HD22	2.00	0.42
12:1L:202:PHE:HB2	41:1p:113:GLN:HE21	1.84	0.42
13:1M:10:MET:HA	13:1M:10:MET:HE3	2.00	0.42
17:1Q:112:LYS:O	17:1Q:114:LYS:HD3	2.20	0.42
22:1W:18:LYS:HE2	22:1W:18:LYS:HB2	1.83	0.42
23:1X:36:ASP:OD1	23:1X:36:ASP:C	2.62	0.42
27:1b:15:GLU:HG2	27:1b:15:GLU:O	2.20	0.42
29:1d:30:ARG:HH21	29:1d:76:LEU:HD22	1.85	0.42
29:1d:49:ARG:C	29:1d:50:ARG:HG2	2.45	0.42
41:1p:167:LYS:HB3	41:1p:167:LYS:HE2	1.74	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:112:MET:HA	4:1D:115:GLU:CD	2.44	0.42
4:1D:269:LEU:HD21	4:1D:373:GLU:HG3	2.00	0.42
4:1D:354:GLU:OE2	4:1D:357:GLN:NE2	2.52	0.42
5:1E:16:ASN:O	5:1E:19:THR:OG1	2.34	0.42
10:1J:34:ILE:HD12	10:1J:34:ILE:HA	1.88	0.42
12:1L:90:ILE:O	12:1L:94:LEU:HG	2.20	0.42
12:1L:381:THR:HG22	12:1L:420:ALA:HA	2.01	0.42
12:1L:439:PRO:HB3	35:1j:12:ARG:HD2	2.01	0.42
12:1L:479:ASN:C	12:1L:482:MET:HE1	2.45	0.42
12:1L:485:TYR:CE1	12:1L:486:MET:HG3	2.54	0.42
12:1L:559:GLU:OE1	12:1L:564:LYS:HE2	2.19	0.42
13:1M:42:LEU:HA	13:1M:63:ALA:HB1	2.00	0.42
14:1N:167:TRP:HA	14:1N:288:LEU:HD13	2.02	0.42
15:1O:90:ASP:OD1	15:1O:91:GLY:N	2.52	0.42
17:1Q:112:LYS:HG2	17:1Q:113:PRO:CD	2.49	0.42
19:1S:32:VAL:HG11	19:1S:62:PRO:HB3	2.01	0.42
20:1T:29:LYS:HA	20:1T:29:LYS:HD3	1.66	0.42
21:1V:3:LEU:HD22	21:1V:4:LEU:N	2.33	0.42
22:1W:100:ARG:O	22:1W:104:MET:HG2	2.19	0.42
26:1a:58:ASN:O	26:1a:58:ASN:ND2	2.51	0.42
32:1g:100:ARG:HD3	32:1g:107:LEU:C	2.45	0.42
42:1q:83:PRO:HB2	42:1q:85:GLU:OE2	2.20	0.42
2:1B:77:ARG:HB3	2:1B:82:GLN:HB3	2.01	0.42
3:1C:136:ASP:HB3	3:1C:137:MET:HE3	2.02	0.42
3:1C:168:LEU:HD22	3:1C:194:PHE:CD2	2.55	0.42
6:1F:68:ARG:HB2	6:1F:227:THR:OG1	2.19	0.42
7:1G:110:GLN:HB3	7:1G:114:CYS:HB2	2.00	0.42
7:1G:175:THR:N	7:1G:182:GLN:O	2.53	0.42
7:1G:243:ARG:HD2	7:1G:244:THR:OG1	2.19	0.42
10:1J:169:MET:HE2	10:1J:169:MET:HB2	1.91	0.42
11:1K:55:LEU:HD22	30:1e:25:PRO:HD3	2.02	0.42
12:1L:438:PRO:HA	12:1L:439:PRO:HD3	1.95	0.42
13:1M:207:MET:HB2	13:1M:207:MET:HE2	1.68	0.42
16:1P:191:VAL:HG11	16:1P:242:VAL:HG11	2.01	0.42
20:1U:70:LEU:HA	20:1U:75:GLU:OE2	2.19	0.42
23:1X:42:PHE:CD2	23:1X:43:MET:HG2	2.55	0.42
25:1Z:98:MET:HE2	25:1Z:98:MET:HA	2.00	0.42
33:1h:73:ARG:NH2	41:1p:61:TYR:O	2.52	0.42
36:1k:15:LEU:H	36:1k:15:LEU:CD2	2.32	0.42
1:1A:46:SER:C	1:1A:48:ARG:H	2.28	0.42
2:1B:125:TYR:HD1	9:1I:89:ALA:HB2	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1D:901:3PE:H292	45:1D:901:3PE:H372	2.01	0.42
6:1F:199:LYS:HZ1	17:1Q:131:SER:C	2.26	0.42
7:1G:32:LYS:HB2	7:1G:32:LYS:HE2	1.81	0.42
8:1H:190:LEU:HD23	8:1H:195:ARG:HB3	2.01	0.42
8:1H:299:ALA:HB1	27:1b:24:ILE:HB	2.00	0.42
9:1I:81:LYS:HE2	9:1I:94:ILE:HG22	2.01	0.42
9:1I:159:ASP:OD1	9:1I:159:ASP:C	2.63	0.42
10:1J:94:VAL:HA	10:1J:97:LEU:HG	2.02	0.42
12:1L:137:LEU:HD12	12:1L:137:LEU:HA	1.85	0.42
12:1L:144:TRP:CZ3	12:1L:259:LEU:HD12	2.55	0.42
12:1L:486:MET:O	12:1L:489:THR:HG22	2.19	0.42
13:1M:114:GLU:HA	13:1M:114:GLU:OE1	2.20	0.42
13:1M:150:LEU:HD12	13:1M:154:LEU:HG	2.02	0.42
13:1M:391:ILE:O	13:1M:394:ILE:HG22	2.20	0.42
14:1N:71:MET:O	14:1N:75:ILE:N	2.47	0.42
14:1N:86:ILE:HG23	14:1N:86:ILE:O	2.19	0.42
14:1N:245:MET:HG3	14:1N:302:LEU:CD2	2.49	0.42
14:1N:271:THR:HG22	14:1N:276:ILE:HG22	2.01	0.42
18:1R:16:GLN:OE1	18:1R:33:LYS:NZ	2.50	0.42
24:1Y:139:LYS:HG3	33:1h:112:ARG:HG3	2.00	0.42
25:1Z:56:GLU:O	25:1Z:60:LEU:HD23	2.20	0.42
42:1q:73:THR:OG1	42:1q:73:THR:O	2.37	0.42
2:1B:41:ARG:HA	8:1H:54:LYS:HG3	2.01	0.42
3:1C:32:ILE:HG21	3:1C:63:PHE:CZ	2.55	0.42
6:1F:343:ILE:HD12	6:1F:344:VAL:N	2.35	0.42
7:1G:611:LEU:HD13	7:1G:611:LEU:HA	1.92	0.42
7:1G:683:THR:HA	7:1G:686:LYS:HD2	2.01	0.42
8:1H:145:THR:O	8:1H:149:ILE:HD12	2.20	0.42
12:1L:209:PRO:HG2	12:1L:213:LEU:HD22	2.01	0.42
14:1N:150:ASN:HB3	14:1N:153:LEU:HB3	2.02	0.42
14:1N:217:MET:SD	14:1N:326:LEU:HA	2.59	0.42
16:1P:122:LYS:HE3	16:1P:160:PHE:CE2	2.54	0.42
20:1U:32:VAL:HG22	20:1U:74:GLN:HB2	2.01	0.42
22:1W:46:THR:O	22:1W:50:PHE:HB2	2.19	0.42
22:1W:62:LYS:NZ	22:1W:107:PHE:HA	2.35	0.42
26:1a:5:ILE:HD13	26:1a:5:ILE:HA	1.81	0.42
39:1n:93:TYR:O	39:1n:97:LYS:HG3	2.19	0.42
43:1r:108:ASP:OD1	43:1r:108:ASP:C	2.63	0.42
4:1D:221:ARG:NE	43:1r:24:GLN:HG3	2.35	0.42
4:1D:425:PHE:O	4:1D:429:ASP:HB3	2.20	0.42
5:1E:39:PRO:HD2	6:1F:216:PHE:CZ	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:164:LEU:HD13	5:1E:164:LEU:HA	1.95	0.42
5:1E:193:CYS:O	6:1F:266:CYS:HB2	2.20	0.42
6:1F:342:ASP:HB3	6:1F:345:LYS:HE3	2.02	0.42
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	2.01	0.42
8:1H:170:GLU:HG3	25:1Z:53:TRP:CZ2	2.54	0.42
8:1H:241:LEU:HB3	8:1H:242:PHE:CD2	2.54	0.42
10:1J:61:LEU:O	10:1J:65:LEU:HB2	2.20	0.42
11:1K:96:LEU:HD23	11:1K:96:LEU:O	2.20	0.42
12:1L:100:ILE:HG21	12:1L:246:LEU:HD12	2.01	0.42
12:1L:241:THR:O	12:1L:245:ALA:N	2.49	0.42
12:1L:406:ALA:HB2	37:1l:122:TYR:O	2.20	0.42
13:1M:84:LEU:O	13:1M:92:LYS:NZ	2.31	0.42
13:1M:200:ILE:O	13:1M:204:MET:HG2	2.20	0.42
15:1O:61:SER:HA	15:1O:66:GLY:HA2	2.01	0.42
15:1O:78:SER:OG	15:1O:80:GLU:OE1	2.32	0.42
16:1P:108:ASP:O	16:1P:113:ILE:HG12	2.20	0.42
16:1P:147:ARG:O	16:1P:151:VAL:HG12	2.20	0.42
18:1R:23:TYR:O	18:1R:26:VAL:HG12	2.20	0.42
20:1T:64:ASP:O	22:1W:30:ARG:NH1	2.53	0.42
21:1V:3:LEU:HD13	21:1V:4:LEU:O	2.19	0.42
21:1V:81:LEU:O	21:1V:85:ASN:HB2	2.19	0.42
31:1f:35:THR:HB	31:1f:38:ARG:HE	1.84	0.42
35:1j:38:TRP:HA	36:1k:77:PHE:CE1	2.55	0.42
37:1l:9:PHE:CD2	38:1m:69:TYR:HD2	2.37	0.42
38:1m:84:LYS:HD3	38:1m:84:LYS:HA	1.89	0.42
41:1p:40:VAL:C	41:1p:43:PRO:HD2	2.45	0.42
43:1r:42:VAL:HB	43:1r:46:HIS:CD2	2.55	0.42
3:1C:70:ALA:HB1	3:1C:72:PHE:HD1	1.85	0.42
4:1D:23:LYS:HD2	4:1D:23:LYS:HA	1.90	0.42
6:1F:256:PHE:CD1	6:1F:332:ALA:HB1	2.55	0.42
6:1F:300:GLY:HA2	6:1F:333:ALA:N	2.34	0.42
6:1F:349:ARG:HA	6:1F:349:ARG:HD2	1.89	0.42
6:1F:351:ILE:C	6:1F:351:ILE:HD12	2.45	0.42
7:1G:100:ASN:OD1	7:1G:179:ASN:ND2	2.39	0.42
7:1G:117:GLN:NE2	47:1G:801:SF4:S4	2.92	0.42
7:1G:349:PHE:CB	7:1G:509:PRO:HB2	2.50	0.42
8:1H:24:GLU:HG2	8:1H:228:TYR:OH	2.20	0.42
8:1H:179:TRP:HE1	25:1Z:43:LEU:HB2	1.84	0.42
8:1H:200:LEU:HD11	8:1H:280:PHE:O	2.20	0.42
10:1J:74:MET:SD	11:1K:82:SER:OG	2.63	0.42
12:1L:204:LEU:HD13	12:1L:204:LEU:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:335:PHE:HE1	12:1L:380:LEU:HD23	1.84	0.42
12:1L:473:PRO:O	12:1L:475:MET:HG3	2.20	0.42
14:1N:312:LYS:HE3	15:1O:76:ASN:OD1	2.19	0.42
16:1P:74:ASN:O	16:1P:80:SER:OG	2.26	0.42
16:1P:331:MET:H	16:1P:331:MET:CE	2.32	0.42
20:1T:43:ASP:OD1	20:1T:44:SER:N	2.53	0.42
25:1Z:120:MET:CG	30:1e:68:ARG:HD3	2.50	0.42
3:1C:93:VAL:HG22	3:1C:108:LYS:HB2	2.02	0.41
3:1C:164:LYS:HB3	17:1Q:84:LEU:HD21	2.02	0.41
3:1C:196:LYS:HD3	7:1G:223:ARG:HG3	2.02	0.41
4:1D:62:LEU:HD13	4:1D:425:PHE:CE1	2.54	0.41
4:1D:371:LYS:HG2	4:1D:422:ASP:OD2	2.20	0.41
7:1G:19:MET:HE2	7:1G:19:MET:HA	2.02	0.41
8:1H:213:VAL:HB	8:1H:214:GLU:OE1	2.20	0.41
11:1K:55:LEU:CD2	30:1e:25:PRO:HD3	2.50	0.41
12:1L:106:TRP:NE1	12:1L:450:LEU:HD22	2.35	0.41
12:1L:470:ASN:OD1	12:1L:471:ASN:N	2.53	0.41
12:1L:525:MET:N	12:1L:525:MET:SD	2.93	0.41
12:1L:530:PRO:HA	12:1L:534:HIS:CD2	2.55	0.41
13:1M:271:MET:HE2	13:1M:271:MET:HB2	1.90	0.41
13:1M:398:MET:O	13:1M:401:MET:HB3	2.20	0.41
14:1N:25:HIS:HE2	30:1e:17:MET:HB3	1.83	0.41
14:1N:209:ILE:HD13	14:1N:209:ILE:HA	1.91	0.41
19:1S:35:PHE:CD2	19:1S:36:ILE:HG23	2.55	0.41
23:1X:112:ASP:OD1	23:1X:112:ASP:C	2.63	0.41
28:1c:19:LEU:O	28:1c:23:THR:HG22	2.20	0.41
33:1h:87:TYR:CE2	41:1p:89:MET:HG3	2.54	0.41
36:1k:42:ASP:OD1	36:1k:42:ASP:C	2.63	0.41
38:1m:61:ASP:O	38:1m:65:ILE:HG12	2.20	0.41
39:1n:51:LYS:NZ	56:1n:201:EHZ:O5	2.53	0.41
40:1o:21:MET:HB3	40:1o:100:GLU:OE2	2.20	0.41
40:1o:62:LEU:HG	40:1o:86:TRP:NE1	2.35	0.41
42:1q:106:ARG:HG3	42:1q:109:ILE:HD11	2.02	0.41
2:1B:50:PHE:CE2	2:1B:100:LEU:HD13	2.55	0.41
2:1B:81:ARG:HB2	8:1H:213:VAL:O	2.19	0.41
3:1C:21:GLN:OE1	43:1r:97:ALA:HA	2.20	0.41
4:1D:105:ARG:NH2	9:1I:117:ILE:HD11	2.35	0.41
4:1D:146:ARG:HD3	4:1D:370:PRO:HG3	2.02	0.41
6:1F:89:ARG:NH1	6:1F:219:PRO:HD3	2.36	0.41
6:1F:136:ILE:HG13	6:1F:176:PHE:O	2.20	0.41
6:1F:322:LEU:HB3	6:1F:327:THR:HG23	2.00	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:582:GLN:O	7:1G:584:LYS:NZ	2.53	0.41
7:1G:588:THR:OG1	17:1Q:63:GLU:HA	2.19	0.41
8:1H:77:LEU:HD22	8:1H:115:SER:HB3	2.02	0.41
8:1H:82:ALA:HB1	8:1H:229:ALA:HB3	2.03	0.41
8:1H:187:ILE:HD12	8:1H:188:SER:N	2.35	0.41
10:1J:52:LEU:HD23	10:1J:139:GLU:HG3	2.02	0.41
11:1K:53:PHE:C	11:1K:53:PHE:CD1	2.98	0.41
11:1K:62:ILE:HA	11:1K:65:VAL:CG2	2.45	0.41
12:1L:4:PHE:HB3	12:1L:61:MET:SD	2.60	0.41
12:1L:161:ARG:HB3	39:1n:91:GLU:HG3	2.01	0.41
13:1M:75:LEU:HG	13:1M:440:HIS:CD2	2.55	0.41
15:1O:25:ILE:HB	15:1O:123:VAL:HG22	2.02	0.41
16:1P:48:PRO:HG3	16:1P:84:VAL:HG11	2.02	0.41
16:1P:211:SER:O	16:1P:215:ILE:HD12	2.20	0.41
16:1P:281:ARG:HE	16:1P:281:ARG:HB2	1.60	0.41
17:1Q:37:ILE:HG22	17:1Q:57:MET:HA	2.02	0.41
19:1S:63:LYS:HZ1	19:1S:77:SER:HA	1.85	0.41
22:1W:36:TYR:OH	22:1W:64:ARG:HG2	2.20	0.41
22:1W:84:ILE:H	22:1W:84:ILE:HG13	1.64	0.41
25:1Z:108:GLU:CD	30:1e:74:ARG:HH22	2.27	0.41
29:1d:30:ARG:NH2	29:1d:76:LEU:HD22	2.35	0.41
33:1h:10:ILE:H	33:1h:10:ILE:HG13	1.79	0.41
33:1h:43:VAL:HA	33:1h:47:ILE:HD12	2.01	0.41
34:1i:46:TRP:HE3	34:1i:49:PHE:HE1	1.67	0.41
37:1l:131:LYS:HD2	40:1o:97:ARG:NH1	2.34	0.41
41:1p:74:THR:OG1	41:1p:75:GLU:N	2.53	0.41
41:1p:143:SER:O	41:1p:145:LEU:HD12	2.20	0.41
42:1q:3:LEU:O	42:1q:7:LEU:HD23	2.19	0.41
42:1q:25:ARG:HE	42:1q:25:ARG:HB2	1.59	0.41
42:1q:43:LYS:NZ	42:1q:111:THR:O	2.41	0.41
1:1A:85:LYS:HB3	46:1J:201:PC1:H151	2.01	0.41
3:1C:97:LEU:HD13	3:1C:104:ARG:HG2	2.03	0.41
3:1C:132:ARG:NH2	3:1C:151:ILE:HD13	2.35	0.41
4:1D:17:ALA:N	4:1D:30:PRO:HG3	2.35	0.41
4:1D:29:LYS:HE2	4:1D:30:PRO:HD2	2.01	0.41
4:1D:164:MET:O	4:1D:167:PHE:HB3	2.19	0.41
4:1D:204:PRO:HA	9:1I:175:TYR:CE2	2.55	0.41
5:1E:42:HIS:CD2	5:1E:42:HIS:N	2.89	0.41
5:1E:76:PRO:HB2	5:1E:79:ARG:HG2	2.02	0.41
8:1H:179:TRP:NE1	25:1Z:43:LEU:HD22	2.35	0.41
8:1H:288:LEU:HD11	46:1H:401:PC1:O22	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:98:PRO:HA	9:1I:104:ARG:HB2	2.03	0.41
11:1K:40:LEU:HD21	14:1N:71:MET:HB3	2.01	0.41
12:1L:231:PRO:C	12:1L:234:PRO:HD2	2.45	0.41
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.56	0.41
14:1N:69:MET:HG2	14:1N:97:MET:SD	2.60	0.41
14:1N:72:MET:O	14:1N:76:ILE:HG12	2.19	0.41
14:1N:235:ASN:ND2	15:1O:289:SER:HB3	2.35	0.41
14:1N:245:MET:HG3	14:1N:302:LEU:HD23	2.02	0.41
15:1O:279:LEU:HB2	15:1O:282:ILE:HB	2.03	0.41
16:1P:203:GLN:HB2	16:1P:235:ARG:HG3	2.03	0.41
16:1P:236:TYR:CE2	16:1P:310:LEU:HD23	2.55	0.41
19:1S:21:HIS:CD2	19:1S:55:ARG:HB2	2.55	0.41
19:1S:38:LYS:H	19:1S:38:LYS:HD2	1.86	0.41
24:1Y:123:LEU:HA	24:1Y:126:MET:HB2	2.01	0.41
32:1g:72:LEU:HD21	33:1h:32:THR:OG1	2.20	0.41
32:1g:97:VAL:HG23	32:1g:107:LEU:HB2	2.01	0.41
33:1h:7:ARG:HD3	33:1h:7:ARG:H	1.85	0.41
38:1m:91:LEU:O	38:1m:96:PRO:HD3	2.20	0.41
3:1C:25:PHE:CD2	43:1r:96:PRO:HG3	2.54	0.41
4:1D:407:LYS:HB2	4:1D:407:LYS:HE3	1.81	0.41
6:1F:15:LEU:HB2	6:1F:271:GLU:N	2.34	0.41
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.61	0.41
7:1G:276:ARG:HA	42:1q:135:GLN:NE2	2.35	0.41
7:1G:405:LYS:HE2	7:1G:439:PHE:HE1	1.85	0.41
7:1G:552:VAL:C	7:1G:555:PRO:HD2	2.45	0.41
7:1G:619:VAL:O	7:1G:623:LEU:HD12	2.20	0.41
8:1H:72:ILE:C	8:1H:75:PRO:HD2	2.45	0.41
10:1J:71:THR:O	10:1J:76:THR:HB	2.19	0.41
12:1L:61:MET:O	12:1L:82:MET:N	2.53	0.41
12:1L:174:TYR:CD1	12:1L:229:LEU:HA	2.55	0.41
13:1M:216:LEU:HG	13:1M:291:VAL:HG22	2.02	0.41
45:1M:501:3PE:H321	24:1Y:132:TRP:CH2	2.56	0.41
16:1P:99:TRP:CZ2	16:1P:276:GLU:HG3	2.56	0.41
16:1P:253:PHE:O	16:1P:254:LEU:HD23	2.21	0.41
20:1U:23:ASP:OD1	20:1U:23:ASP:N	2.53	0.41
22:1W:38:ALA:O	22:1W:42:GLU:HB2	2.20	0.41
22:1W:68:MET:HA	22:1W:71:ALA:CB	2.51	0.41
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	2.03	0.41
26:1a:69:ILE:H	26:1a:69:ILE:HG13	1.75	0.41
28:1c:23:THR:O	28:1c:27:LEU:HB2	2.20	0.41
29:1d:44:ILE:O	29:1d:48:ILE:HD12	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:32:GLU:HA	31:1f:35:THR:HG23	2.02	0.41
32:1g:88:TRP:O	32:1g:92:GLU:HG2	2.20	0.41
40:1o:46:ASN:OD1	40:1o:46:ASN:C	2.63	0.41
1:1A:79:SER:HA	1:1A:87:MET:HE3	2.01	0.41
1:1A:82:ASN:ND2	27:1b:46:ARG:HG2	2.36	0.41
1:1A:82:ASN:HD21	27:1b:46:ARG:HG2	1.84	0.41
2:1B:72:PHE:CD2	2:1B:161:LEU:HD21	2.55	0.41
2:1B:112:TYR:HD1	2:1B:143:ASP:OD2	2.03	0.41
5:1E:104:THR:HG21	5:1E:141:GLU:HB2	2.01	0.41
5:1E:196:ALA:HB3	6:1F:264:HIS:ND1	2.35	0.41
6:1F:22:PHE:HD1	6:1F:117:LYS:HD2	1.85	0.41
6:1F:419:ILE:O	6:1F:423:ARG:HB2	2.20	0.41
7:1G:669:LYS:H	7:1G:669:LYS:HG3	1.57	0.41
8:1H:6:ILE:HD13	8:1H:95:LEU:HD11	2.03	0.41
8:1H:294:LEU:HD12	8:1H:294:LEU:HA	1.82	0.41
9:1I:62:ARG:HA	9:1I:133:GLU:HB3	2.03	0.41
11:1K:65:VAL:O	11:1K:69:CYS:HB2	2.21	0.41
12:1L:293:ILE:O	12:1L:425:ARG:NH1	2.53	0.41
12:1L:374:ILE:O	12:1L:378:LEU:HD23	2.19	0.41
13:1M:77:LEU:HA	13:1M:77:LEU:HD23	1.80	0.41
13:1M:358:TRP:CZ3	13:1M:441:ILE:HG21	2.55	0.41
15:1O:102:ALA:HA	15:1O:105:LEU:HB3	2.02	0.41
15:1O:266:LYS:HD3	15:1O:266:LYS:HA	1.86	0.41
17:1Q:124:TRP:HD1	17:1Q:125:ASN:OD1	2.03	0.41
18:1R:27:ARG:NH2	42:1q:127:TYR:HA	2.36	0.41
21:1V:93:MET:HE2	21:1V:93:MET:HA	2.02	0.41
30:1e:76:SER:O	30:1e:80:ARG:HB2	2.19	0.41
33:1h:50:ALA:HB2	41:1p:60:TYR:CE2	2.54	0.41
40:1o:99:LYS:HA	40:1o:99:LYS:HD2	1.96	0.41
42:1q:13:GLN:HE21	42:1q:34:ARG:HA	1.85	0.41
44:1s:43:HIS:HA	44:1s:46:TYR:CZ	2.56	0.41
4:1D:148:LEU:HD23	4:1D:148:LEU:HA	1.78	0.41
4:1D:178:PHE:HA	4:1D:181:TYR:HB2	2.01	0.41
4:1D:270:ARG:HE	4:1D:368:GLU:HG2	1.85	0.41
6:1F:63:SER:OG	6:1F:64:GLY:N	2.52	0.41
7:1G:145:LEU:HB2	7:1G:269:PHE:CE2	2.55	0.41
7:1G:273:GLY:HA3	7:1G:677:ILE:HG23	2.03	0.41
7:1G:437:HIS:CD2	7:1G:438:PRO:HD2	2.55	0.41
8:1H:26:LYS:HB2	8:1H:37:PRO:HD2	2.02	0.41
10:1J:34:ILE:HD11	10:1J:61:LEU:HG	2.02	0.41
11:1K:16:LEU:O	11:1K:20:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:289:ALA:O	12:1L:293:ILE:HG12	2.21	0.41
12:1L:327:LEU:O	12:1L:331:MET:HG2	2.21	0.41
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.20	0.41
13:1M:116:ILE:HG22	23:1X:168:PHE:HE1	1.85	0.41
14:1N:36:ASN:O	14:1N:40:MET:HB2	2.20	0.41
14:1N:58:LYS:O	14:1N:62:THR:HG23	2.20	0.41
15:1O:42:ILE:HG22	15:1O:235:VAL:HG12	2.01	0.41
15:1O:245:LYS:HE2	15:1O:245:LYS:HB3	1.73	0.41
16:1P:172:PHE:CD2	16:1P:204:PRO:HB2	2.55	0.41
20:1T:55:GLU:HB2	20:1T:60:PHE:O	2.20	0.41
24:1Y:4:LEU:H	24:1Y:4:LEU:HD22	1.86	0.41
24:1Y:30:ALA:O	24:1Y:34:ILE:HG13	2.20	0.41
33:1h:38:ILE:HD12	33:1h:38:ILE:C	2.46	0.41
37:1l:135:TYR:OH	40:1o:40:ALA:O	2.38	0.41
38:1m:45:GLU:OE1	38:1m:46:TYR:N	2.54	0.41
39:1n:75:HIS:HD2	39:1n:76:PRO:HD2	1.85	0.41
40:1o:24:PHE:HB2	40:1o:107:LEU:HD13	2.02	0.41
41:1p:29:VAL:HA	41:1p:32:LEU:HD23	2.02	0.41
1:1A:81:THR:C	27:1b:45:ASN:HD22	2.28	0.41
2:1B:100:LEU:HA	2:1B:103:VAL:HG12	2.03	0.41
6:1F:268:VAL:HG21	6:1F:283:HIS:HB3	2.02	0.41
7:1G:359:ARG:HA	7:1G:362:TYR:CE1	2.56	0.41
7:1G:385:ARG:HB2	7:1G:415:LEU:HD12	2.03	0.41
7:1G:543:ILE:N	7:1G:558:ASP:OD2	2.43	0.41
7:1G:547:GLY:O	7:1G:563:GLY:N	2.34	0.41
8:1H:139:THR:HG21	10:1J:65:LEU:HD21	2.02	0.41
9:1I:31:VAL:O	9:1I:35:GLY:N	2.47	0.41
13:1M:43:ASN:HD21	33:1h:80:TYR:HE1	1.69	0.41
13:1M:44:GLN:HE22	13:1M:59:ASP:HA	1.85	0.41
13:1M:423:ILE:HD13	13:1M:426:ILE:CD1	2.51	0.41
14:1N:45:MET:HA	14:1N:52:ALA:HB1	2.02	0.41
14:1N:109:SER:C	14:1N:111:PHE:N	2.79	0.41
14:1N:218:LEU:HD12	14:1N:326:LEU:HD11	2.01	0.41
15:1O:294:GLN:O	15:1O:297:THR:OG1	2.38	0.41
17:1Q:94:ALA:O	17:1Q:98:LYS:HG2	2.20	0.41
20:1U:83:LYS:HA	20:1U:83:LYS:HD2	1.62	0.41
31:1f:56:TRP:HE1	33:1h:88:GLU:CD	2.28	0.41
35:1j:45:ASP:OD1	35:1j:50:HIS:HB2	2.20	0.41
36:1k:17:ASP:OD2	36:1k:19:LYS:HG2	2.20	0.41
40:1o:53:GLN:OE1	40:1o:53:GLN:N	2.44	0.41
42:1q:55:PHE:CE2	42:1q:58:ARG:HD3	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:109:VAL:HG12	4:1D:152:MET:CE	2.50	0.41
7:1G:475:GLN:O	7:1G:479:LEU:N	2.53	0.41
7:1G:523:PHE:CG	7:1G:544:ILE:HD11	2.55	0.41
8:1H:156:MET:HE3	8:1H:156:MET:HB2	1.83	0.41
12:1L:298:ILE:CD1	12:1L:426:ILE:HD11	2.51	0.41
12:1L:360:GLY:O	12:1L:435:PRO:HA	2.19	0.41
12:1L:368:PHE:HB3	12:1L:445:GLU:OE1	2.21	0.41
13:1M:71:TRP:HH2	13:1M:439:LEU:HD22	1.86	0.41
13:1M:122:PHE:HE1	13:1M:206:LYS:HD2	1.85	0.41
13:1M:378:GLU:C	13:1M:378:GLU:OE1	2.64	0.41
14:1N:231:SER:O	14:1N:234:TRP:HD1	2.03	0.41
14:1N:299:SER:HA	14:1N:305:PHE:HE2	1.86	0.41
16:1P:141:SER:OG	16:1P:146:LEU:HB2	2.21	0.41
21:1V:113:TRP:CZ3	21:1V:115:ILE:HG13	2.56	0.41
24:1Y:103:ARG:HA	24:1Y:103:ARG:HD2	1.77	0.41
31:1f:2:ASN:O	31:1f:5:GLN:N	2.54	0.41
35:1j:12:ARG:HE	36:1k:50:TRP:CD1	2.39	0.41
39:1n:163:PRO:HA	39:1n:164:PRO:HD3	1.96	0.41
41:1p:6:LYS:HE2	41:1p:6:LYS:HB2	1.69	0.41
44:1s:40:ASN:HB3	44:1s:43:HIS:ND1	2.36	0.41
44:1s:47:SER:H	44:1s:50:THR:CG2	2.33	0.41
2:1B:49:THR:HG22	2:1B:76:PHE:HB3	2.02	0.41
47:1B:201:SF4:S1	4:1D:105:ARG:HD3	2.60	0.41
3:1C:96:LEU:HB2	3:1C:105:ILE:CG2	2.50	0.41
4:1D:35:ASP:OD2	14:1N:176:ARG:NH2	2.45	0.41
4:1D:151:ILE:HG21	4:1D:174:ARG:HB2	2.03	0.41
4:1D:169:TRP:HH2	8:1H:31:MET:O	2.04	0.41
4:1D:243:GLY:O	4:1D:296:ARG:NH2	2.53	0.41
5:1E:41:GLY:HA3	44:1s:68:SER:HB3	2.03	0.41
5:1E:48:LEU:HD11	5:1E:87:TYR:CE2	2.56	0.41
5:1E:91:ASN:OD1	5:1E:91:ASN:N	2.54	0.41
5:1E:169:ILE:C	5:1E:169:ILE:HD12	2.46	0.41
5:1E:172:ILE:HG13	5:1E:182:PRO:CG	2.51	0.41
6:1F:256:PHE:CD2	6:1F:270:GLU:HB3	2.55	0.41
6:1F:304:THR:HB	6:1F:327:THR:OG1	2.21	0.41
6:1F:345:LYS:HE3	6:1F:345:LYS:HB3	1.91	0.41
7:1G:170:ASP:OD1	7:1G:170:ASP:N	2.36	0.41
7:1G:276:ARG:HA	42:1q:135:GLN:HE22	1.86	0.41
7:1G:339:ASP:HA	19:1S:16:ARG:HH22	1.86	0.41
7:1G:634:ASP:OD1	7:1G:634:ASP:O	2.39	0.41
8:1H:191:ALA:HA	8:1H:198:PHE:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:257:ILE:HD13	26:1a:17:PHE:HZ	1.86	0.41
8:1H:261:LEU:HD13	8:1H:261:LEU:HA	1.92	0.41
8:1H:299:ALA:HA	8:1H:302:MET:HE3	2.03	0.41
8:1H:300:LEU:HD12	8:1H:300:LEU:H	1.85	0.41
46:1I:203:PC1:O21	46:1I:203:PC1:H322	2.19	0.41
11:1K:22:TYR:HE1	12:1L:588:PHE:CG	2.39	0.41
11:1K:25:HIS:HB2	11:1K:88:ASP:OD2	2.20	0.41
12:1L:172:ILE:HD11	12:1L:176:ARG:HH21	1.86	0.41
12:1L:426:ILE:HD12	12:1L:426:ILE:HA	1.80	0.41
13:1M:32:LEU:HD23	13:1M:32:LEU:HA	1.90	0.41
13:1M:107:ILE:HD12	13:1M:107:ILE:HA	1.87	0.41
13:1M:210:TYR:HB2	13:1M:268:GLY:HA3	2.02	0.41
13:1M:390:ASN:O	13:1M:393:ILE:HG22	2.21	0.41
13:1M:401:MET:O	13:1M:405:LEU:HD23	2.21	0.41
14:1N:147:GLN:HB2	33:1h:125:TYR:CD2	2.56	0.41
14:1N:156:THR:O	14:1N:160:LEU:HD12	2.21	0.41
14:1N:205:LEU:O	14:1N:209:ILE:HG12	2.21	0.41
14:1N:324:LYS:H	14:1N:324:LYS:HG2	1.52	0.41
16:1P:51:CYS:SG	16:1P:52:GLU:N	2.94	0.41
16:1P:59:LEU:HB2	16:1P:70:PHE:HZ	1.85	0.41
16:1P:134:HIS:CE1	54:1P:501:NDP:H41N	2.56	0.41
16:1P:171:ILE:HD12	16:1P:171:ILE:HA	1.86	0.41
16:1P:282:ASP:CG	16:1P:286:ARG:HH12	2.29	0.41
18:1R:13:HIS:HA	18:1R:39:PHE:CE2	2.56	0.41
19:1S:12:LYS:CD	19:1S:13:LEU:H	2.33	0.41
20:1T:27:PRO:HA	20:1T:30:LEU:HB3	2.02	0.41
20:1U:14:ARG:HG2	20:1U:58:PHE:HE1	1.86	0.41
20:1U:87:TYR:CZ	34:1i:22:LEU:HD21	2.55	0.41
22:1W:72:HIS:CD2	22:1W:72:HIS:N	2.89	0.41
51:1X:201:CDL:H612	51:1X:201:CDL:H232	2.03	0.41
25:1Z:97:ILE:HD13	30:1e:91:TYR:CD2	2.56	0.41
29:1d:36:PHE:CD1	29:1d:36:PHE:C	2.98	0.41
30:1e:6:GLN:CD	30:1e:13:LEU:HB2	2.46	0.41
30:1e:68:ARG:NH1	30:1e:71:THR:OG1	2.54	0.41
30:1e:87:LYS:HE3	30:1e:87:LYS:HB3	1.92	0.41
32:1g:68:ILE:HA	32:1g:72:LEU:HG	2.02	0.41
38:1m:84:LYS:O	38:1m:88:LEU:HD23	2.21	0.41
39:1n:139:LEU:O	39:1n:142:GLU:HG2	2.21	0.41
43:1r:19:LEU:H	43:1r:19:LEU:HD12	1.86	0.41
44:1s:58:LEU:HD11	44:1s:62:ARG:NH1	2.35	0.41
2:1B:80:PRO:C	2:1B:82:GLN:H	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:116:PRO:C	3:1C:117:ILE:HD13	2.46	0.41
4:1D:63:ARG:HB3	4:1D:79:HIS:HB2	2.01	0.41
4:1D:176:LYS:HE3	4:1D:176:LYS:HB3	1.87	0.41
6:1F:82:MET:HB2	6:1F:129:MET:HG3	2.03	0.41
6:1F:376:MET:HB2	6:1F:392:LEU:HD11	2.02	0.41
8:1H:74:ALA:O	8:1H:115:SER:HB2	2.21	0.41
8:1H:135:ALA:O	8:1H:139:THR:HG22	2.20	0.41
8:1H:294:LEU:O	8:1H:298:LEU:HG	2.21	0.41
10:1J:17:PHE:CD2	11:1K:11:ALA:HB1	2.56	0.41
10:1J:120:ASN:OD1	10:1J:121:GLY:N	2.48	0.41
12:1L:204:LEU:HD21	38:1m:124:PHE:CD2	2.56	0.41
13:1M:19:LYS:O	13:1M:23:ILE:HG23	2.20	0.41
13:1M:31:SER:HB3	13:1M:73:LEU:HD12	2.03	0.41
13:1M:225:ILE:H	13:1M:225:ILE:HD12	1.86	0.41
16:1P:14:SER:OG	16:1P:64:ASP:OD2	2.38	0.41
17:1Q:20:THR:HA	17:1Q:23:THR:HG22	2.01	0.41
20:1U:26:ASP:HA	20:1U:27:PRO:HD3	1.92	0.41
21:1V:63:ASP:OD1	21:1V:63:ASP:C	2.64	0.41
29:1d:14:LEU:HD11	29:1d:77:LYS:CB	2.49	0.41
32:1g:113:PHE:N	41:1p:158:GLN:HE22	2.10	0.41
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.53	0.41
33:1h:138:LYS:HB2	33:1h:143:ASN:HD21	1.86	0.41
40:1o:14:LYS:HA	40:1o:112:LYS:NZ	2.36	0.41
1:1A:88:LEU:O	1:1A:92:LEU:HB2	2.21	0.40
4:1D:76:CYS:SG	4:1D:403:ASP:HA	2.61	0.40
5:1E:196:ALA:HB3	6:1F:264:HIS:HD1	1.86	0.40
6:1F:228:VAL:O	6:1F:232:PRO:HD3	2.21	0.40
7:1G:51:ASN:OD1	7:1G:51:ASN:N	2.54	0.40
7:1G:651:LEU:HD23	7:1G:651:LEU:HA	1.88	0.40
8:1H:121:TRP:HD1	8:1H:121:TRP:O	2.04	0.40
8:1H:140:ILE:HD13	8:1H:140:ILE:HA	1.94	0.40
9:1I:70:TYR:OH	18:1R:68:HIS:HB3	2.21	0.40
9:1I:146:GLU:OE1	9:1I:146:GLU:HA	2.21	0.40
11:1K:22:TYR:CE1	12:1L:584:ILE:HG22	2.56	0.40
11:1K:94:ASN:C	11:1K:94:ASN:OD1	2.63	0.40
12:1L:82:MET:N	12:1L:82:MET:HE2	2.36	0.40
12:1L:210:ASN:O	12:1L:214:ILE:HG22	2.21	0.40
12:1L:353:GLU:OE2	12:1L:354:GLN:N	2.55	0.40
15:1O:49:ARG:N	15:1O:120:GLN:HE22	2.19	0.40
22:1W:69:LYS:HG2	22:1W:70:ASN:ND2	2.36	0.40
24:1Y:46:ALA:HB3	24:1Y:50:GLU:OE2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:97:ILE:HD13	30:1e:91:TYR:HD2	1.86	0.40
25:1Z:97:ILE:HG23	25:1Z:98:MET:HE3	2.02	0.40
26:1a:40:HIS:N	26:1a:44:GLN:OE1	2.54	0.40
28:1c:46:ASN:HB2	28:1c:48:LEU:HD22	2.03	0.40
29:1d:42:GLY:HA2	29:1d:64:TYR:CD2	2.56	0.40
34:1i:34:LEU:HD22	34:1i:35:PRO:HD2	2.03	0.40
35:1j:34:PHE:CD1	35:1j:34:PHE:C	2.99	0.40
37:1l:126:GLN:O	37:1l:128:VAL:N	2.53	0.40
40:1o:44:GLU:HA	40:1o:47:ASP:HB2	2.03	0.40
40:1o:49:GLN:HB3	41:1p:118:GLU:HB2	2.03	0.40
1:1A:106:TRP:CD1	1:1A:106:TRP:C	2.99	0.40
4:1D:128:ILE:HD13	4:1D:128:ILE:HA	1.94	0.40
4:1D:165:THR:HG21	8:1H:275:ALA:HB1	2.02	0.40
4:1D:177:MET:HA	4:1D:180:PHE:HD2	1.86	0.40
4:1D:335:ARG:NH2	9:1I:126:CYS:O	2.44	0.40
7:1G:496:ILE:HD13	7:1G:496:ILE:HA	1.89	0.40
8:1H:260:VAL:HG22	26:1a:16:LEU:HB3	2.04	0.40
9:1I:27:TRP:HB3	9:1I:30:LEU:HB3	2.02	0.40
10:1J:17:PHE:CE2	11:1K:39:SER:HB3	2.56	0.40
13:1M:2:LEU:HD23	31:1f:27:ASP:HA	2.02	0.40
13:1M:449:LEU:HD22	13:1M:449:LEU:H	1.87	0.40
14:1N:86:ILE:HD12	14:1N:86:ILE:HA	1.81	0.40
15:1O:259:LEU:HD23	15:1O:259:LEU:HA	1.94	0.40
16:1P:196:LEU:HD23	16:1P:196:LEU:HA	1.90	0.40
16:1P:222:ASP:N	16:1P:222:ASP:OD1	2.53	0.40
20:1T:66:ASP:HB3	20:1T:79:TYR:CE1	2.56	0.40
24:1Y:103:ARG:HA	24:1Y:103:ARG:HH11	1.87	0.40
45:1Y:802:3PE:H321	45:1Y:802:3PE:H31	1.62	0.40
25:1Z:105:LYS:HB3	25:1Z:108:GLU:HB3	2.03	0.40
37:1l:121:ILE:HD12	37:1l:121:ILE:C	2.46	0.40
43:1r:50:ASN:O	43:1r:50:ASN:ND2	2.54	0.40
1:1A:7:LEU:O	1:1A:11:VAL:HG13	2.21	0.40
2:1B:158:TYR:CZ	42:1q:116:ASN:ND2	2.88	0.40
3:1C:58:ILE:CG2	3:1C:59:PRO:HD3	2.51	0.40
6:1F:143:TYR:CZ	44:1s:51:PHE:HB2	2.56	0.40
6:1F:257:ASN:HA	6:1F:267:THR:HA	2.04	0.40
8:1H:141:SER:HA	8:1H:290:TRP:HE1	1.86	0.40
8:1H:150:LEU:HD23	8:1H:150:LEU:HA	1.92	0.40
8:1H:253:GLU:O	8:1H:256:THR:OG1	2.36	0.40
10:1J:157:THR:O	10:1J:161:LEU:HD23	2.21	0.40
12:1L:94:LEU:HA	12:1L:97:THR:HG22	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:552:LEU:HG	12:1L:553:LEU:HD23	2.02	0.40
14:1N:62:THR:HG21	14:1N:114:TRP:HB3	2.04	0.40
14:1N:128:LEU:HD21	14:1N:213:LEU:HA	2.03	0.40
16:1P:35:VAL:HG23	16:1P:62:MET:HG2	2.04	0.40
16:1P:269:LEU:HD12	16:1P:269:LEU:H	1.85	0.40
17:1Q:79:LEU:HD12	17:1Q:82:LEU:HD23	2.03	0.40
19:1S:33:ARG:O	19:1S:37:GLU:HG3	2.21	0.40
19:1S:68:TYR:N	19:1S:72:GLN:O	2.54	0.40
20:1T:12:LYS:NZ	20:1T:77:VAL:HG11	2.37	0.40
24:1Y:21:ALA:O	24:1Y:25:THR:HG23	2.20	0.40
30:1e:12:ASP:OD1	30:1e:12:ASP:C	2.65	0.40
31:1f:16:VAL:HB	31:1f:17:PRO:HD3	2.03	0.40
32:1g:49:LYS:HD3	32:1g:49:LYS:O	2.20	0.40
33:1h:105:LEU:HD23	33:1h:105:LEU:HA	1.90	0.40
38:1m:2:PHE:CE1	39:1n:68:GLU:HG2	2.57	0.40
39:1n:80:ILE:HD11	39:1n:84:SER:OG	2.21	0.40
2:1B:55:CYS:SG	2:1B:117:GLY:HA3	2.62	0.40
4:1D:36:VAL:HG23	14:1N:50:PRO:HD2	2.02	0.40
4:1D:43:LEU:HD23	4:1D:43:LEU:HA	1.79	0.40
5:1E:73:LEU:HB3	5:1E:75:VAL:HG23	2.03	0.40
5:1E:126:ILE:HD11	5:1E:130:GLU:HB2	2.02	0.40
6:1F:13:GLY:HA3	6:1F:274:VAL:HG22	2.03	0.40
6:1F:49:LEU:HD13	6:1F:127:ARG:HB2	2.03	0.40
6:1F:81:PHE:HD1	6:1F:81:PHE:HA	1.81	0.40
6:1F:134:ALA:HB3	6:1F:175:VAL:HA	2.02	0.40
7:1G:158:ARG:HA	7:1G:161:ARG:HH21	1.86	0.40
7:1G:201:ASP:HA	17:1Q:45:MET:CG	2.51	0.40
7:1G:333:ASP:HA	7:1G:336:ASN:HB2	2.04	0.40
7:1G:651:LEU:O	7:1G:653:ASN:N	2.54	0.40
8:1H:55:LEU:HD23	8:1H:55:LEU:HA	1.82	0.40
13:1M:25:ILE:O	13:1M:29:VAL:HG13	2.21	0.40
13:1M:86:LYS:HE3	13:1M:86:LYS:HB3	1.99	0.40
13:1M:344:LEU:HD13	38:1m:64:LEU:HD22	2.03	0.40
14:1N:122:ILE:O	14:1N:176:ARG:NH1	2.54	0.40
14:1N:162:ILE:HA	14:1N:185:ALA:HA	2.03	0.40
16:1P:169:SER:HB3	16:1P:231:VAL:HG23	2.03	0.40
16:1P:216:ASN:HA	16:1P:219:LYS:HZ1	1.86	0.40
32:1g:68:ILE:HG22	32:1g:72:LEU:HD12	2.02	0.40
32:1g:92:GLU:HB3	41:1p:64:HIS:NE2	2.35	0.40
33:1h:98:ALA:HB2	41:1p:81:ILE:HG13	2.03	0.40
40:1o:3:HIS:HA	40:1o:6:ARG:HH21	1.85	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:143:SER:O	41:1p:144:ASP:HB3	2.21	0.40
42:1q:72:ASP:OD1	42:1q:72:ASP:C	2.64	0.40
1:1A:41:PHE:HD2	4:1D:50:ASN:HD21	1.69	0.40
2:1B:41:ARG:NH1	2:1B:110:PRO:HG3	2.36	0.40
2:1B:78:ALA:O	4:1D:54:GLN:NE2	2.50	0.40
4:1D:51:PHE:HB3	4:1D:64:LEU:HB3	2.03	0.40
6:1F:68:ARG:HA	6:1F:68:ARG:HD3	1.68	0.40
6:1F:321:ALA:CA	6:1F:324:GLN:HE21	2.30	0.40
7:1G:94:MET:HE1	7:1G:116:LEU:HD22	2.03	0.40
8:1H:27:VAL:HA	26:1a:5:ILE:HD11	2.04	0.40
8:1H:31:MET:HE2	8:1H:31:MET:HB2	1.81	0.40
8:1H:231:ILE:HD11	8:1H:270:PHE:HB3	2.03	0.40
11:1K:53:PHE:HE1	11:1K:55:LEU:HB2	1.87	0.40
12:1L:103:PHE:CE2	12:1L:242:PRO:HG3	2.56	0.40
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	2.02	0.40
13:1M:72:LEU:HD21	13:1M:233:ALA:HB3	2.04	0.40
16:1P:311:GLU:H	16:1P:311:GLU:CD	2.26	0.40
17:1Q:26:PRO:HG2	17:1Q:29:HIS:HD2	1.86	0.40
19:1S:44:LYS:HA	19:1S:44:LYS:HD2	1.77	0.40
20:1U:3:ALA:HA	20:1U:4:PRO:HD3	1.99	0.40
27:1b:29:ILE:O	27:1b:32:PRO:HD2	2.22	0.40
29:1d:106:LYS:H	29:1d:106:LYS:HG2	1.70	0.40
33:1h:51:GLU:OE2	41:1p:59:ARG:NE	2.54	0.40
33:1h:62:GLU:H	33:1h:62:GLU:HG3	1.73	0.40
37:1l:9:PHE:HD2	38:1m:69:TYR:HD2	1.68	0.40
37:1l:131:LYS:HA	40:1o:97:ARG:HH22	1.86	0.40
40:1o:51:MET:O	40:1o:55:ARG:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	106 (94%)	6 (5%)	1 (1%)	14	45
2	1B	153/258 (59%)	145 (95%)	8 (5%)	0	100	100
3	1C	207/264 (78%)	191 (92%)	15 (7%)	1 (0%)	24	57
4	1D	427/430 (99%)	406 (95%)	21 (5%)	0	100	100
5	1E	212/249 (85%)	184 (87%)	27 (13%)	1 (0%)	24	57
6	1F	430/464 (93%)	408 (95%)	21 (5%)	1 (0%)	43	73
7	1G	697/727 (96%)	648 (93%)	47 (7%)	2 (0%)	36	67
8	1H	315/318 (99%)	297 (94%)	17 (5%)	1 (0%)	36	67
9	1I	174/239 (73%)	159 (91%)	15 (9%)	0	100	100
10	1J	171/175 (98%)	159 (93%)	9 (5%)	3 (2%)	6	33
11	1K	95/98 (97%)	88 (93%)	7 (7%)	0	100	100
12	1L	603/606 (100%)	554 (92%)	48 (8%)	1 (0%)	43	73
13	1M	456/459 (99%)	432 (95%)	24 (5%)	0	100	100
14	1N	344/347 (99%)	321 (93%)	23 (7%)	0	100	100
15	1O	318/357 (89%)	305 (96%)	13 (4%)	0	100	100
16	1P	340/377 (90%)	326 (96%)	14 (4%)	0	100	100
17	1Q	127/175 (73%)	118 (93%)	9 (7%)	0	100	100
18	1R	94/123 (76%)	90 (96%)	4 (4%)	0	100	100
19	1S	85/99 (86%)	83 (98%)	2 (2%)	0	100	100
20	1T	83/156 (53%)	78 (94%)	5 (6%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	100 (88%)	12 (11%)	1 (1%)	14	45
22	1W	113/128 (88%)	106 (94%)	6 (5%)	1 (1%)	14	45
23	1X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	1Y	137/141 (97%)	133 (97%)	3 (2%)	1 (1%)	18	51
25	1Z	139/144 (96%)	134 (96%)	5 (4%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/122 (96%)	107 (92%)	9 (8%)	1 (1%)	14	45
30	1e	97/106 (92%)	84 (87%)	12 (12%)	1 (1%)	12	43
31	1f	55/58 (95%)	49 (89%)	6 (11%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
32	1g	98/154 (64%)	84 (86%)	14 (14%)	0	100	100
33	1h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	1i	126/128 (98%)	118 (94%)	7 (6%)	1 (1%)	16	48
35	1j	69/105 (66%)	63 (91%)	6 (9%)	0	100	100
36	1k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	1l	154/186 (83%)	141 (92%)	13 (8%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	21	54
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
41	1p	171/176 (97%)	164 (96%)	7 (4%)	0	100	100
42	1q	143/145 (99%)	136 (95%)	7 (5%)	0	100	100
43	1r	90/112 (80%)	84 (93%)	6 (7%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
All	All	8189/9618 (85%)	7661 (94%)	510 (6%)	18 (0%)	44	73

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	46	SER
3	1C	89	ARG
7	1G	499	GLN
8	1H	208	VAL
10	1J	4	TYR
12	1L	30	ASN
24	1Y	46	ALA
30	1e	18	THR
7	1G	416	THR
10	1J	116	ILE
29	1d	3	SER
6	1F	33	LEU
34	1i	5	PRO
21	1V	108	ALA
5	1E	157	ASN
10	1J	151	THR
22	1W	96	VAL
39	1n	31	VAL

5.3.2 Protein sidechains ⓘ

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	100/100 (100%)	99 (99%)	1 (1%)	68	74
2	1B	131/212 (62%)	129 (98%)	2 (2%)	57	69
3	1C	191/228 (84%)	188 (98%)	3 (2%)	55	68
4	1D	371/371 (100%)	371 (100%)	0	100	100
5	1E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	346 (100%)	0	100	100
7	1G	588/610 (96%)	586 (100%)	2 (0%)	86	84
8	1H	274/275 (100%)	270 (98%)	4 (2%)	57	69
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	139/141 (99%)	139 (100%)	0	100	100
11	1K	84/85 (99%)	82 (98%)	2 (2%)	43	62
12	1L	539/540 (100%)	535 (99%)	4 (1%)	76	77
13	1M	408/409 (100%)	405 (99%)	3 (1%)	76	77
14	1N	310/311 (100%)	308 (99%)	2 (1%)	78	79
15	1O	283/307 (92%)	283 (100%)	0	100	100
16	1P	296/323 (92%)	294 (99%)	2 (1%)	76	77
17	1Q	117/152 (77%)	117 (100%)	0	100	100
18	1R	79/97 (81%)	78 (99%)	1 (1%)	61	71
19	1S	77/82 (94%)	77 (100%)	0	100	100
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	78 (99%)	1 (1%)	61	71
21	1V	100/101 (99%)	99 (99%)	1 (1%)	68	74
22	1W	107/112 (96%)	105 (98%)	2 (2%)	50	66
23	1X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	100 (99%)	1 (1%)	68	74
25	1Z	123/124 (99%)	122 (99%)	1 (1%)	73	76

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%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	106/109 (97%)	103 (97%)	3 (3%)	38	58
30	1e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/55 (98%)	53 (98%)	1 (2%)	50	66
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	73
33	1h	121/158 (77%)	119 (98%)	2 (2%)	53	67
34	1i	120/120 (100%)	118 (98%)	2 (2%)	53	67
35	1j	62/84 (74%)	61 (98%)	1 (2%)	55	68
36	1k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	141 (100%)	0	100	100
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%)	109 (99%)	1 (1%)	70	74
41	1p	154/156 (99%)	154 (100%)	0	100	100
42	1q	131/131 (100%)	130 (99%)	1 (1%)	73	76
43	1r	85/97 (88%)	84 (99%)	1 (1%)	63	72
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7220/8187 (88%)	7175 (99%)	45 (1%)	76	79

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	68	GLU
2	1B	162	GLN
2	1B	173	LEU
3	1C	71	GLN
3	1C	85	THR
3	1C	175	ARG
7	1G	493	LEU
7	1G	666	LEU
8	1H	46	LEU
8	1H	183	MET
8	1H	286	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1H	287	HIS
11	1K	47	ILE
11	1K	61	ILE
12	1L	133	THR
12	1L	206	ASN
12	1L	274	GLN
12	1L	359	MET
13	1M	42	LEU
13	1M	75	LEU
13	1M	214	LEU
14	1N	9	LEU
14	1N	266	ILE
16	1P	201	VAL
16	1P	236	TYR
18	1R	75	LEU
20	1U	33	ASN
21	1V	13	LEU
22	1W	18	LYS
22	1W	72	HIS
24	1Y	114	CYS
25	1Z	10	MET
29	1d	2	MET
29	1d	19	ARG
29	1d	86	ARG
31	1f	51	ASN
32	1g	36	ASN
33	1h	24	LEU
33	1h	80	TYR
34	1i	5	PRO
34	1i	9	LEU
35	1j	38	TRP
40	1o	63	ILE
42	1q	27	LEU
43	1r	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	28	ASN
2	1B	94	ASN
2	1B	162	GLN
3	1C	88	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1C	192	GLN
4	1D	5	GLN
4	1D	129	GLN
4	1D	149	ASN
5	1E	55	GLN
5	1E	57	GLN
5	1E	99	HIS
6	1F	324	GLN
6	1F	438	GLN
7	1G	182	GLN
7	1G	402	ASN
7	1G	472	ASN
7	1G	475	GLN
7	1G	517	ASN
7	1G	581	GLN
8	1H	5	ASN
8	1H	157	ASN
8	1H	194	ASN
8	1H	235	ASN
8	1H	258	ASN
10	1J	175	ASN
11	1K	25	HIS
12	1L	109	HIS
12	1L	139	GLN
12	1L	199	GLN
12	1L	205	ASN
12	1L	210	ASN
12	1L	447	ASN
12	1L	518	GLN
12	1L	541	ASN
13	1M	20	HIS
13	1M	220	HIS
13	1M	424	ASN
14	1N	171	ASN
14	1N	310	ASN
14	1N	322	GLN
15	1O	97	GLN
15	1O	309	ASN
16	1P	103	ASN
16	1P	203	GLN
16	1P	234	ASN
16	1P	341	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1Q	44	ASN
18	1R	36	ASN
19	1S	21	HIS
19	1S	72	GLN
20	1T	47	GLN
21	1V	72	GLN
22	1W	51	GLN
22	1W	72	HIS
23	1X	94	GLN
24	1Y	128	GLN
25	1Z	85	GLN
29	1d	79	GLN
30	1e	44	HIS
32	1g	57	ASN
32	1g	86	GLN
33	1h	44	ASN
33	1h	69	HIS
33	1h	143	ASN
34	1i	12	GLN
34	1i	13	GLN
34	1i	47	ASN
34	1i	127	HIS
35	1j	13	GLN
35	1j	42	HIS
37	1l	3	HIS
37	1l	87	ASN
38	1m	74	ASN
39	1n	25	HIS
41	1p	106	GLN
41	1p	133	GLN
41	1p	158	GLN
42	1q	13	GLN
42	1q	31	ASN
42	1q	54	GLN
42	1q	116	ASN
42	1q	123	GLN
43	1r	109	GLN
44	1s	44	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 46 ligands modelled in this entry, 3 are monoatomic - leaving 43 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	$\# Z > 2$
45	3PE	1L	704	-	41,41,50	0.30	0	44,46,55	0.36	0
47	SF4	1G	802	7	0,12,12	-	-	-		
46	PC1	1M	502	-	34,34,53	0.32	0	40,42,61	0.36	0
52	GTP	1O	401	53	33,34,34	0.60	0	50,54,54	0.61	0
51	CDL	1L	702	-	75,75,99	0.31	0	81,87,111	0.37	0
46	PC1	1B	203	-	47,47,53	0.27	0	53,55,61	0.37	0
47	SF4	1I	202	9	0,12,12	-	-	-		
46	PC1	1A	202	-	25,25,53	0.36	0	29,32,61	0.53	0
49	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.65	1 (2%)
46	PC1	1I	203	-	43,43,53	0.30	0	49,51,61	0.43	0
45	3PE	1Y	804	-	34,34,50	0.31	0	37,39,55	0.57	1 (2%)
48	FES	1G	803	7	0,4,4	-	-	-		
46	PC1	1L	703	-	37,37,53	0.29	0	43,45,61	0.32	0
46	PC1	1h	201	33	46,46,53	0.28	0	52,54,61	0.30	0
47	SF4	1B	201	2	0,12,12	-	-	-		
51	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.43	0
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.33	0
45	3PE	1L	701	-	45,45,50	0.28	0	48,50,55	0.38	0
45	3PE	1A	201	-	30,30,50	0.33	0	33,35,55	0.40	0
47	SF4	1F	502	6	0,12,12	-	-	-		
54	NDP	1P	501	-	51,52,52	0.50	0	71,80,80	0.78	1 (1%)
46	PC1	1d	201	-	38,38,53	0.31	0	44,46,61	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	1I	201	9	0,12,12	-	-	-		
45	3PE	1M	503	-	37,37,50	0.30	0	40,42,55	0.39	0
46	PC1	1f	101	31,13	33,33,53	0.30	0	39,41,61	0.36	0
51	CDL	1N	401	-	64,64,99	0.32	0	70,76,111	0.36	0
46	PC1	1Y	803	-	45,45,53	0.28	0	51,53,61	0.33	0
45	3PE	1Y	802	-	39,39,50	0.30	0	42,44,55	0.37	0
46	PC1	1H	401	-	53,53,53	0.27	0	59,61,61	0.40	0
51	CDL	1H	402	-	50,50,99	0.36	0	56,62,111	0.54	1 (1%)
45	3PE	1Y	801	-	30,30,50	0.35	0	33,35,55	1.28	4 (12%)
51	CDL	1N	402	-	66,66,99	0.30	0	72,78,111	0.46	0
51	CDL	1X	201	-	85,85,99	0.29	0	91,97,111	0.33	0
45	3PE	1D	901	-	45,45,50	0.28	0	48,50,55	0.33	0
48	FES	1E	301	5	0,4,4	-	-	-		
56	EHZ	1n	201	-	31,36,37	0.17	0	36,44,47	1.14	1 (2%)
45	3PE	1f	102	-	50,50,50	0.29	0	53,55,55	0.99	3 (5%)
46	PC1	1J	201	-	31,31,53	0.33	0	37,39,61	0.35	0
56	EHZ	1W	201	-	31,36,37	0.21	0	36,44,47	1.44	1 (2%)
57	MYR	1l	201	-	13,14,15	0.30	0	12,13,15	0.32	0
45	3PE	1M	501	-	37,37,50	0.31	0	40,42,55	0.46	0
46	PC1	1Z	201	-	33,33,53	0.33	0	39,41,61	0.39	0
47	SF4	1G	801	7	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1L	704	-	-	2/45/45/54	-
47	SF4	1G	802	7	-	-	0/6/5/5
46	PC1	1M	502	-	-	3/38/38/57	-
52	GTP	1O	401	53	-	1/22/38/38	0/3/3/3
51	CDL	1L	702	-	-	10/86/86/110	-
46	PC1	1B	203	-	-	8/51/51/57	-
47	SF4	1I	202	9	-	-	0/6/5/5
46	PC1	1A	202	-	-	4/28/28/57	-
49	FMN	1F	501	-	-	0/18/18/18	0/3/3/3
46	PC1	1I	203	-	-	7/47/47/57	-
45	3PE	1Y	804	-	-	6/38/38/54	-
48	FES	1G	803	7	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	PC1	1L	703	-	-	4/40/40/57	-
46	PC1	1h	201	33	-	18/50/50/57	-
47	SF4	1B	201	2	-	-	0/6/5/5
51	CDL	1a	101	-	-	4/71/71/110	-
46	PC1	1B	202	-	-	9/37/37/57	-
45	3PE	1L	701	-	-	4/49/49/54	-
45	3PE	1A	201	-	-	3/34/34/54	-
54	NDP	1P	501	-	-	9/34/77/77	0/5/5/5
47	SF4	1F	502	6	-	-	0/6/5/5
46	PC1	1d	201	-	-	11/42/42/57	-
47	SF4	1I	201	9	-	-	0/6/5/5
45	3PE	1M	503	-	-	8/41/41/54	-
46	PC1	1f	101	31,13	-	10/36/36/57	-
51	CDL	1N	401	-	-	11/75/75/110	-
46	PC1	1Y	803	-	-	6/49/49/57	-
45	3PE	1Y	802	-	-	11/43/43/54	-
46	PC1	1H	401	-	-	3/57/57/57	-
51	CDL	1H	402	-	-	7/61/61/110	-
45	3PE	1Y	801	-	-	6/34/34/54	-
51	CDL	1N	402	-	-	6/76/76/110	-
51	CDL	1X	201	-	-	19/96/96/110	-
45	3PE	1D	901	-	-	2/49/49/54	-
56	EHZ	1n	201	-	-	7/42/44/45	-
48	FES	1E	301	5	-	-	0/1/1/1
45	3PE	1f	102	-	-	10/54/54/54	-
46	PC1	1J	201	-	-	5/35/35/57	-
56	EHZ	1W	201	-	-	13/42/44/45	-
57	MYR	1l	201	-	-	3/12/12/13	-
45	3PE	1M	501	-	-	6/41/41/54	-
46	PC1	1Z	201	-	-	1/37/37/57	-
47	SF4	1G	801	7	-	-	0/6/5/5

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1W	201	EHZ	C10-S1-C9	8.05	125.63	101.84
56	1n	201	EHZ	C10-S1-C9	6.33	120.56	101.84
45	1Y	801	3PE	O21-C21-C22	5.39	123.14	111.48
45	1f	102	3PE	O21-C21-C22	5.06	122.43	111.48
54	1P	501	NDP	P2B-O2B-C2B	-4.54	111.30	123.43
45	1f	102	3PE	O21-C21-O22	-2.81	117.15	123.70
45	1Y	801	3PE	O21-C21-O22	-2.53	117.78	123.70
45	1f	102	3PE	C2-O21-C21	2.34	123.40	117.80
45	1Y	801	3PE	C2-O21-C21	2.28	123.25	117.80
45	1Y	801	3PE	O21-C2-C3	2.15	116.05	108.34
49	1F	501	FMN	C4-N3-C2	-2.10	121.92	125.64
51	1H	402	CDL	OB6-CB5-C51	2.08	115.99	111.48
45	1Y	804	3PE	O21-C21-C22	2.05	115.91	111.48

There are no chirality outliers.

All (237) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1M	501	3PE	C1-O11-P-O14
45	1M	501	3PE	C12-C11-O13-P
45	1M	503	3PE	C1-O11-P-O13
45	1Y	801	3PE	C2-C1-O11-P
45	1Y	801	3PE	O32-C31-O31-C3
45	1Y	801	3PE	C32-C31-O31-C3
45	1Y	801	3PE	O22-C21-O21-C2
45	1Y	801	3PE	C22-C21-O21-C2
45	1Y	802	3PE	C1-O11-P-O14
45	1Y	802	3PE	O21-C2-C3-O31
45	1Y	802	3PE	O32-C31-O31-C3
45	1Y	802	3PE	C32-C31-O31-C3
45	1Y	804	3PE	O22-C21-O21-C2
45	1Y	804	3PE	C22-C21-O21-C2
45	1f	102	3PE	C2-C1-O11-P
45	1f	102	3PE	O22-C21-O21-C2
45	1f	102	3PE	C22-C21-O21-C2
46	1A	202	PC1	C11-O13-P-O12
46	1A	202	PC1	C11-O13-P-O11
46	1A	202	PC1	C12-C11-O13-P
46	1B	202	PC1	C11-O13-P-O14
46	1B	202	PC1	C1-O11-P-O13
46	1B	202	PC1	C2-C1-O11-P
46	1B	202	PC1	O32-C31-O31-C3
46	1B	202	PC1	C32-C31-O31-C3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	1B	203	PC1	C11-O13-P-O14
46	1I	203	PC1	C11-O13-P-O11
46	1I	203	PC1	C1-O11-P-O14
46	1I	203	PC1	O32-C31-O31-C3
46	1I	203	PC1	C32-C31-O31-C3
46	1J	201	PC1	C11-O13-P-O12
46	1J	201	PC1	C11-O13-P-O14
46	1J	201	PC1	C11-O13-P-O11
46	1L	703	PC1	C11-O13-P-O14
46	1M	502	PC1	C1-O11-P-O14
46	1Y	803	PC1	C11-O13-P-O14
46	1Y	803	PC1	C1-O11-P-O14
46	1d	201	PC1	C11-O13-P-O14
46	1d	201	PC1	C11-O13-P-O11
46	1d	201	PC1	O13-C11-C12-N
46	1d	201	PC1	O22-C21-O21-C2
46	1d	201	PC1	C22-C21-O21-C2
46	1d	201	PC1	O32-C31-O31-C3
46	1d	201	PC1	C32-C31-O31-C3
46	1f	101	PC1	C11-O13-P-O11
46	1f	101	PC1	C2-C1-O11-P
46	1f	101	PC1	O32-C31-O31-C3
46	1f	101	PC1	C32-C31-O31-C3
46	1h	201	PC1	C11-O13-P-O12
46	1h	201	PC1	C11-O13-P-O14
46	1h	201	PC1	C11-O13-P-O11
46	1h	201	PC1	C2-C1-O11-P
46	1h	201	PC1	O32-C31-O31-C3
46	1h	201	PC1	C32-C31-O31-C3
51	1H	402	CDL	C1-CA2-OA2-PA1
51	1H	402	CDL	CA3-OA5-PA1-OA3
51	1H	402	CDL	OB7-CB5-OB6-CB4
51	1H	402	CDL	C51-CB5-OB6-CB4
51	1L	702	CDL	C1-CA2-OA2-PA1
51	1L	702	CDL	OA6-CA4-CA6-OA8
51	1N	401	CDL	CB2-OB2-PB2-OB3
51	1N	402	CDL	CB2-OB2-PB2-OB4
51	1N	402	CDL	CB2-OB2-PB2-OB5
51	1X	201	CDL	CA2-OA2-PA1-OA3
51	1X	201	CDL	CA2-OA2-PA1-OA4
51	1X	201	CDL	CA2-OA2-PA1-OA5
51	1X	201	CDL	CA3-OA5-PA1-OA3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	1X	201	CDL	CA4-CA3-OA5-PA1
51	1X	201	CDL	C1-CB2-OB2-PB2
51	1X	201	CDL	OB9-CB7-OB8-CB6
51	1X	201	CDL	C71-CB7-OB8-CB6
51	1a	101	CDL	CA3-OA5-PA1-OA3
54	1P	501	NDP	C5D-O5D-PN-O1N
56	1W	201	EHZ	N2-C15-C16-C17
56	1W	201	EHZ	N2-C15-C16-O5
56	1W	201	EHZ	O4-C15-C16-C17
56	1W	201	EHZ	O4-C15-C16-O5
56	1W	201	EHZ	C15-C16-C17-C19
56	1W	201	EHZ	C16-C17-C20-O6
56	1W	201	EHZ	C18-C17-C20-O6
56	1W	201	EHZ	C19-C17-C20-O6
56	1W	201	EHZ	O2-C9-S1-C10
56	1W	201	EHZ	C8-C9-S1-C10
56	1n	201	EHZ	C7-C8-C9-S1
56	1n	201	EHZ	O2-C9-S1-C10
56	1n	201	EHZ	C8-C9-S1-C10
57	1l	201	MYR	O1-C1-C2-C3
54	1P	501	NDP	C2D-C1D-N1N-C2N
46	1d	201	PC1	C2-C1-O11-P
51	1N	401	CDL	C1-CA2-OA2-PA1
46	1h	201	PC1	C11-C12-N-C13
46	1h	201	PC1	C11-C12-N-C15
46	1B	203	PC1	O21-C2-C3-O31
54	1P	501	NDP	C2D-C1D-N1N-C6N
46	1h	201	PC1	C11-C12-N-C14
46	1f	101	PC1	C37-C38-C39-C3A
45	1M	501	3PE	C25-C26-C27-C28
46	1Z	201	PC1	C21-C22-C23-C24
51	1N	401	CDL	C37-C38-C39-C40
45	1L	704	3PE	C2-C1-O11-P
51	1X	201	CDL	C33-C34-C35-C36
46	1B	203	PC1	C3A-C3B-C3C-C3D
57	1l	201	MYR	C2-C3-C4-C5
45	1f	102	3PE	O21-C2-C3-O31
46	1h	201	PC1	C36-C37-C38-C39
45	1Y	802	3PE	C1-C2-C3-O31
46	1B	203	PC1	C1-C2-C3-O31
45	1Y	804	3PE	C32-C33-C34-C35
46	1I	203	PC1	C21-C22-C23-C24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
45	1D	901	3PE	C24-C25-C26-C27
51	1N	401	CDL	CA4-CA3-OA5-PA1
54	1P	501	NDP	C4B-C5B-O5B-PA
45	1M	503	3PE	O31-C31-C32-C33
46	1Y	803	PC1	C33-C34-C35-C36
51	1X	201	CDL	C60-C61-C62-C63
51	1N	401	CDL	CA3-CA4-CA6-OA8
46	1h	201	PC1	C31-C32-C33-C34
46	1I	203	PC1	C32-C33-C34-C35
46	1f	101	PC1	O11-C1-C2-O21
51	1H	402	CDL	OB5-CB3-CB4-OB6
51	1X	201	CDL	C24-C25-C26-C27
46	1H	401	PC1	C3B-C3C-C3D-C3E
51	1L	702	CDL	C58-C59-C60-C61
51	1H	402	CDL	CA4-CA3-OA5-PA1
51	1N	401	CDL	C1-CB2-OB2-PB2
51	1a	101	CDL	CA4-CA3-OA5-PA1
56	1n	201	EHZ	C3-C4-C5-C6
51	1N	402	CDL	OB6-CB4-CB6-OB8
51	1L	702	CDL	C40-C41-C42-C43
46	1B	202	PC1	C31-C32-C33-C34
51	1L	702	CDL	C54-C55-C56-C57
46	1h	201	PC1	C2B-C2C-C2D-C2E
45	1f	102	3PE	O11-C1-C2-O21
51	1L	702	CDL	CA3-CA4-CA6-OA8
45	1A	201	3PE	C12-C11-O13-P
45	1L	701	3PE	C12-C11-O13-P
45	1L	704	3PE	C12-C11-O13-P
45	1Y	802	3PE	C12-C11-O13-P
45	1Y	804	3PE	C12-C11-O13-P
45	1f	102	3PE	C12-C11-O13-P
46	1B	202	PC1	C12-C11-O13-P
46	1B	203	PC1	C12-C11-O13-P
46	1J	201	PC1	C12-C11-O13-P
46	1Y	803	PC1	C12-C11-O13-P
46	1d	201	PC1	C12-C11-O13-P
46	1h	201	PC1	C12-C11-O13-P
45	1M	503	3PE	O21-C2-C3-O31
46	1B	203	PC1	C39-C3A-C3B-C3C
51	1L	702	CDL	CA4-CA3-OA5-PA1
46	1A	202	PC1	O13-C11-C12-N
46	1J	201	PC1	O13-C11-C12-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	1L	703	PC1	O13-C11-C12-N
46	1Y	803	PC1	O13-C11-C12-N
46	1h	201	PC1	O13-C11-C12-N
51	1X	201	CDL	C52-C51-CB5-OB6
46	1f	101	PC1	C36-C37-C38-C39
51	1N	401	CDL	C42-C43-C44-C45
46	1f	101	PC1	O11-C1-C2-C3
56	1W	201	EHZ	C15-C16-C17-C20
46	1B	203	PC1	C37-C38-C39-C3A
52	1O	401	GTP	C4'-C5'-O5'-PA
45	1M	501	3PE	O11-C1-C2-O21
45	1Y	801	3PE	O11-C1-C2-O21
45	1M	503	3PE	C34-C35-C36-C37
54	1P	501	NDP	O4D-C1D-N1N-C6N
51	1N	401	CDL	OA6-CA4-CA6-OA8
45	1M	503	3PE	C1-C2-C3-O31
56	1W	201	EHZ	C10-C11-N1-C12
45	1A	201	3PE	C11-O13-P-O14
45	1M	503	3PE	C11-O13-P-O14
45	1Y	802	3PE	C1-O11-P-O13
46	1L	703	PC1	C11-O13-P-O11
46	1M	502	PC1	C1-O11-P-O13
46	1d	201	PC1	C11-O13-P-O12
46	1f	101	PC1	C11-O13-P-O14
46	1h	201	PC1	C1-O11-P-O14
51	1L	702	CDL	CA2-OA2-PA1-OA3
51	1N	402	CDL	CA2-OA2-PA1-OA3
56	1n	201	EHZ	O5-C16-C17-C20
51	1N	401	CDL	C32-C33-C34-C35
45	1D	901	3PE	C2-C1-O11-P
51	1X	201	CDL	C1-CA2-OA2-PA1
54	1P	501	NDP	O4D-C1D-N1N-C2N
45	1M	501	3PE	C21-C22-C23-C24
45	1M	501	3PE	O11-C1-C2-C3
45	1Y	802	3PE	O11-C1-C2-C3
45	1Y	802	3PE	O11-C1-C2-O21
45	1Y	804	3PE	C35-C36-C37-C38
46	1Y	803	PC1	C27-C28-C29-C2A
46	1B	203	PC1	C35-C36-C37-C38
46	1B	202	PC1	O21-C21-C22-C23
54	1P	501	NDP	C2B-O2B-P2B-O3X
51	1X	201	CDL	C32-C33-C34-C35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	1d	201	PC1	C33-C34-C35-C36
51	1X	201	CDL	C54-C55-C56-C57
46	1H	401	PC1	C24-C25-C26-C27
45	1L	701	3PE	C35-C36-C37-C38
45	1M	503	3PE	O32-C31-C32-C33
45	1L	701	3PE	C2-C1-O11-P
51	1H	402	CDL	OB5-CB3-CB4-CB6
54	1P	501	NDP	O4D-C4D-C5D-O5D
46	1f	101	PC1	C33-C34-C35-C36
46	1h	201	PC1	C33-C34-C35-C36
51	1X	201	CDL	CB4-CB3-OB5-PB2
51	1N	402	CDL	CB3-CB4-CB6-OB8
57	1l	201	MYR	C6-C7-C8-C9
51	1X	201	CDL	C55-C56-C57-C58
46	1B	202	PC1	O22-C21-C22-C23
51	1L	702	CDL	C31-C32-C33-C34
51	1X	201	CDL	C20-C21-C22-C23
56	1W	201	EHZ	C15-C16-C17-C18
56	1n	201	EHZ	C21-C1-C2-C3
45	1A	201	3PE	C27-C28-C29-C2A
45	1f	102	3PE	C38-C39-C3A-C3B
45	1M	503	3PE	C3A-C3B-C3C-C3D
56	1n	201	EHZ	O5-C16-C17-C18
46	1I	203	PC1	C24-C25-C26-C27
51	1a	101	CDL	CA5-C11-C12-C13
54	1P	501	NDP	O4B-C4B-C5B-O5B
46	1H	401	PC1	C34-C35-C36-C37
46	1L	703	PC1	C22-C23-C24-C25
46	1M	502	PC1	O21-C2-C3-O31
51	1N	401	CDL	OB6-CB4-CB6-OB8
45	1f	102	3PE	O11-C1-C2-C3
46	1h	201	PC1	O31-C31-C32-C33
51	1X	201	CDL	C23-C24-C25-C26
45	1f	102	3PE	C1-C2-O21-C21
51	1N	401	CDL	C38-C39-C40-C41
45	1Y	802	3PE	C27-C28-C29-C2A
45	1Y	804	3PE	C25-C26-C27-C28
51	1L	702	CDL	C52-C51-CB5-OB6
46	1h	201	PC1	O32-C31-C32-C33
45	1L	701	3PE	C28-C29-C2A-C2B
45	1Y	802	3PE	O31-C31-C32-C33
51	1N	402	CDL	C72-C71-CB7-OB8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
51	1a	101	CDL	C52-C51-CB5-OB6
45	1f	102	3PE	C35-C36-C37-C38

There are no ring outliers.

39 monomers are involved in 124 short contacts:

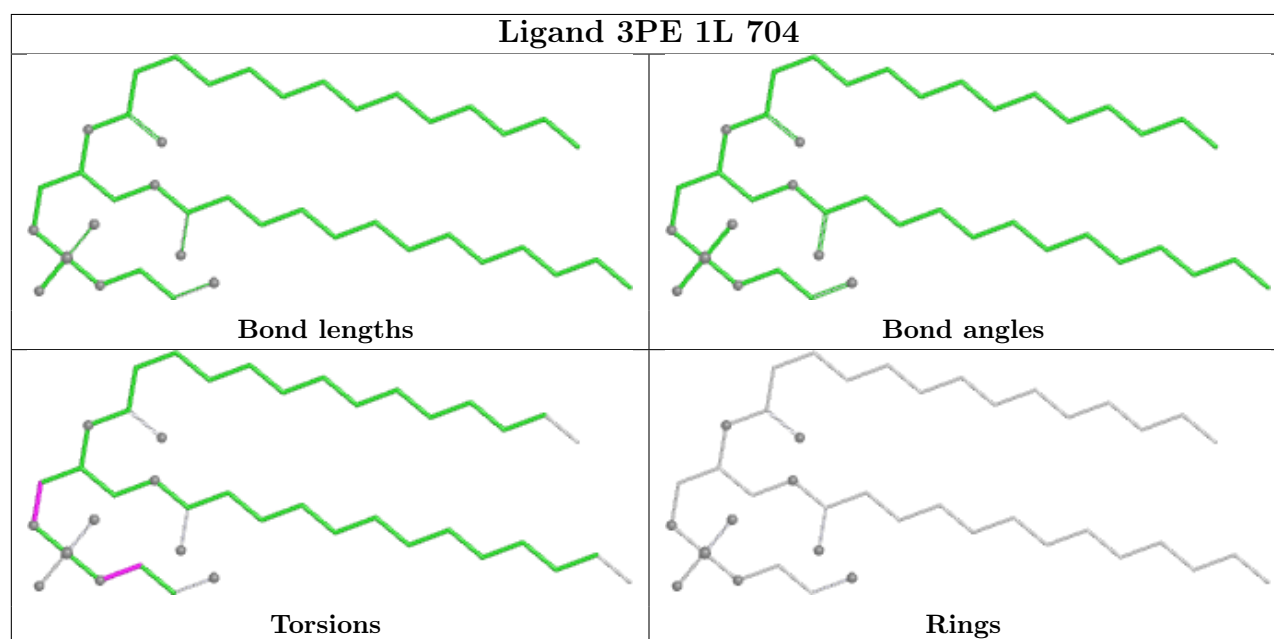
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1L	704	3PE	1	0
46	1M	502	PC1	1	0
52	1O	401	GTP	2	0
51	1L	702	CDL	3	0
46	1A	202	PC1	1	0
49	1F	501	FMN	2	0
46	1I	203	PC1	6	0
45	1Y	804	3PE	4	0
48	1G	803	FES	3	0
46	1L	703	PC1	4	0
46	1h	201	PC1	2	0
47	1B	201	SF4	1	0
51	1a	101	CDL	4	0
46	1B	202	PC1	2	0
45	1L	701	3PE	2	0
45	1A	201	3PE	2	0
47	1F	502	SF4	1	0
54	1P	501	NDP	8	0
46	1d	201	PC1	9	0
47	1I	201	SF4	3	0
45	1M	503	3PE	3	0
46	1f	101	PC1	3	0
51	1N	401	CDL	5	0
46	1Y	803	PC1	2	0
45	1Y	802	3PE	4	0
46	1H	401	PC1	3	0
51	1H	402	CDL	4	0
45	1Y	801	3PE	4	0
51	1N	402	CDL	3	0
51	1X	201	CDL	12	0
45	1D	901	3PE	4	0
48	1E	301	FES	2	0
56	1n	201	EHZ	2	0
45	1f	102	3PE	2	0
46	1J	201	PC1	2	0

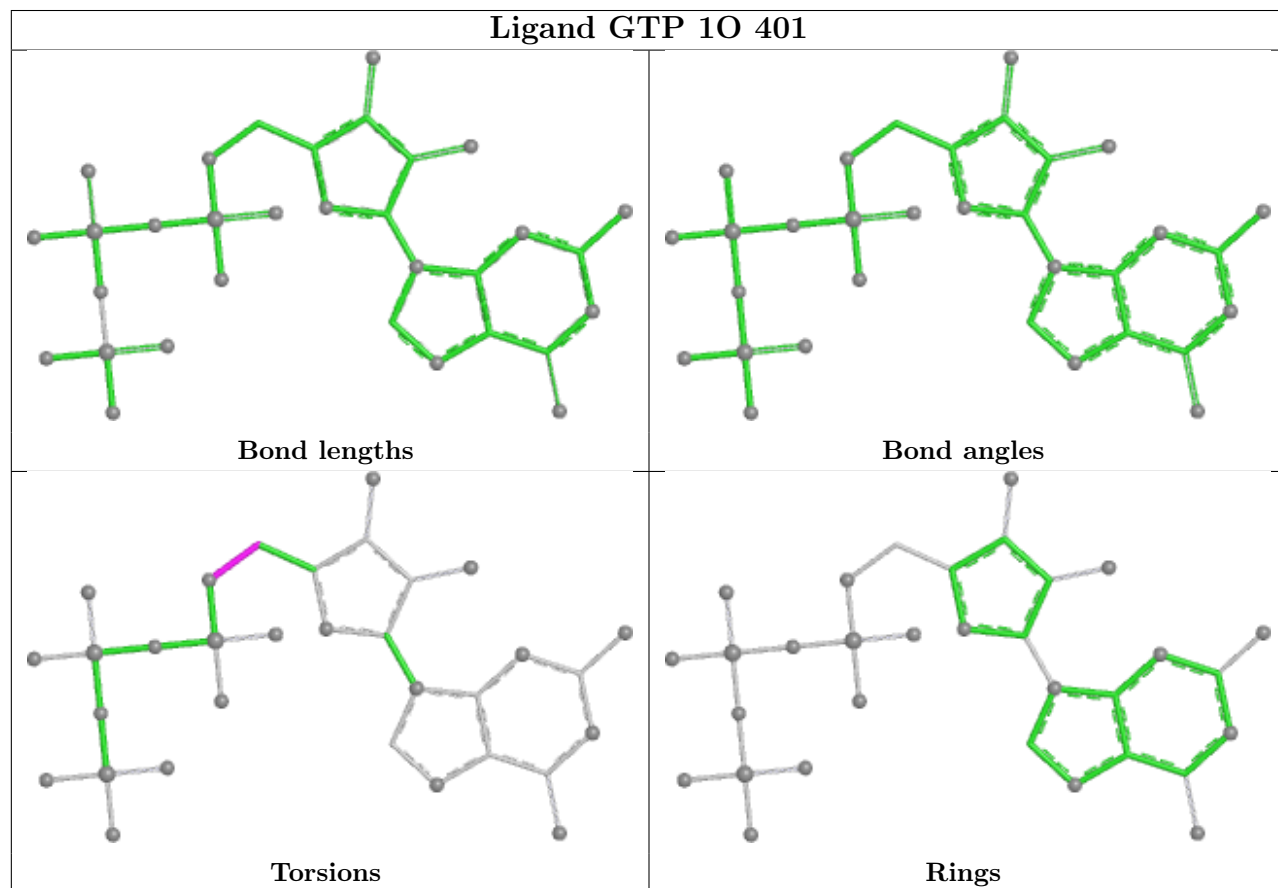
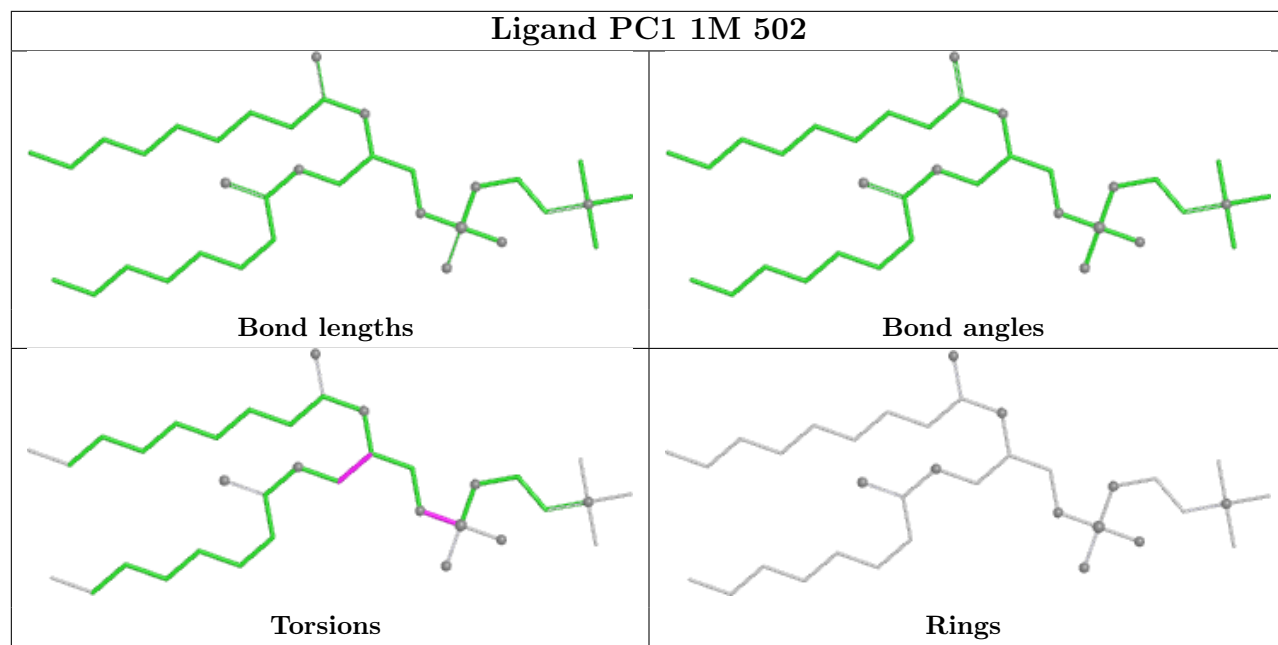
Continued on next page...

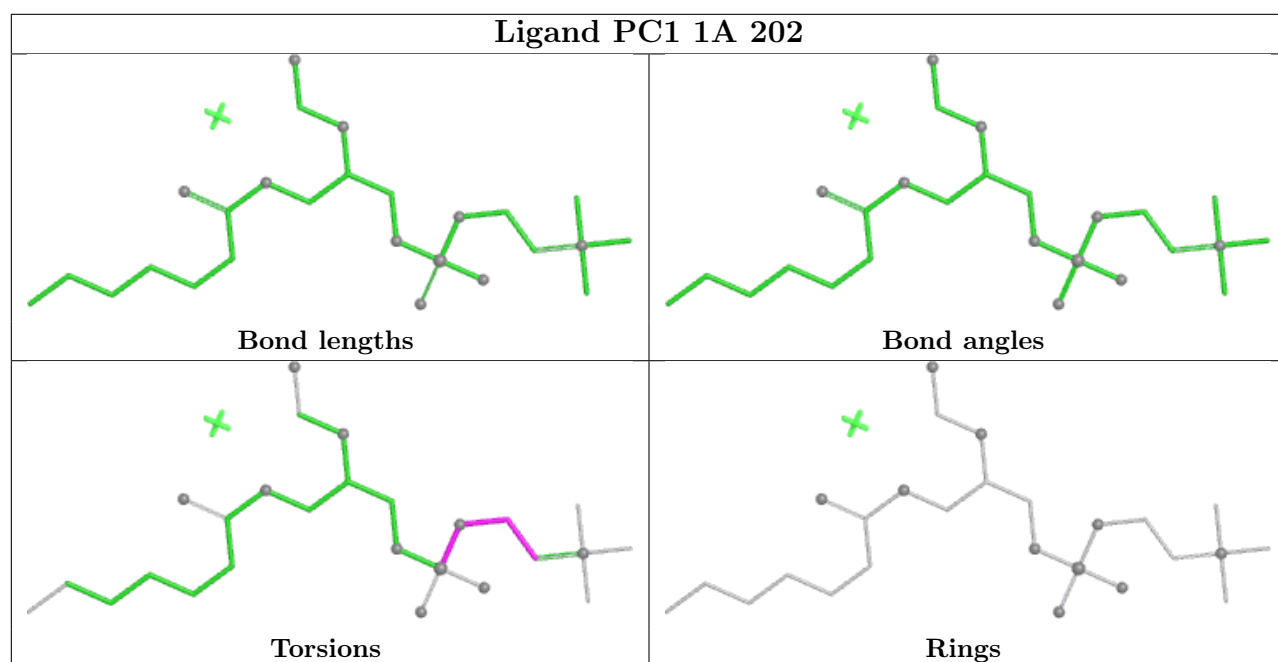
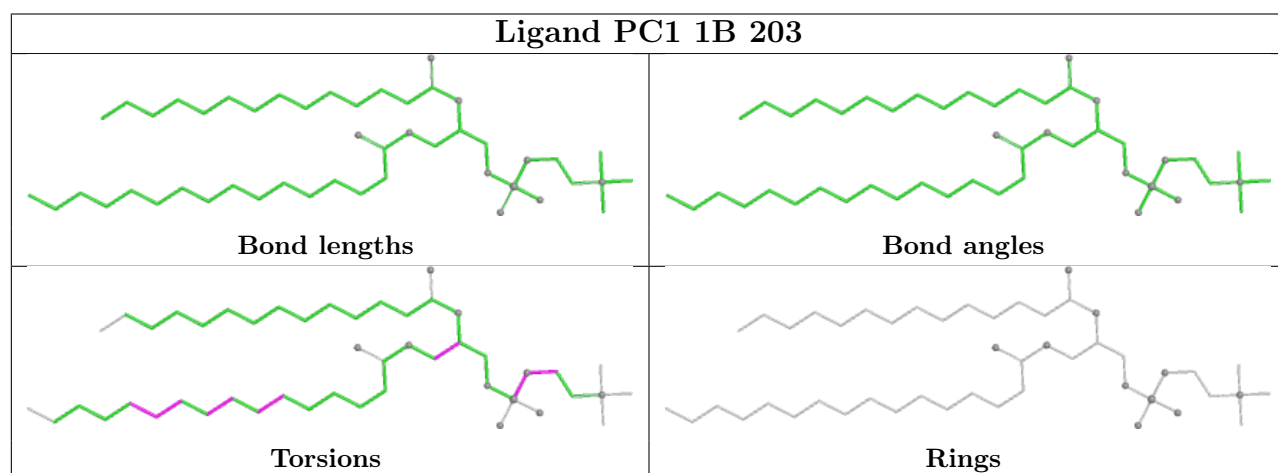
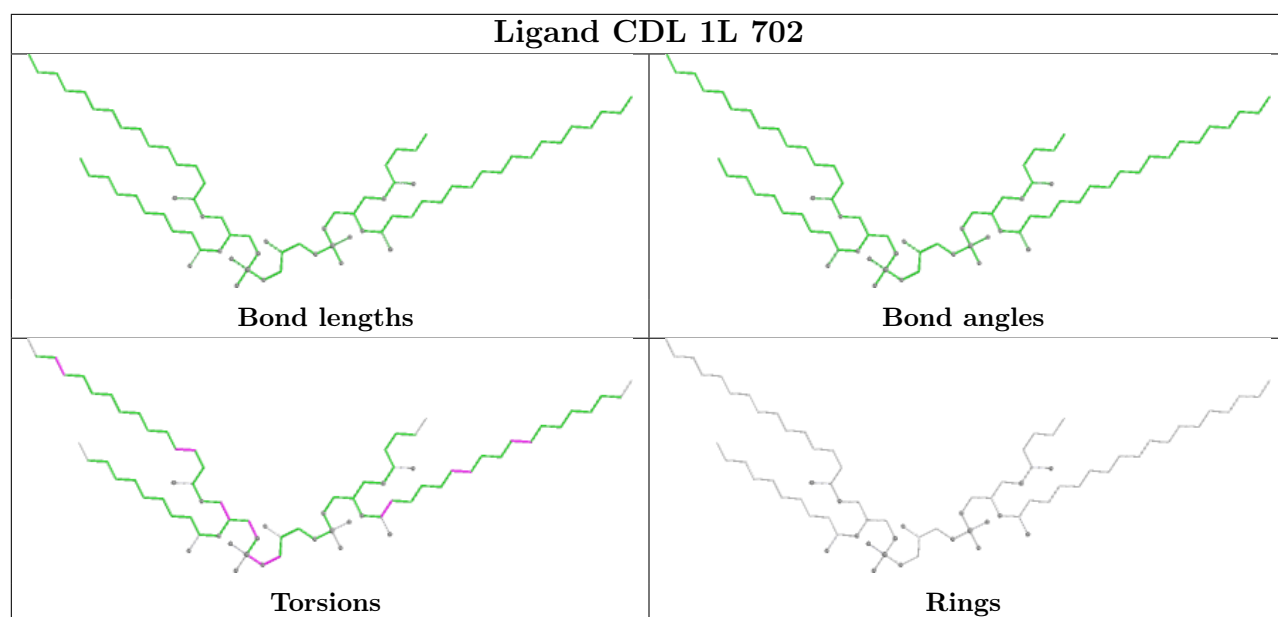
Continued from previous page...

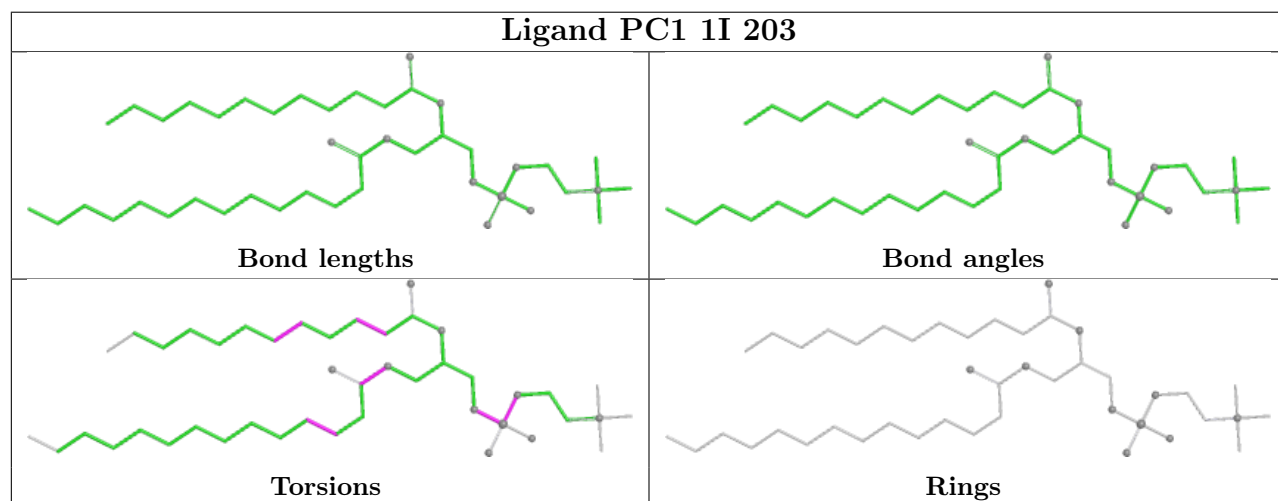
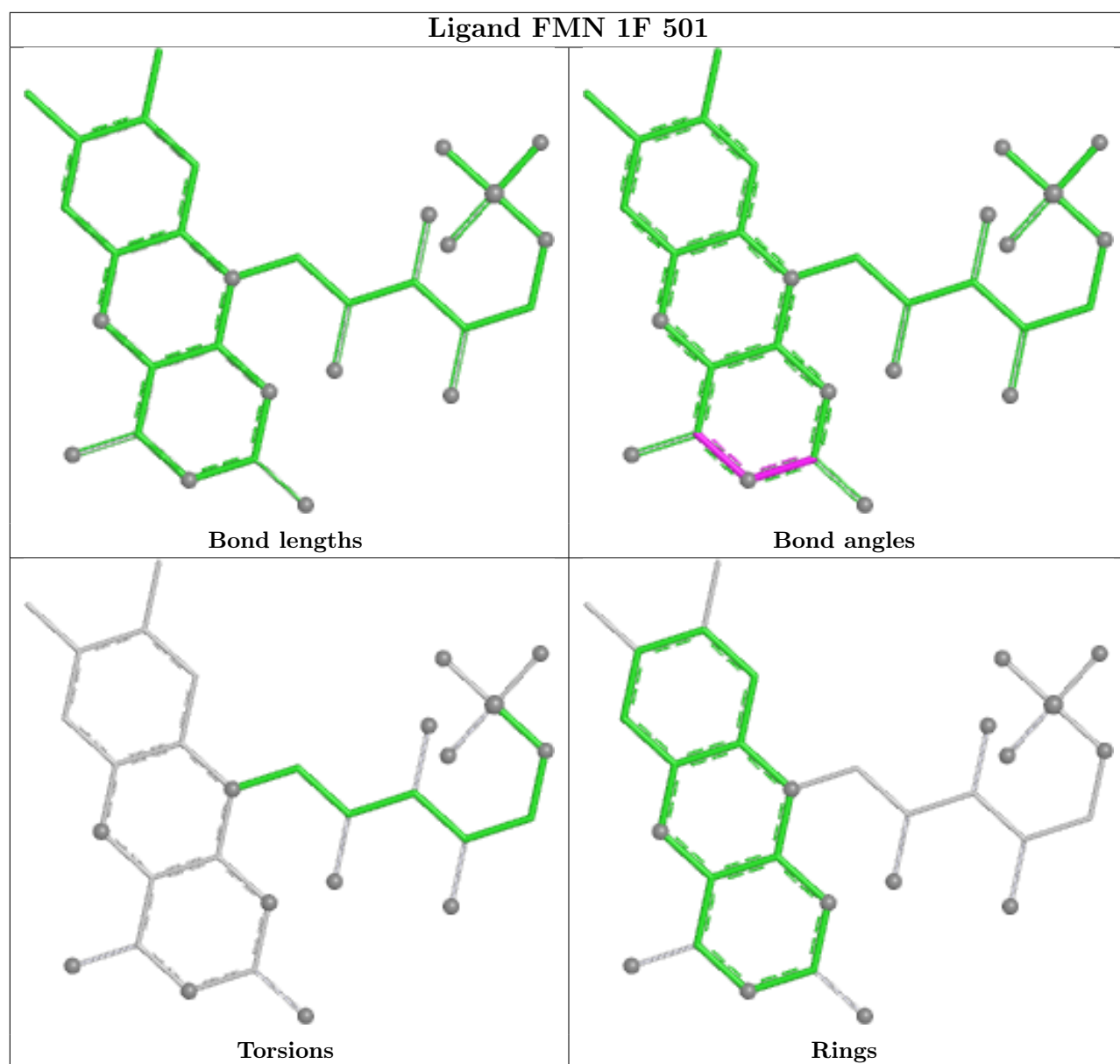
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	1l	201	MYR	2	0
45	1M	501	3PE	1	0
46	1Z	201	PC1	5	0
47	1G	801	SF4	2	0

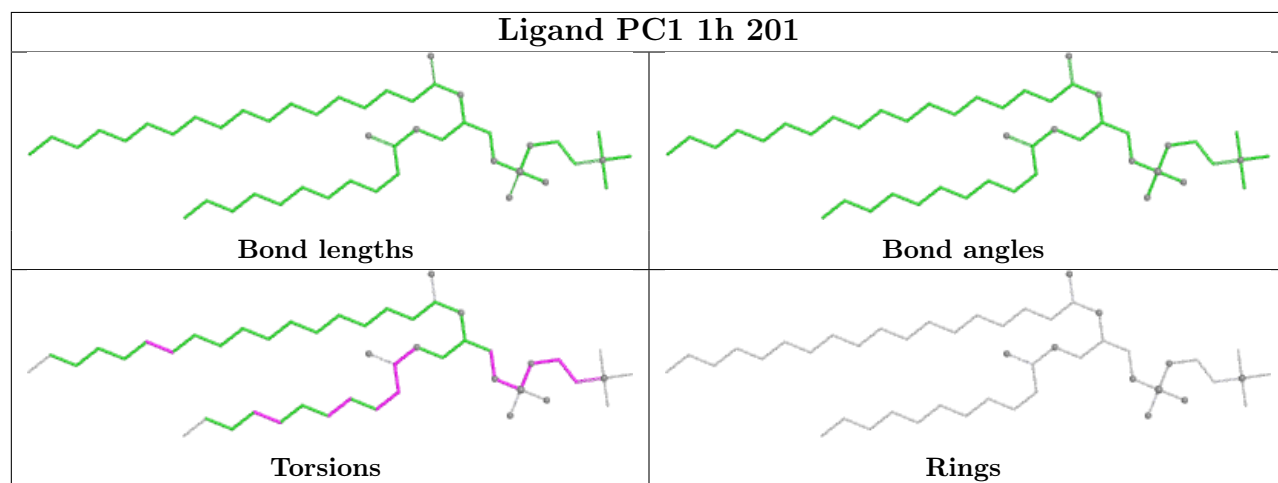
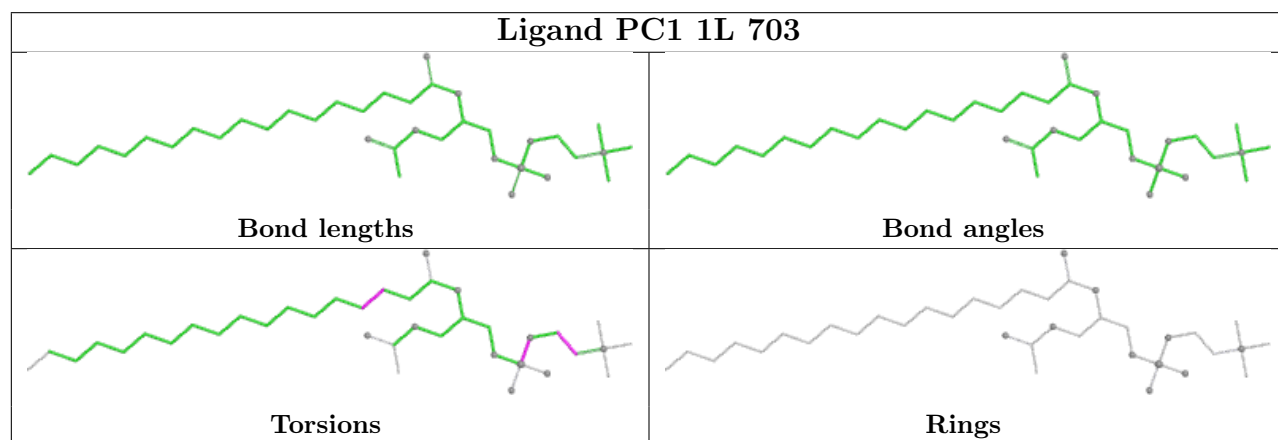
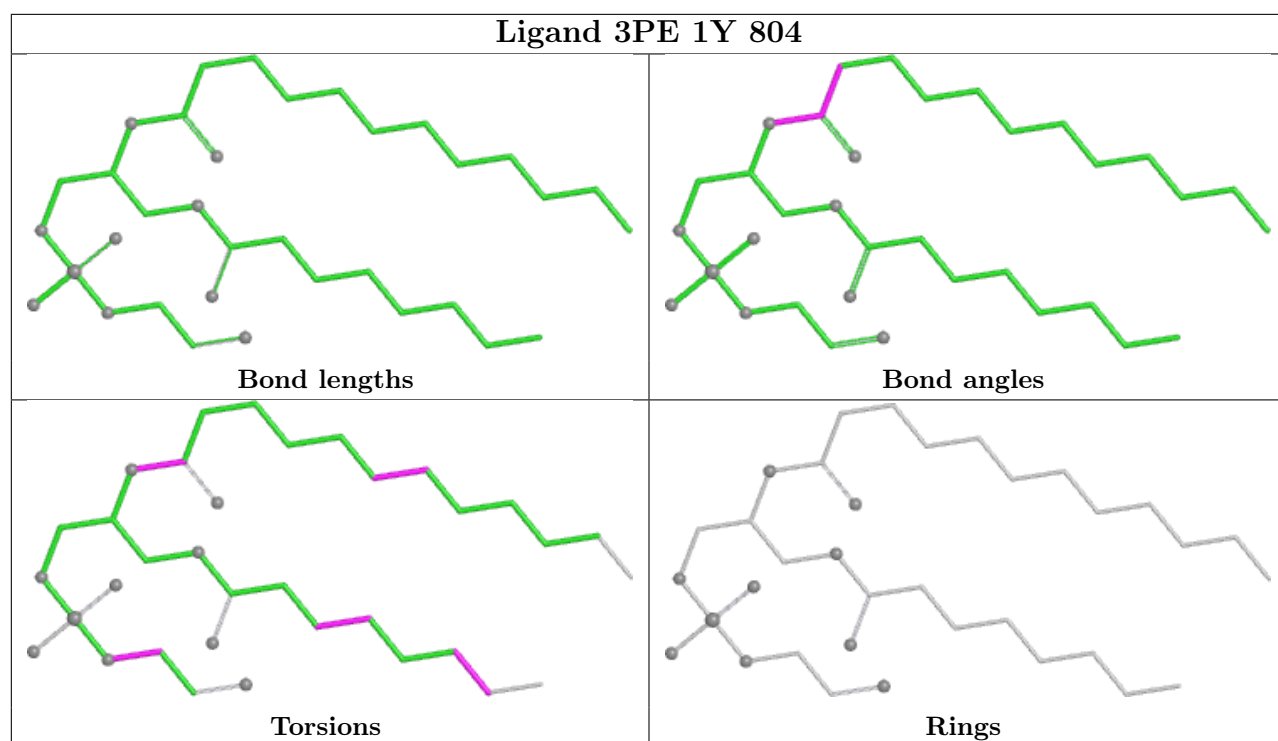
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

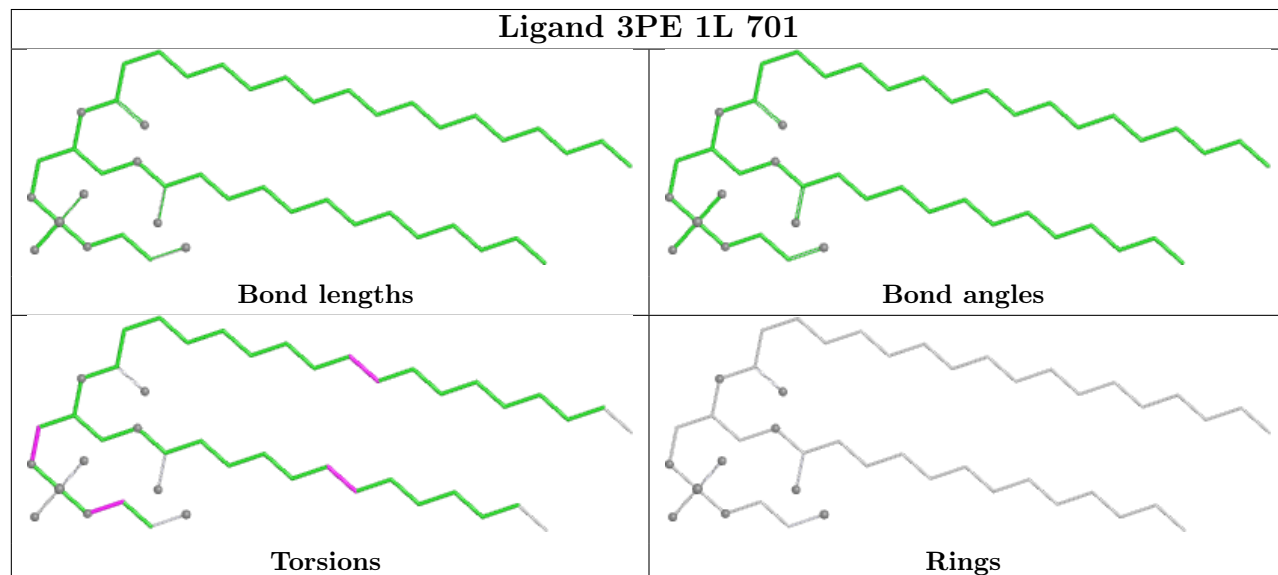
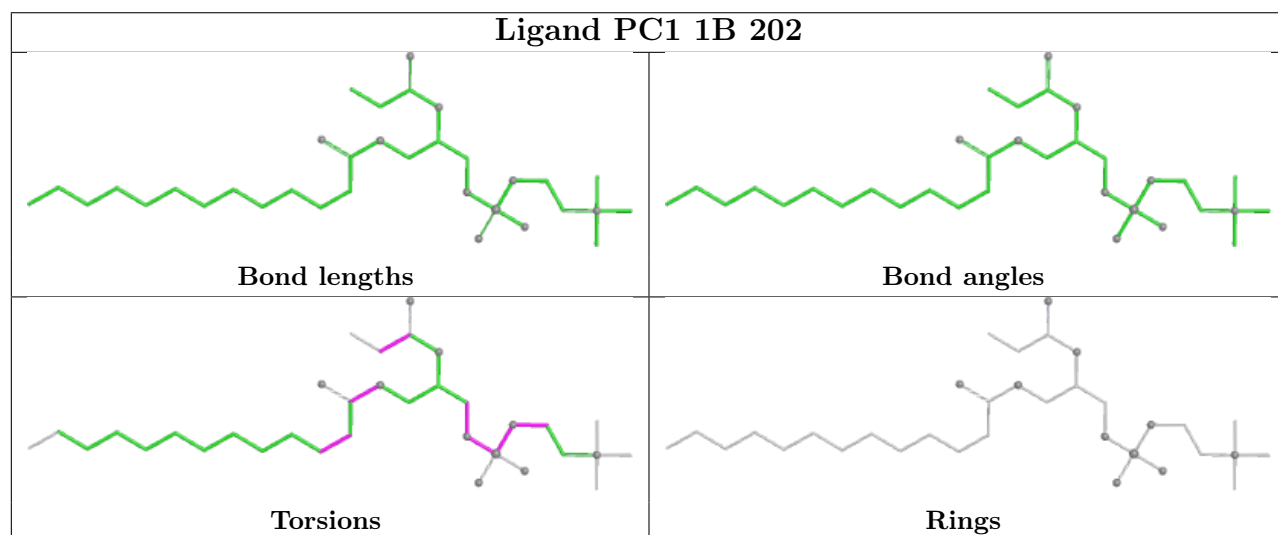
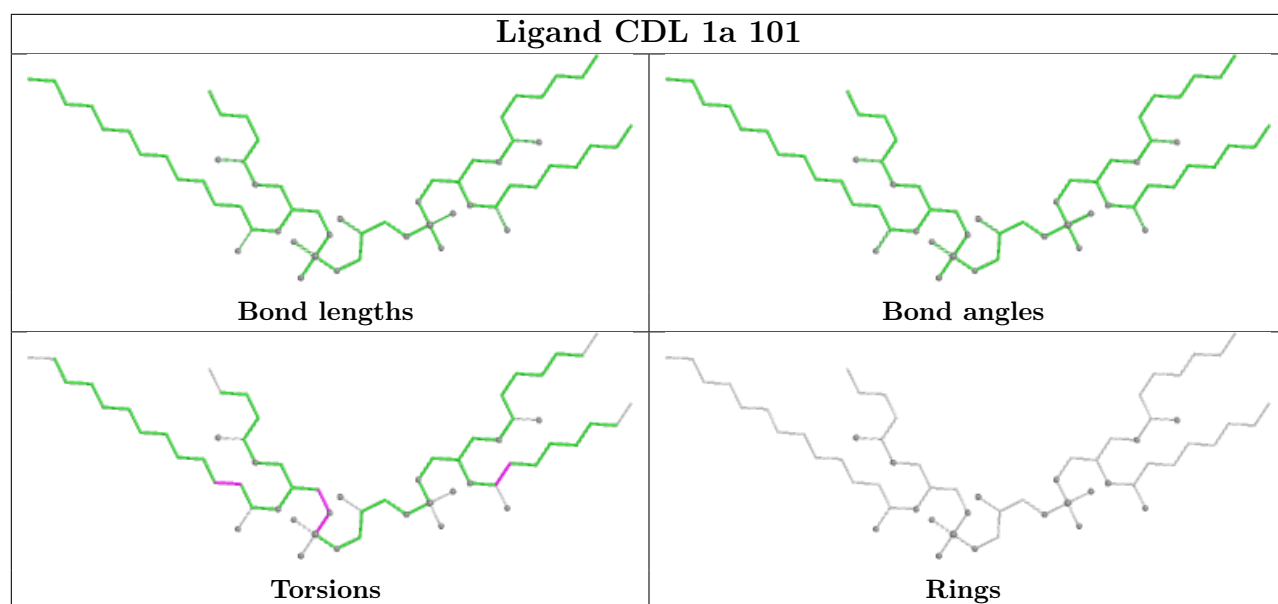


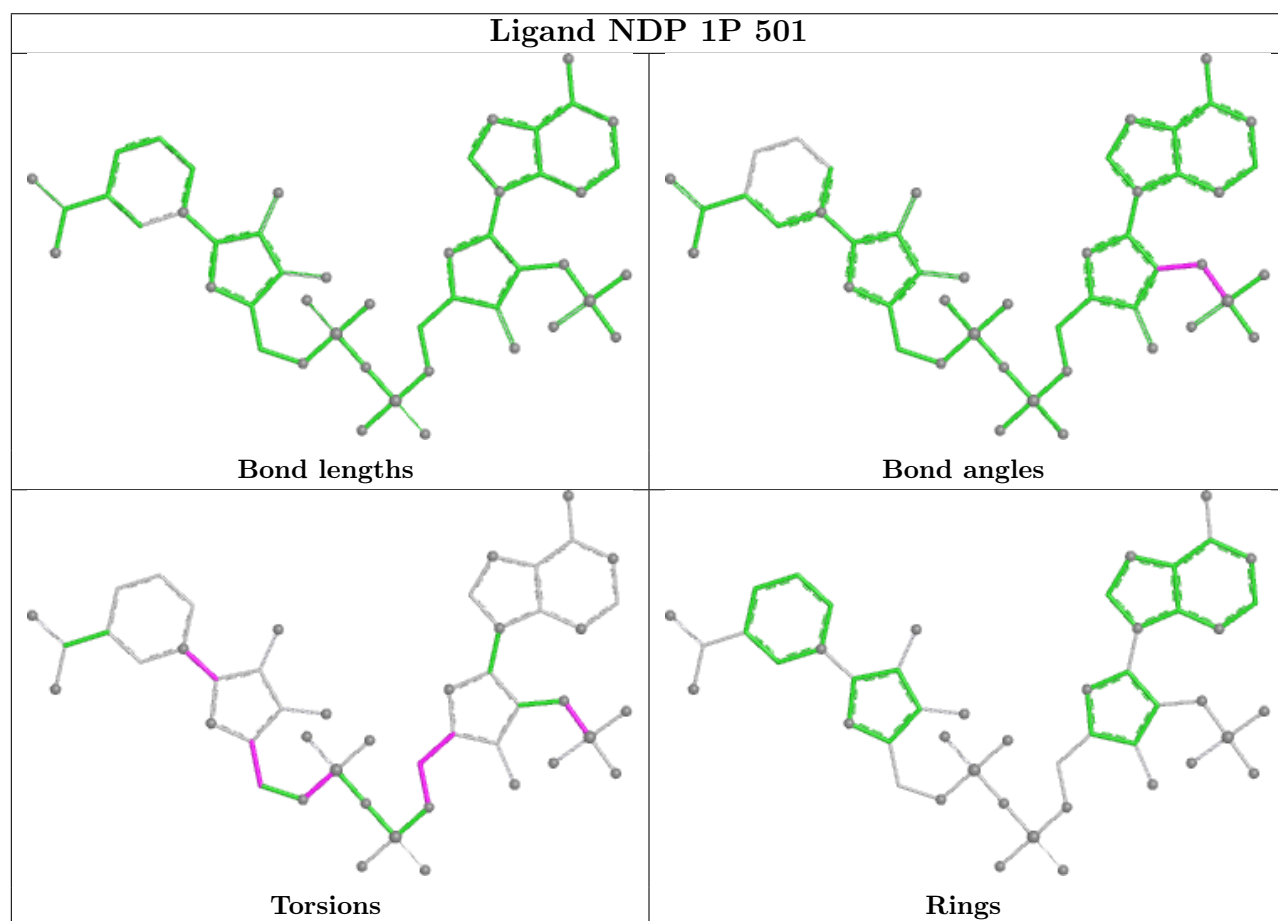
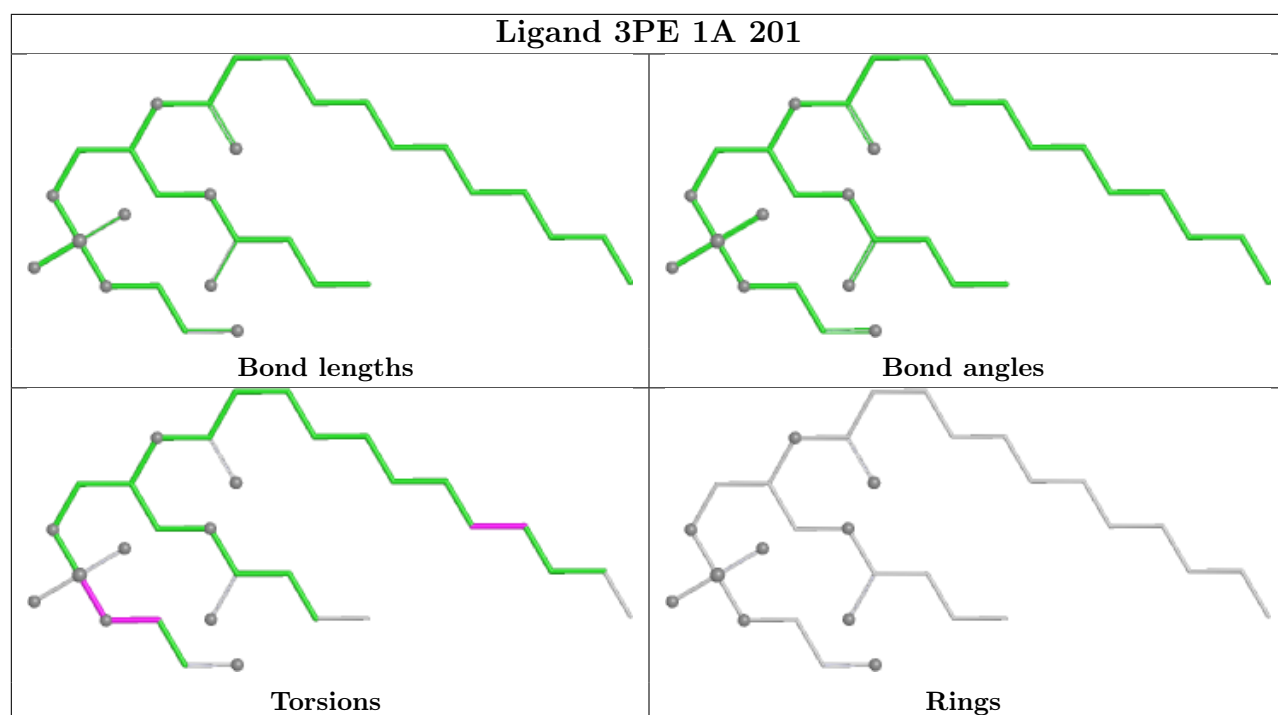


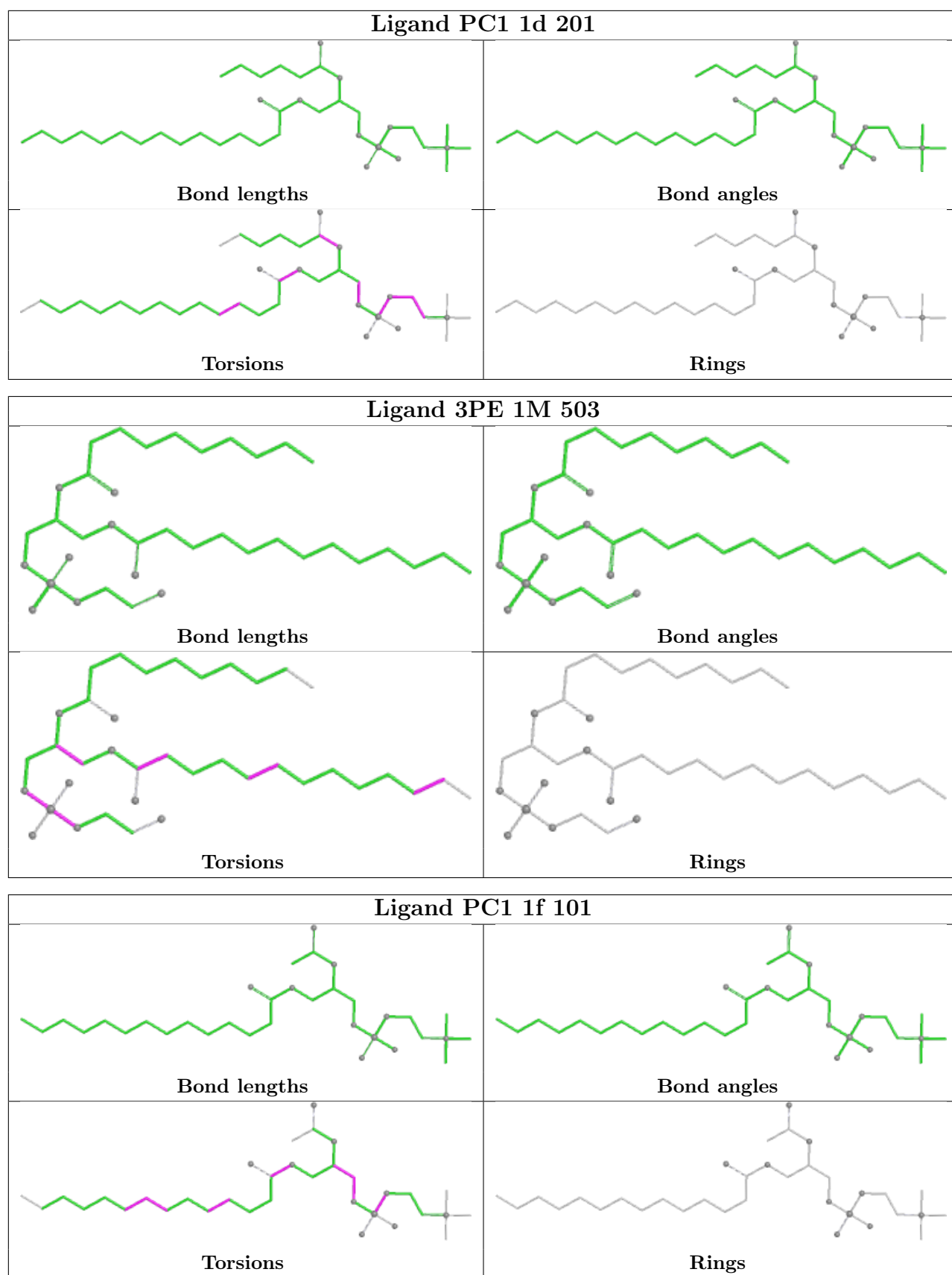


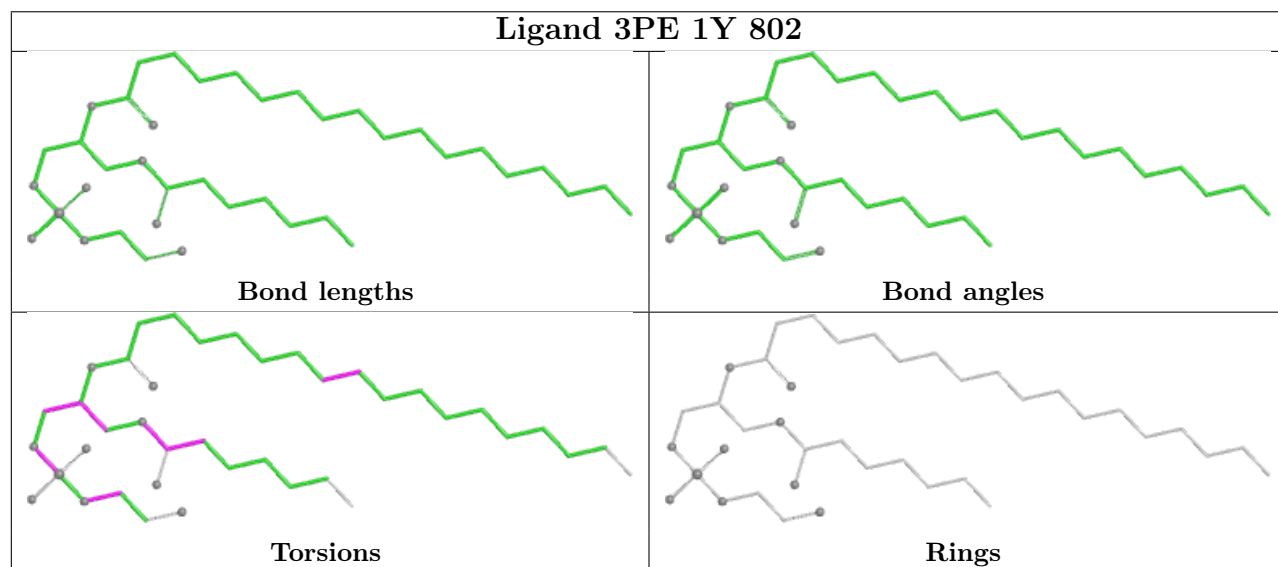
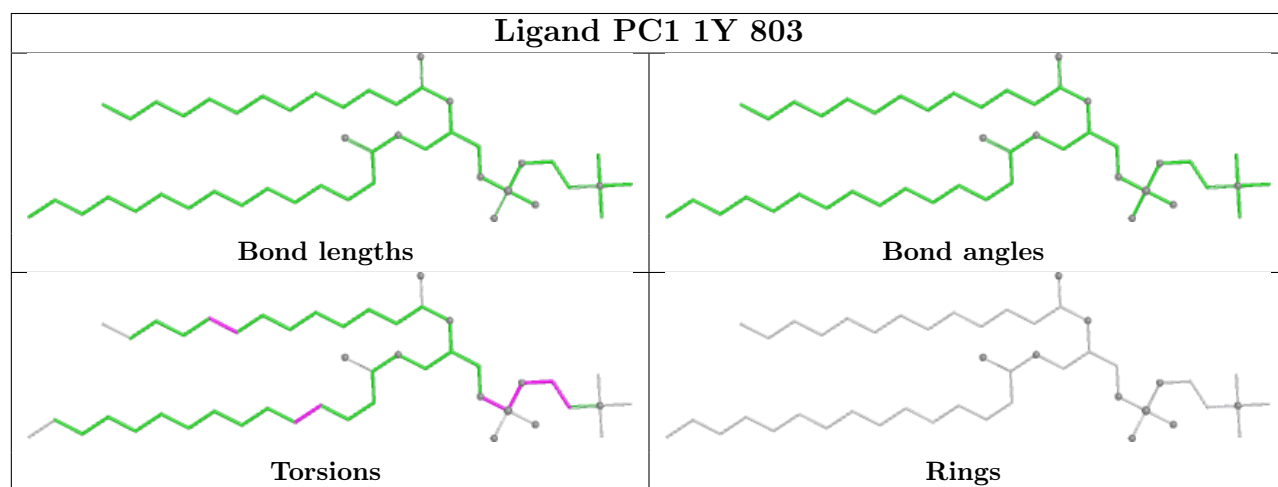
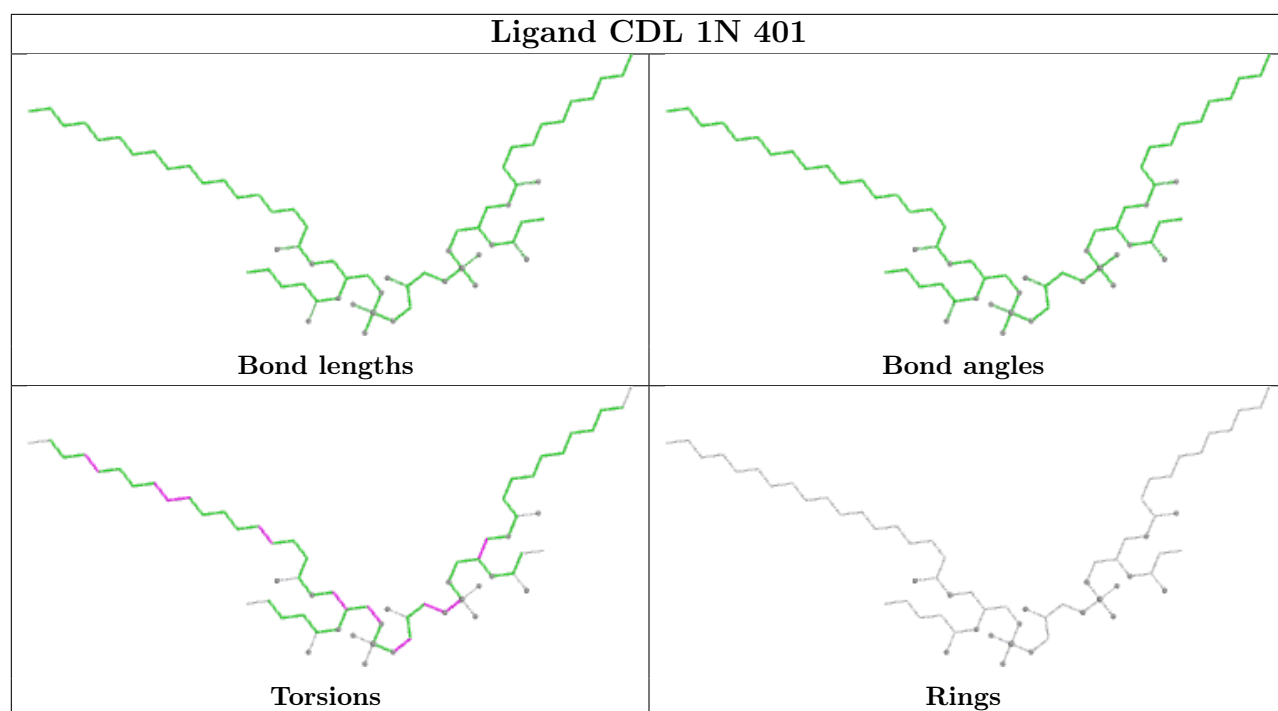


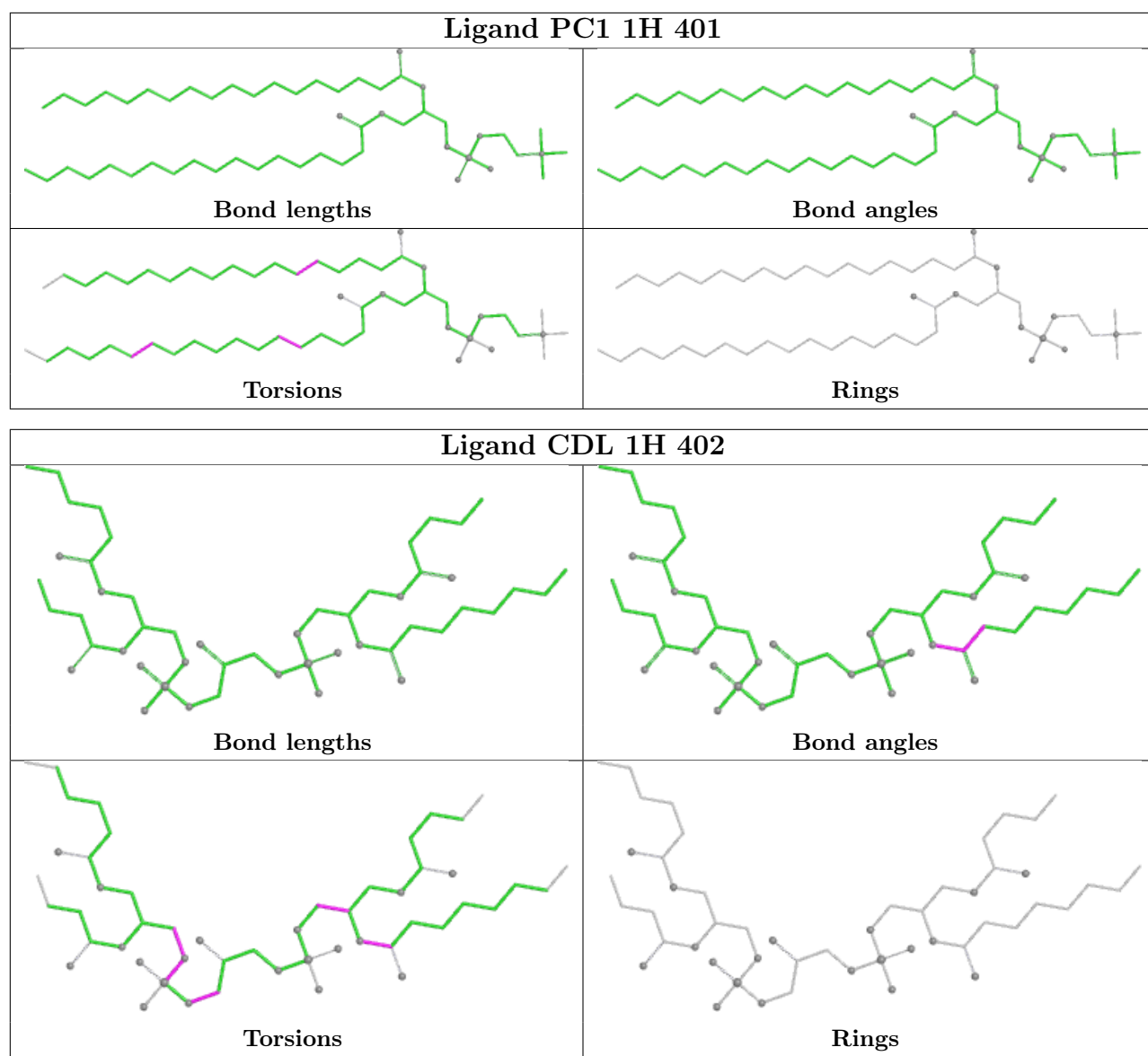


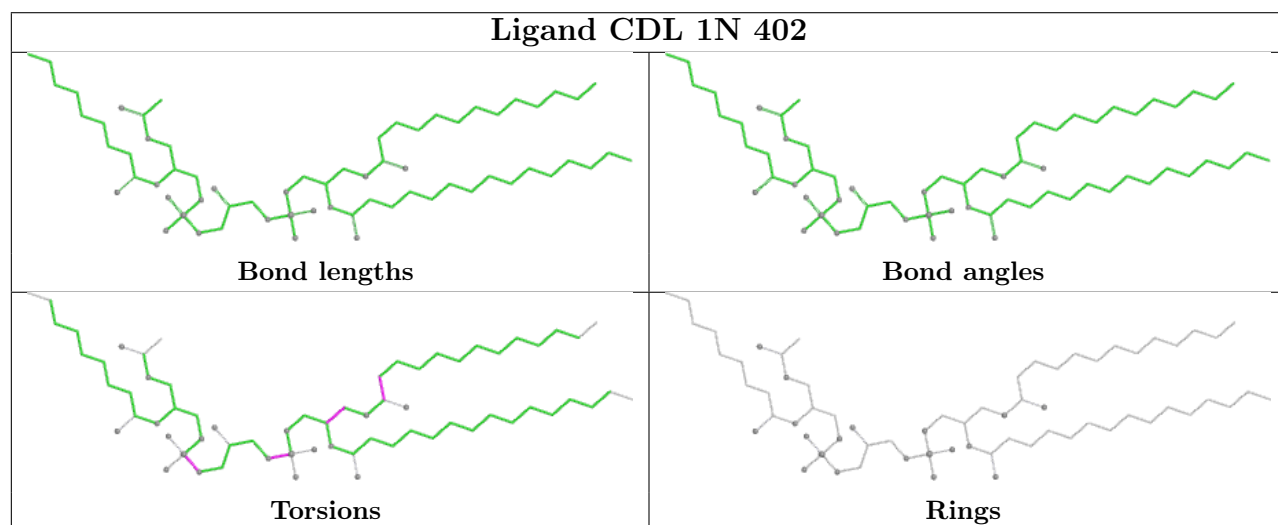
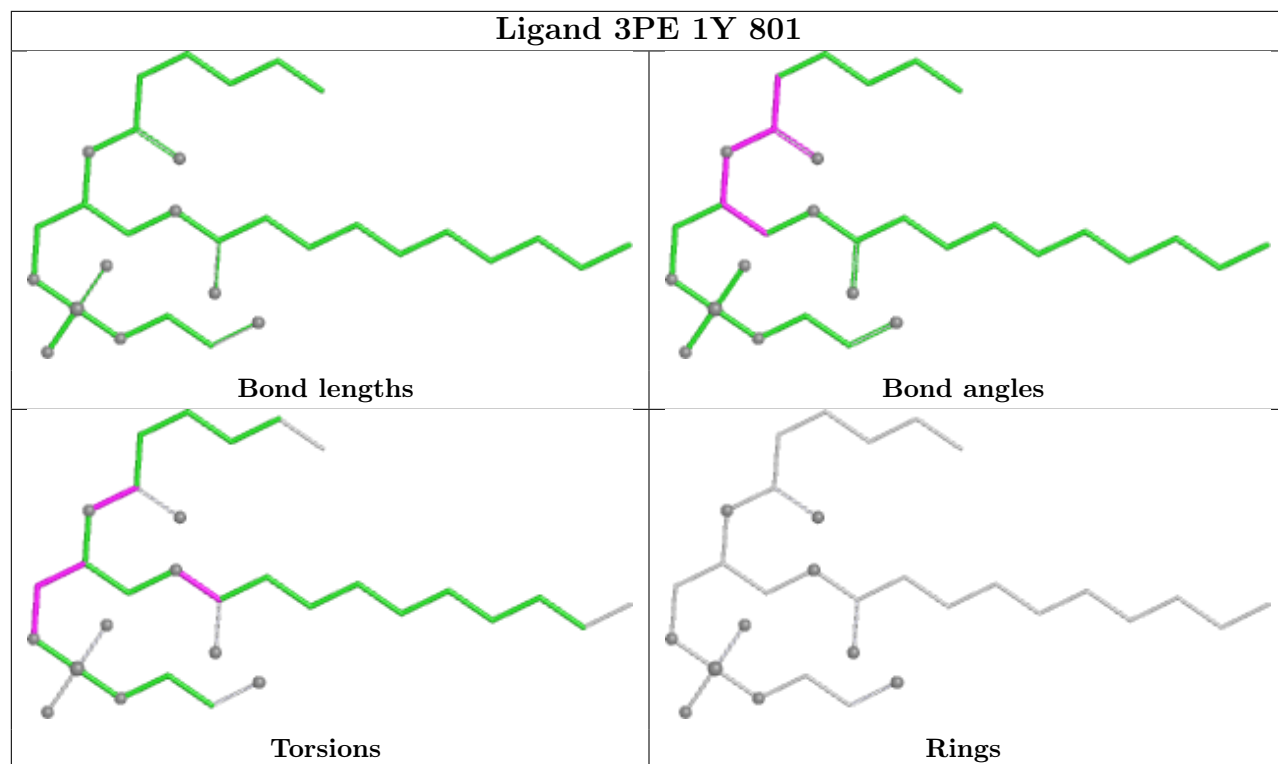


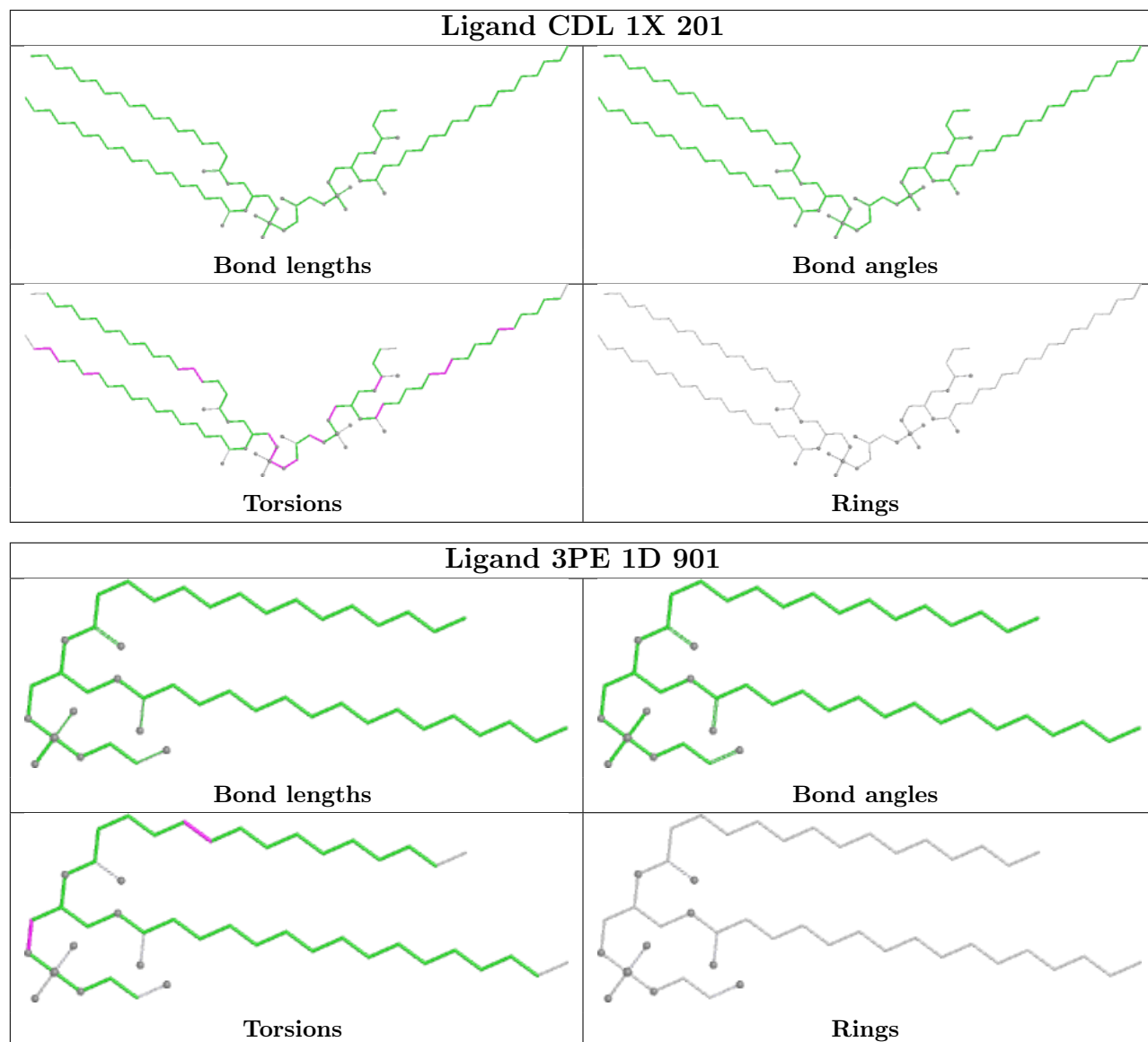


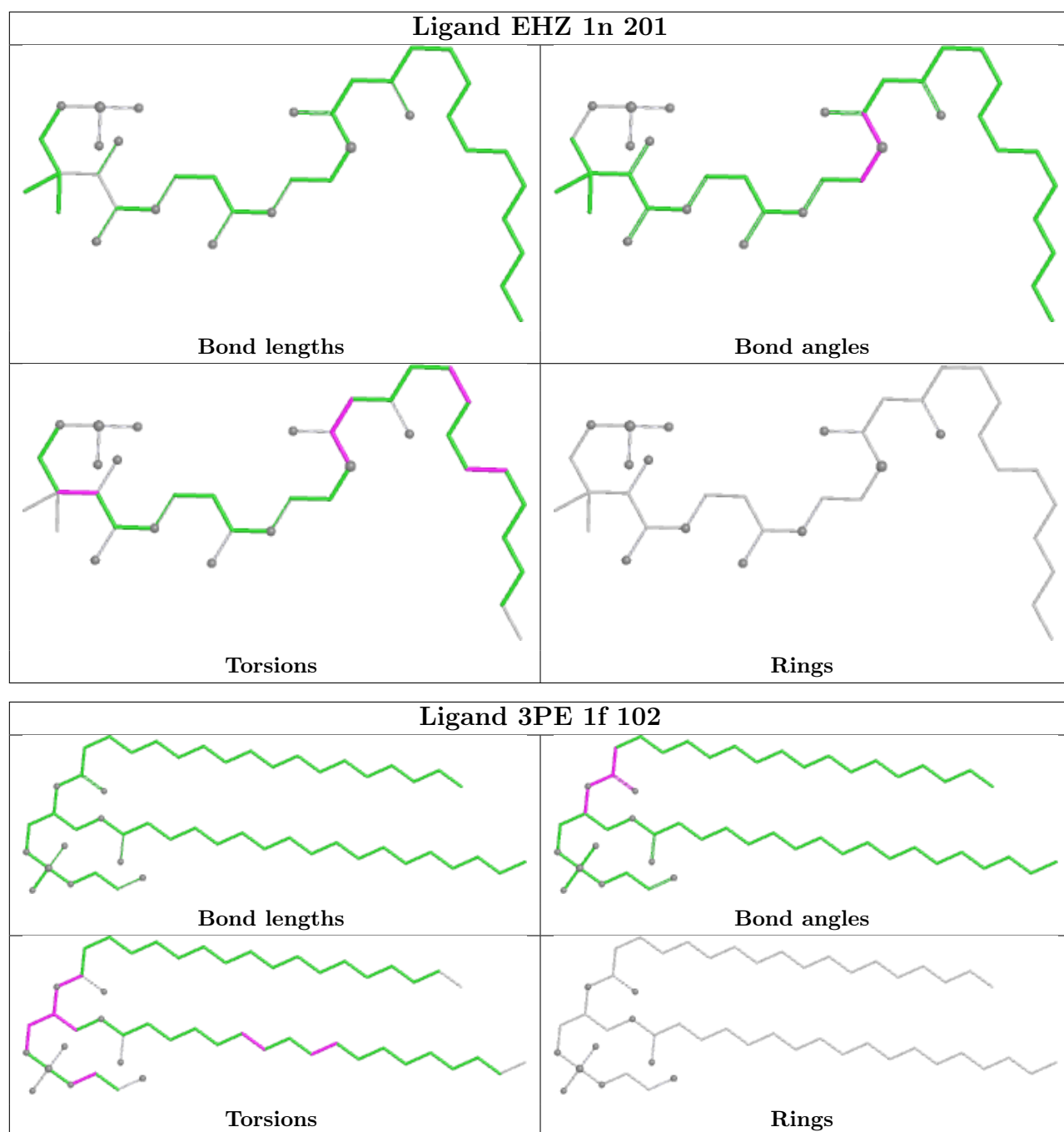


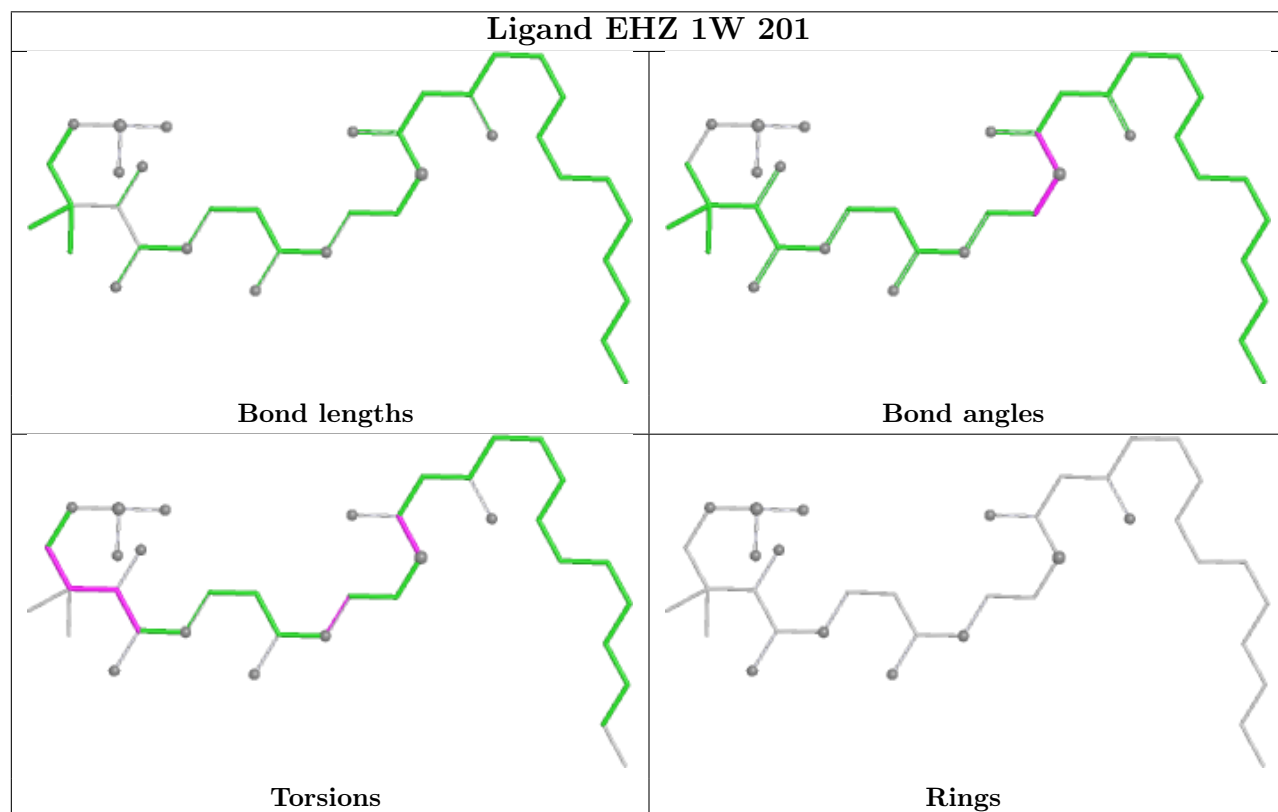
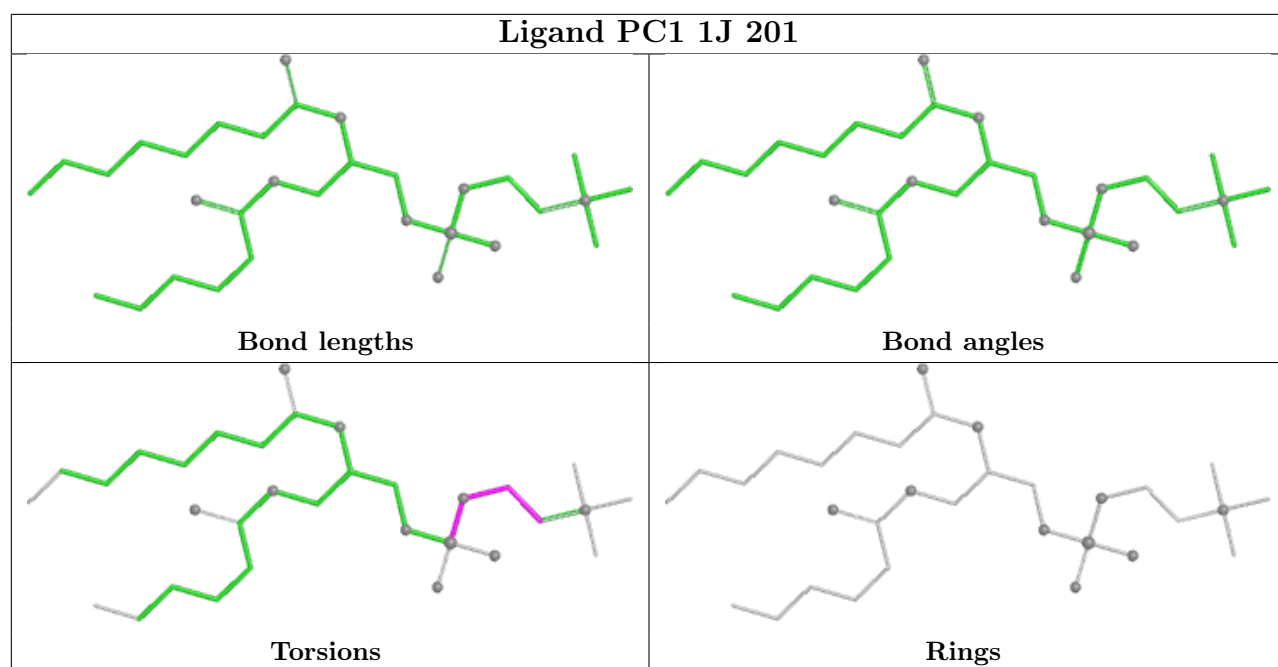


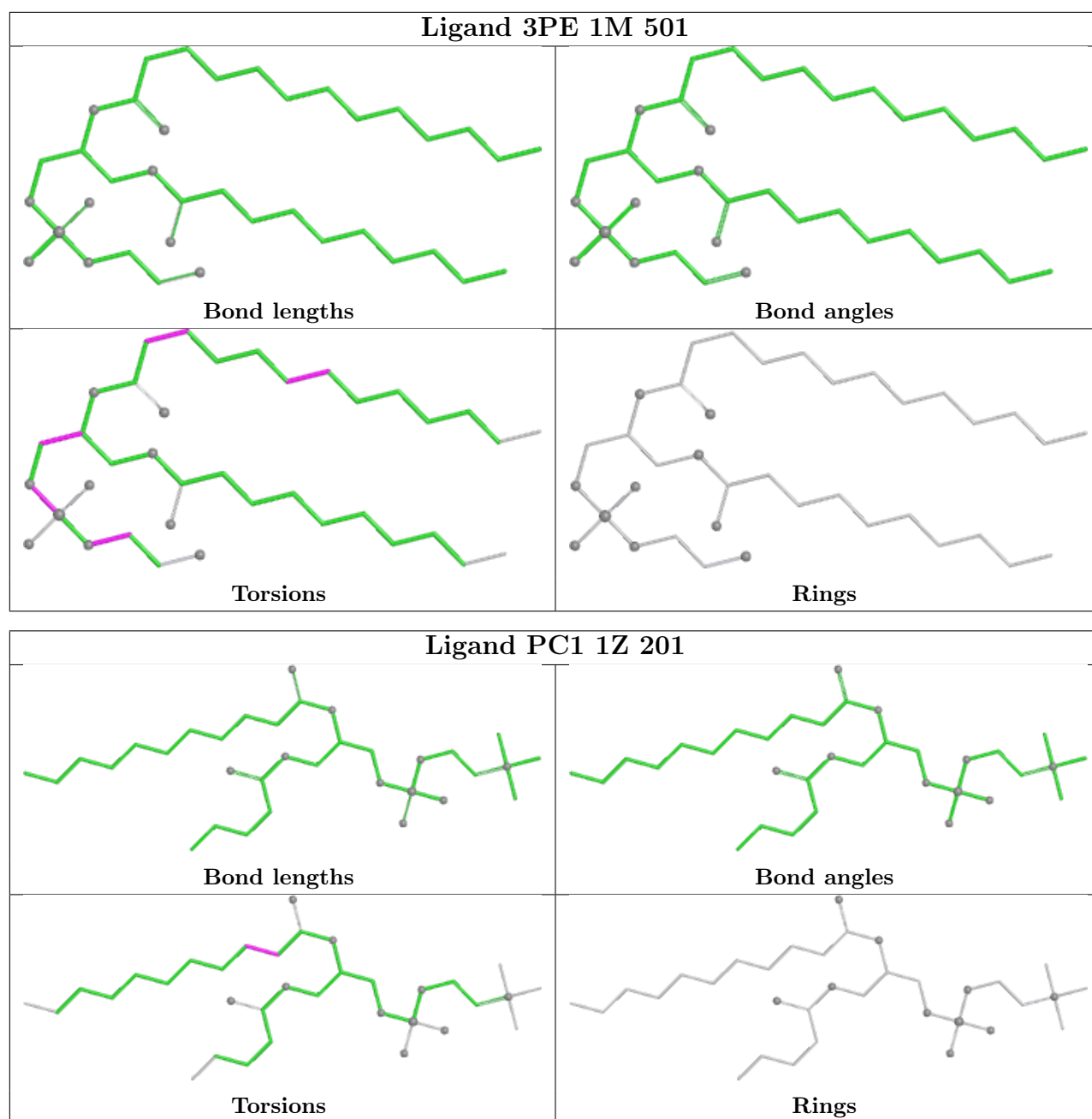












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

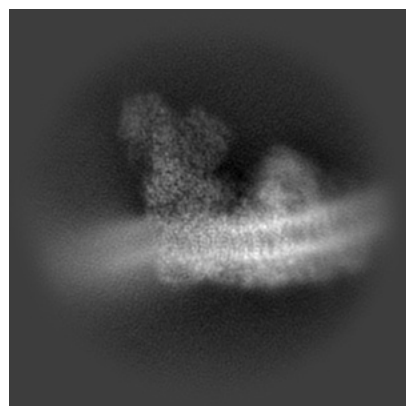
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42165. These allow visual inspection of the internal detail of the map and identification of artifacts.

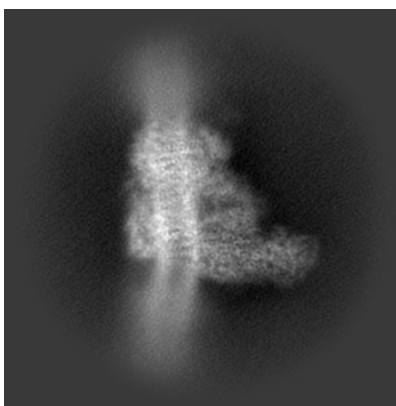
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

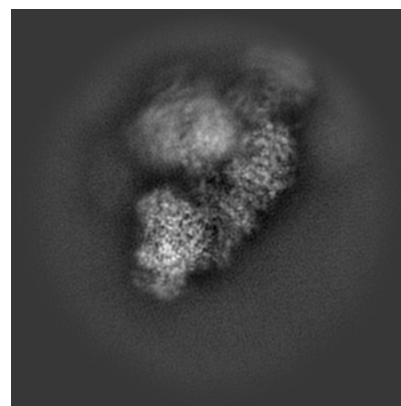
6.1.1 Primary map



X

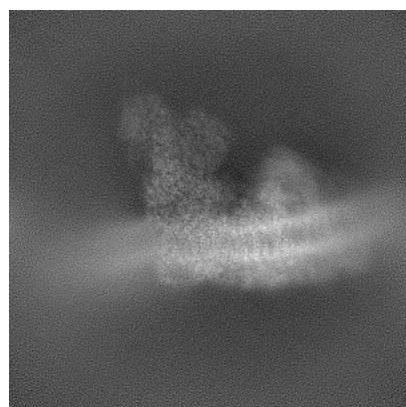


Y

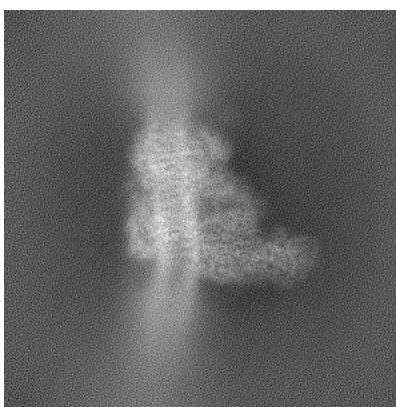


Z

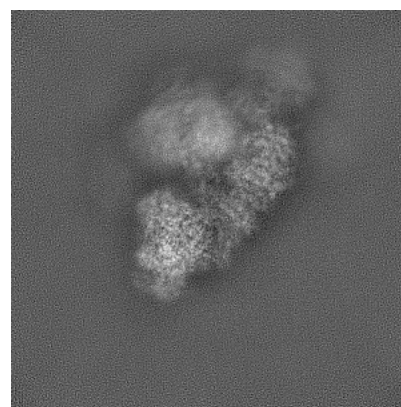
6.1.2 Raw map



X



Y

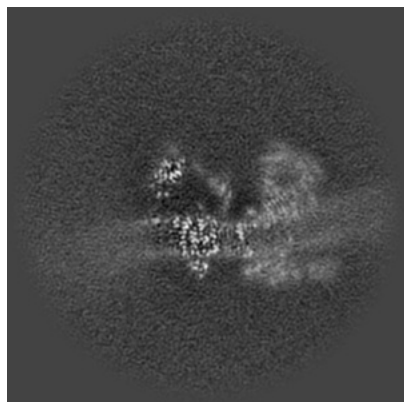


Z

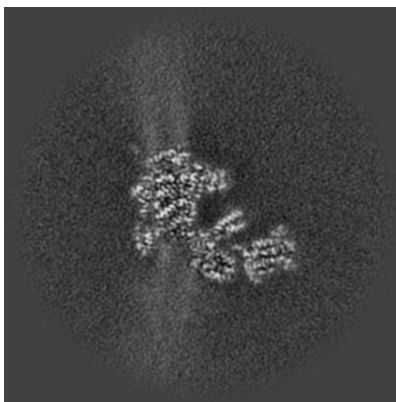
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

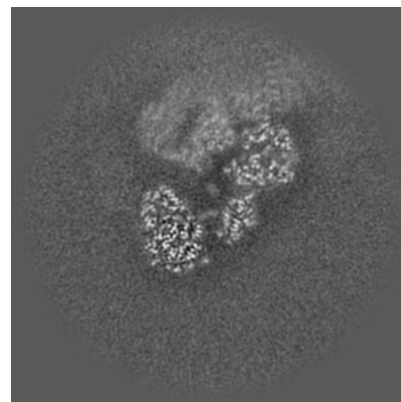
6.2.1 Primary map



X Index: 200

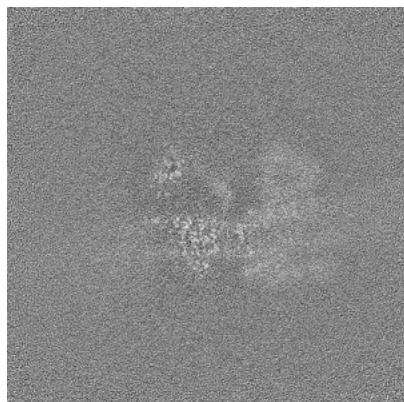


Y Index: 200

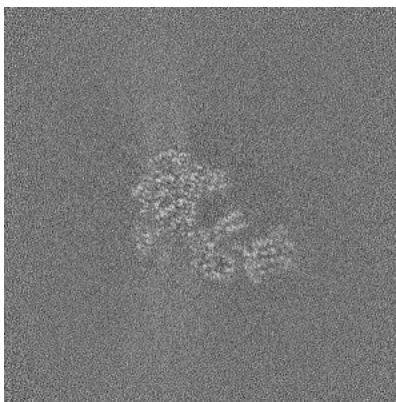


Z Index: 200

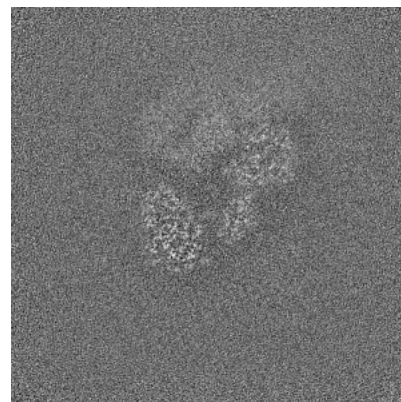
6.2.2 Raw map



X Index: 200



Y Index: 200

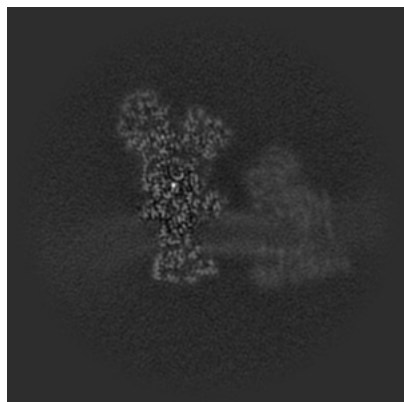


Z Index: 200

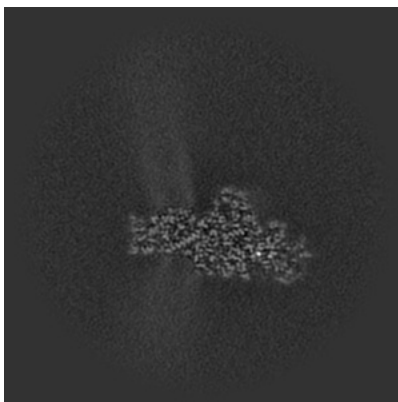
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

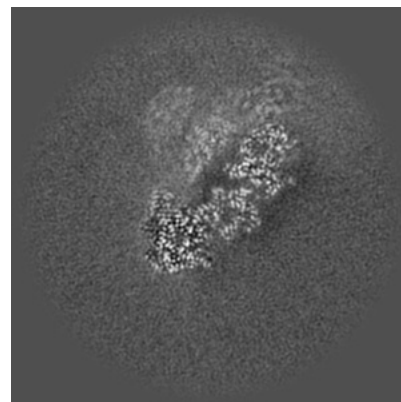
6.3.1 Primary map



X Index: 162

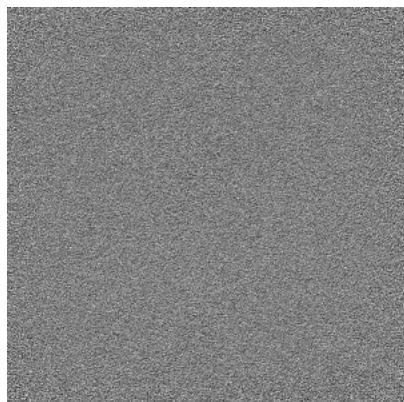


Y Index: 157

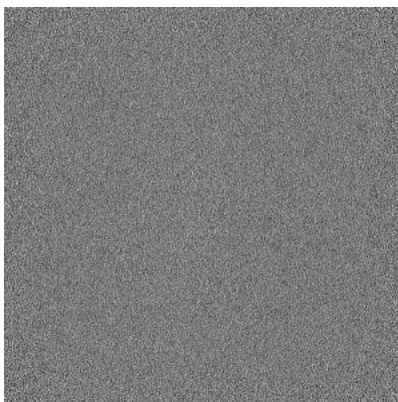


Z Index: 190

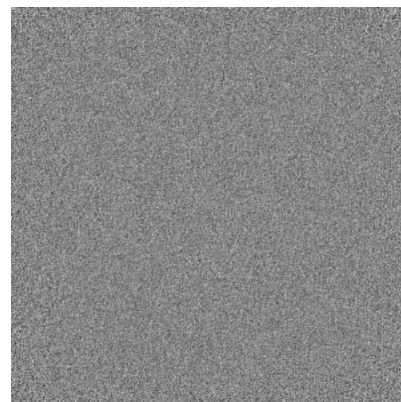
6.3.2 Raw map



X Index: 0



Y Index: 0

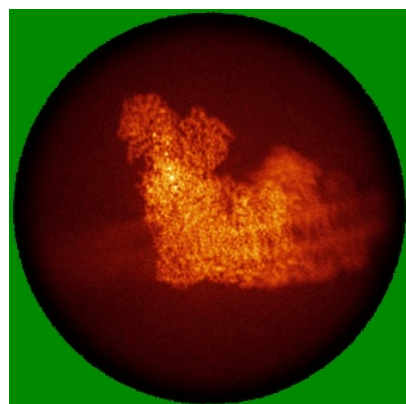


Z Index: 0

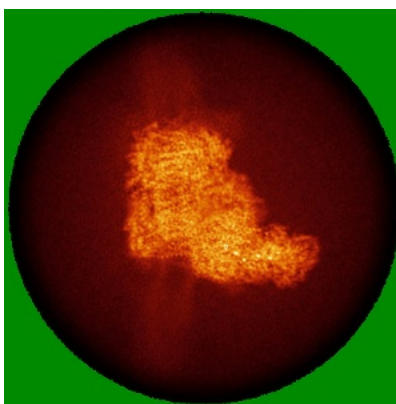
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

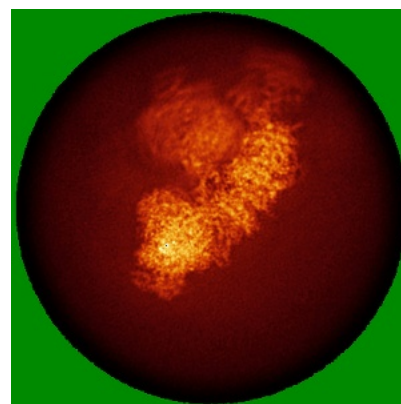
6.4.1 Primary map



X

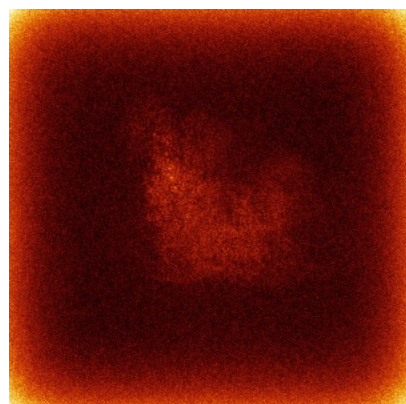


Y

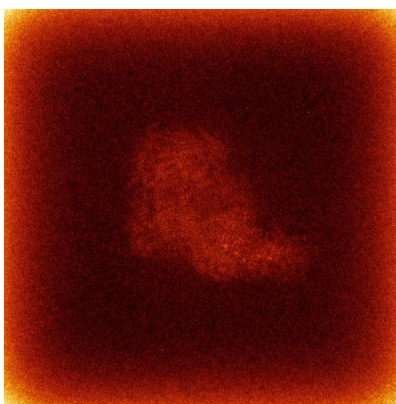


Z

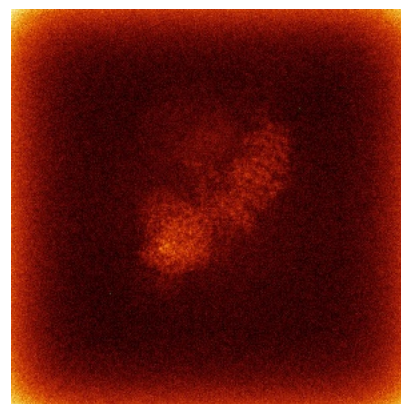
6.4.2 Raw map



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.

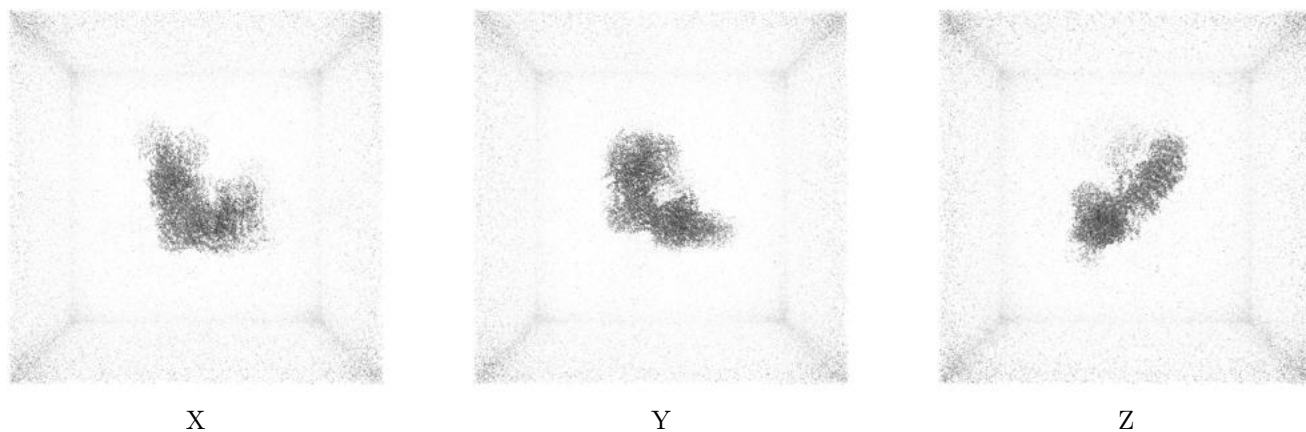
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

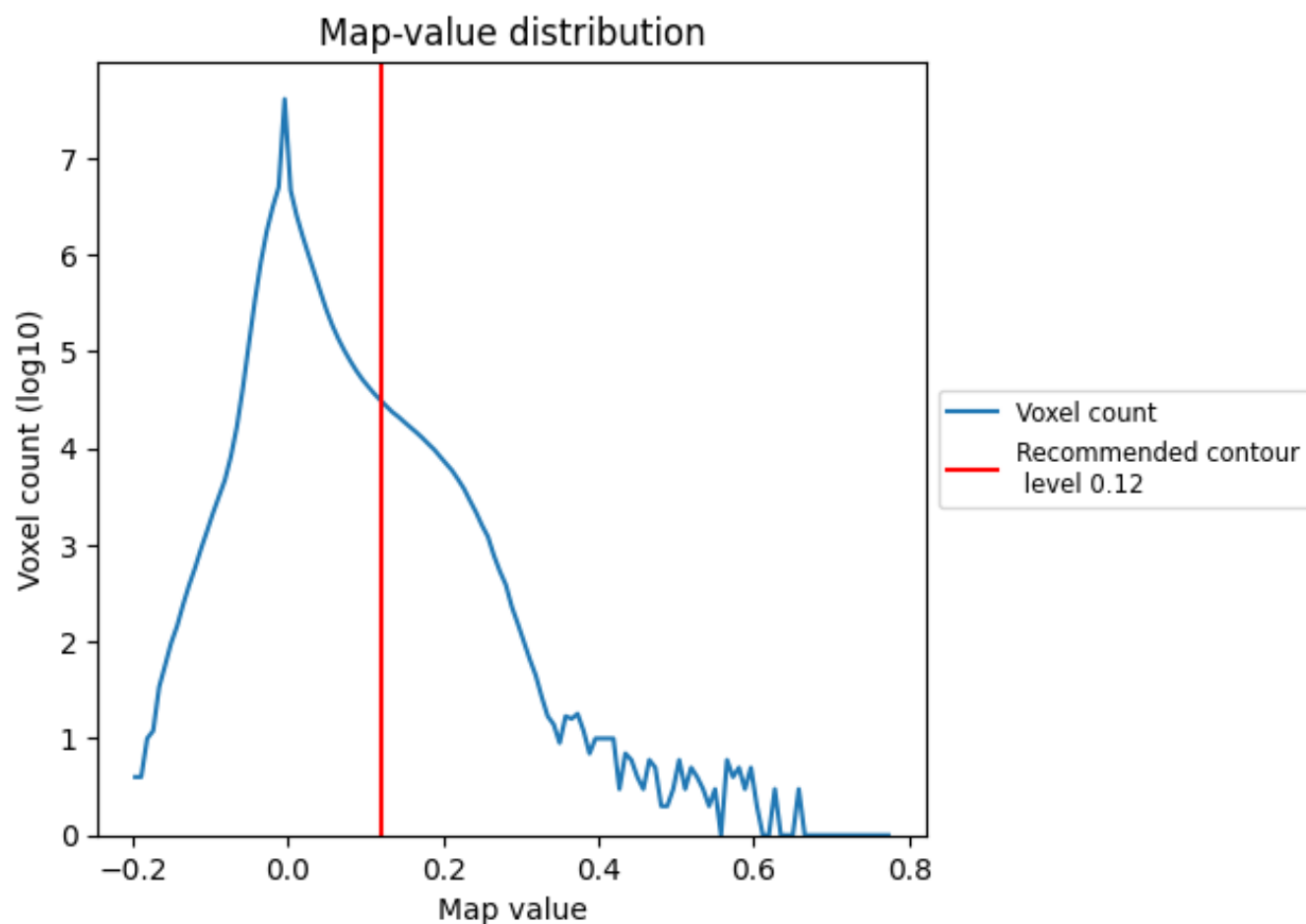
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

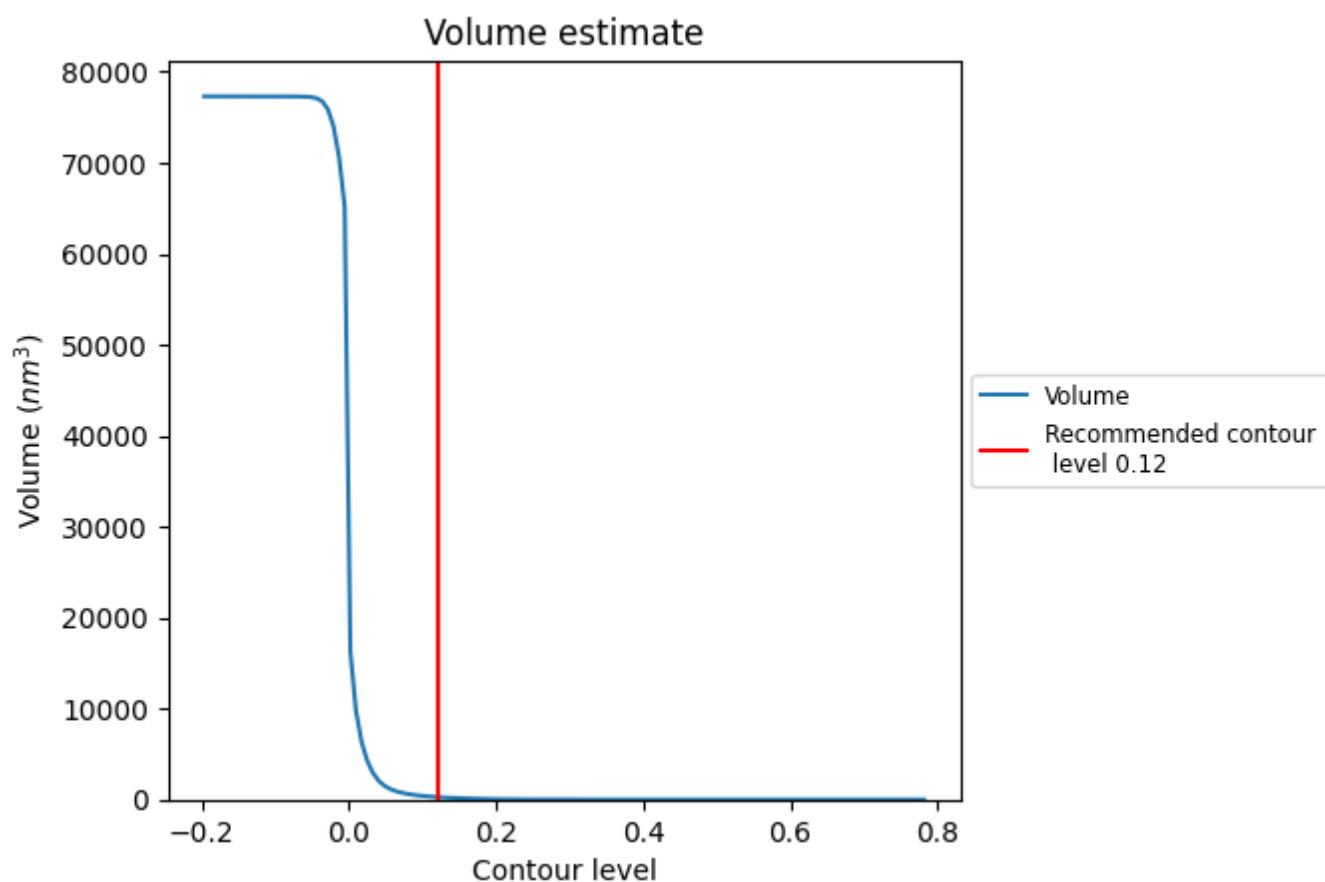
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

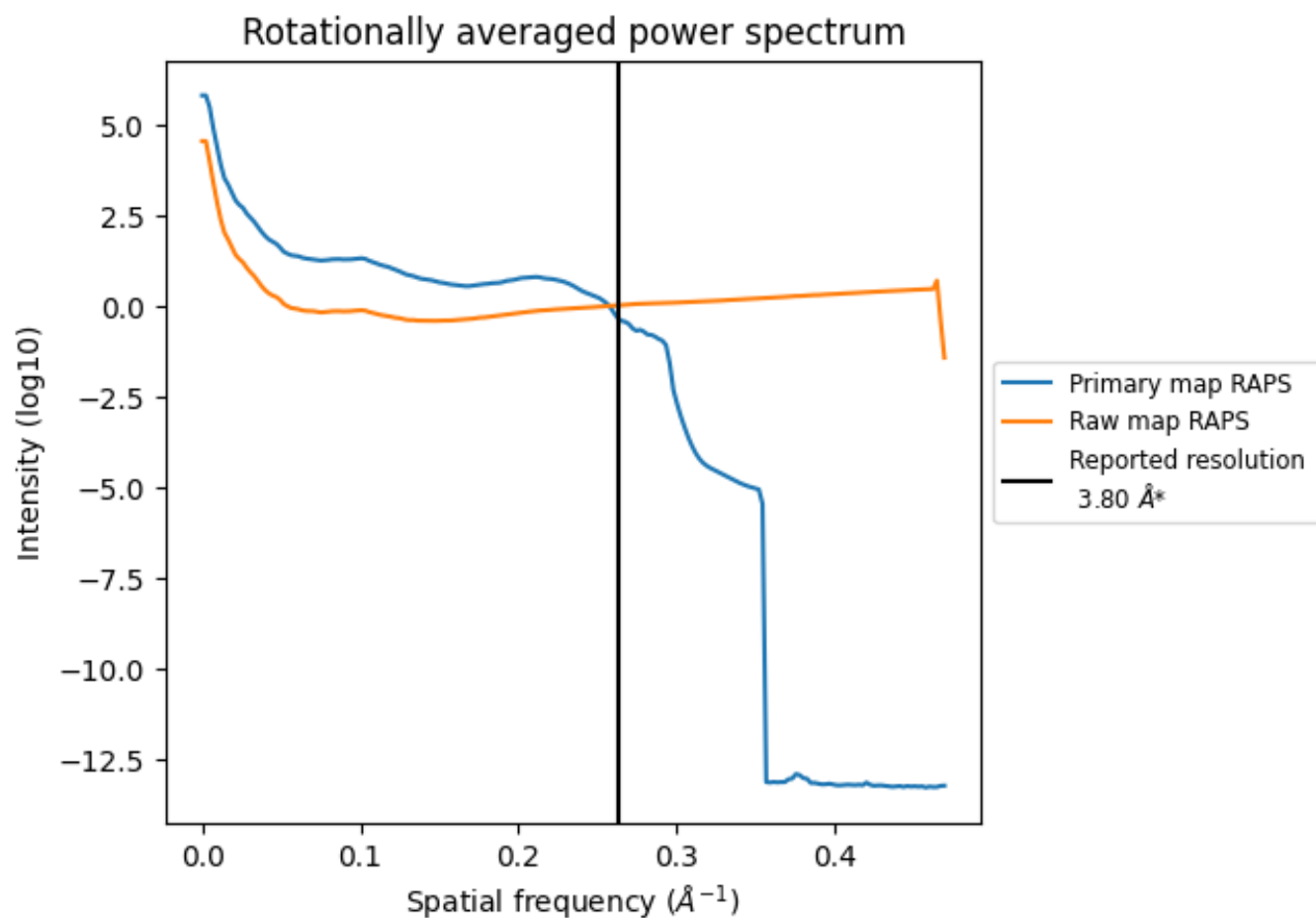
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 269 nm^3 ; this corresponds to an approximate mass of 243 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 ⓘ

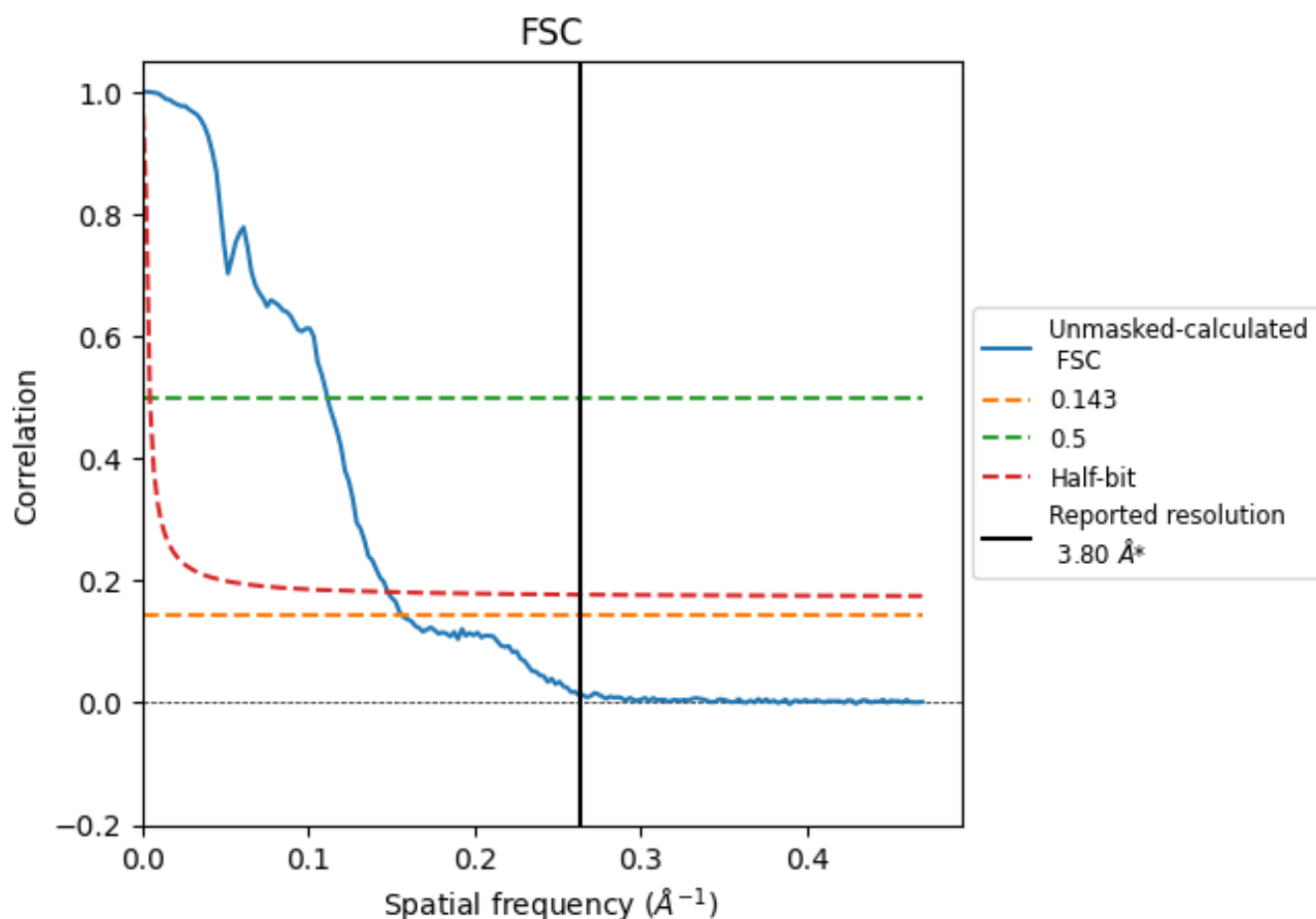


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

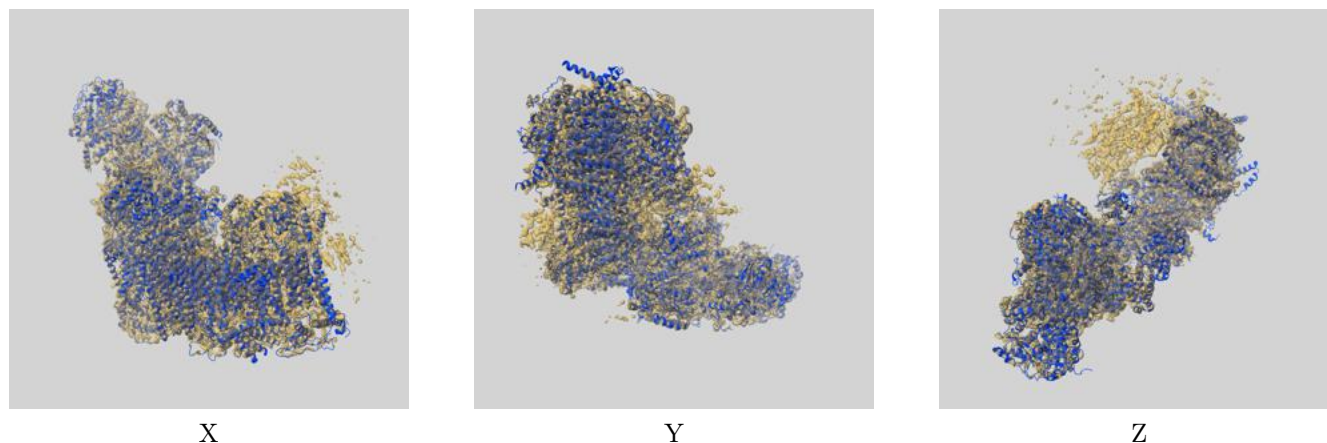
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.39	8.98	6.77

*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 6.39 differs from the reported value 3.8 by more than 10 %

9 Map-model fit [i](#)

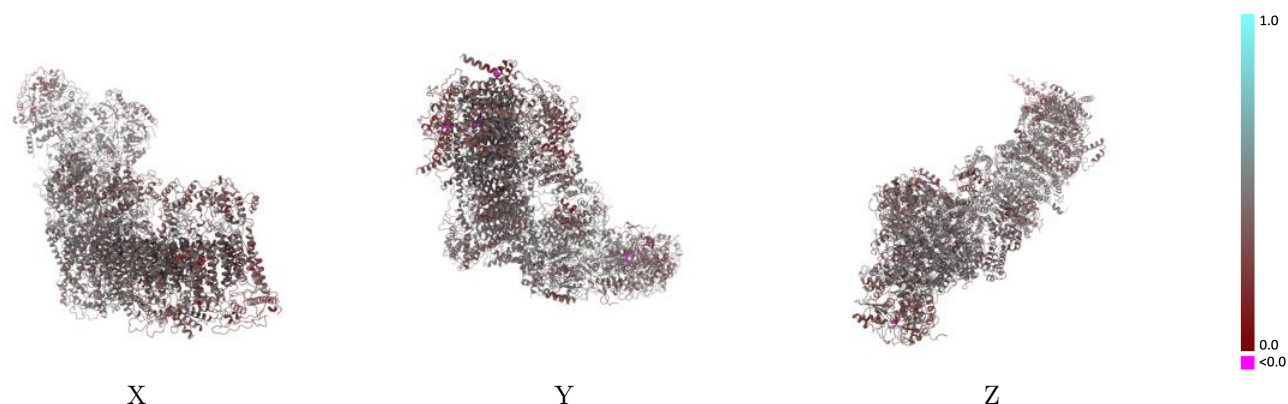
This section contains information regarding the fit between EMDB map EMD-42165 and PDB model 8UEO. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

9.1 Map-model overlay [i](#)



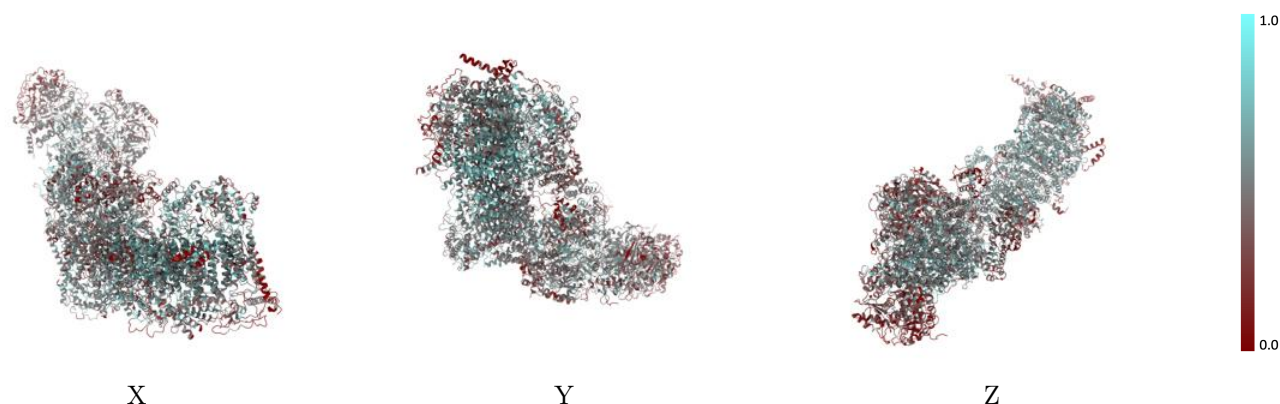
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



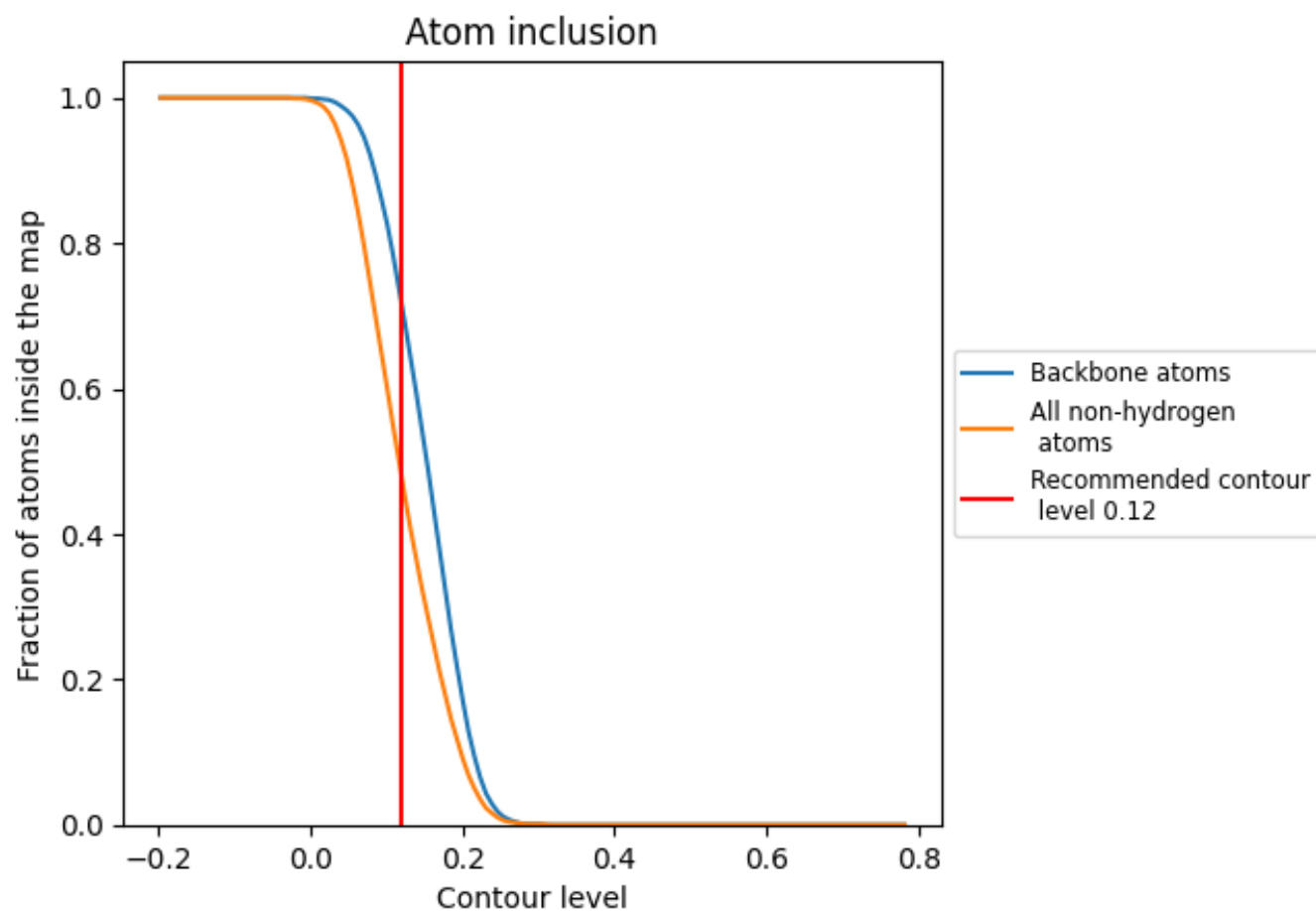
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 48% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4770	 0.4120
1A	 0.4680	 0.4240
1B	 0.5590	 0.4530
1C	 0.5460	 0.4500
1D	 0.5640	 0.4510
1E	 0.3100	 0.3780
1F	 0.3360	 0.3820
1G	 0.4480	 0.4200
1H	 0.5340	 0.4450
1I	 0.5720	 0.4370
1J	 0.4850	 0.4140
1K	 0.5120	 0.4170
1L	 0.5500	 0.4030
1M	 0.6230	 0.4450
1N	 0.5770	 0.4400
1O	 0.3790	 0.3960
1P	 0.4070	 0.4220
1Q	 0.4150	 0.4260
1R	 0.4500	 0.4420
1S	 0.2940	 0.3440
1T	 0.2020	 0.3200
1U	 0.4740	 0.3560
1V	 0.4060	 0.3980
1W	 0.3770	 0.4010
1X	 0.4940	 0.4180
1Y	 0.4990	 0.4060
1Z	 0.5300	 0.4280
1a	 0.5290	 0.4310
1b	 0.4780	 0.4150
1c	 0.3920	 0.3890
1d	 0.5450	 0.4260
1e	 0.5390	 0.4300
1f	 0.3190	 0.3980
1g	 0.4690	 0.3820
1h	 0.5310	 0.4090



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1i	 0.3260	 0.3440
1j	 0.3690	 0.3460
1k	 0.3620	 0.3670
1l	 0.5030	 0.3960
1m	 0.5540	 0.4000
1n	 0.5320	 0.3750
1o	 0.3410	 0.3020
1p	 0.4820	 0.3850
1q	 0.4960	 0.4440
1r	 0.5170	 0.4500
1s	 0.2000	 0.3420