



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 04:47 PM EDT

PDB ID : 8UEZ / pdb_00008uez
EMDB ID : EMD-42176
Title : In-situ complex I, Active-Q10 (State-delta)
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.50 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:

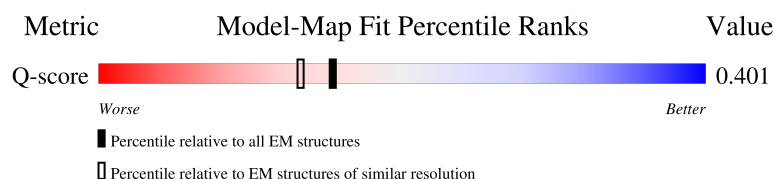
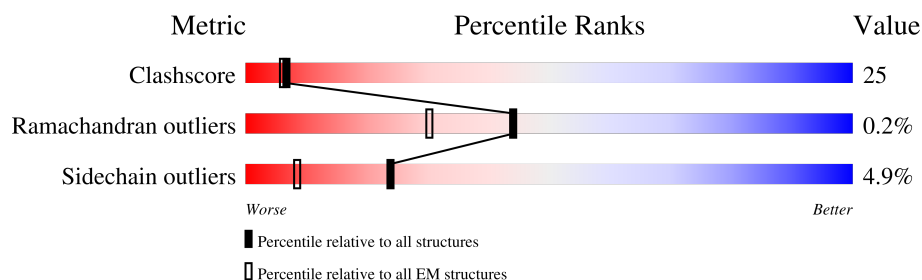
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



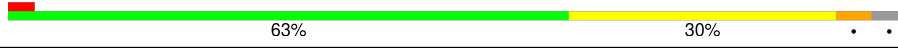
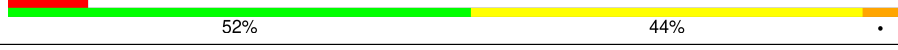
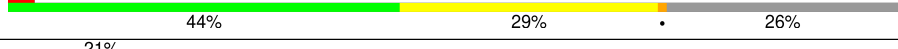
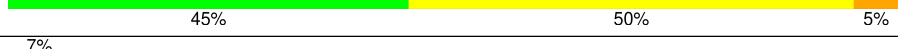
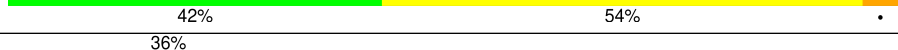
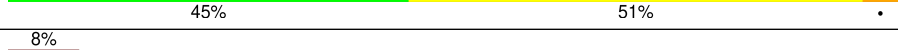
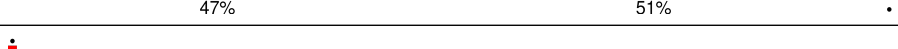
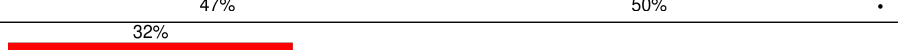
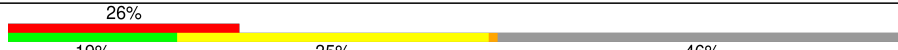
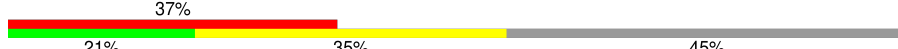
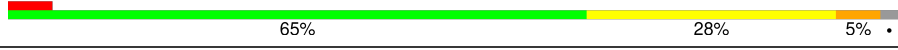
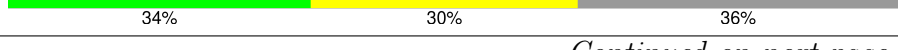
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	
2	1B	258	
3	1C	264	
4	1D	476	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
29	1d	123	
30	1e	106	
31	1f	135	
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	114	
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
45	SF4	1F	502	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67334 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
			916	616	134	159	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
			1740	1125	297	316	2		

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	1R	96	Total	C	N	O	S	0	0
			741	452	140	146	3		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	128	Total	C	N	O	0	0
			1062	691	182	189		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	1n	172	Total	C	N	O	S	0	0
			1495	956	273	258	8		

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

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

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

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

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

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

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

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

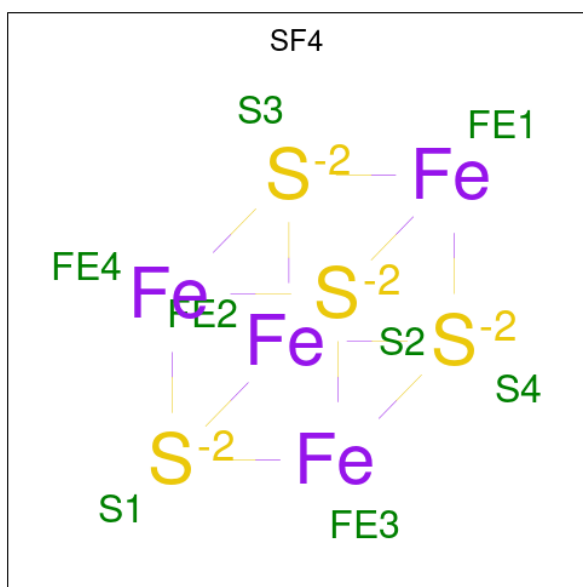
There is a discrepancy between the modelled and reference sequences:

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

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

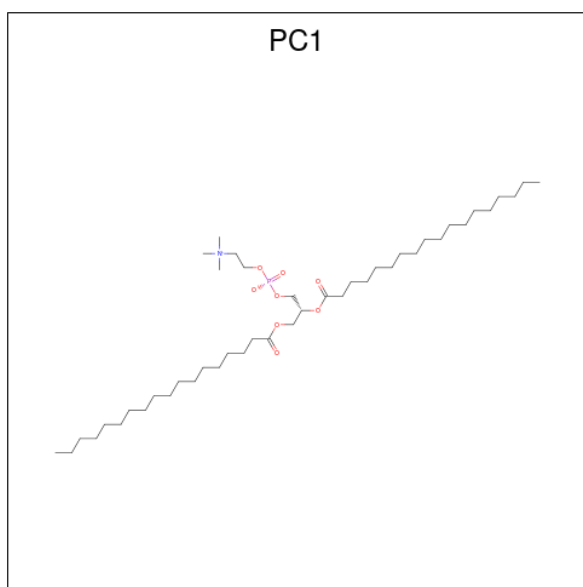
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



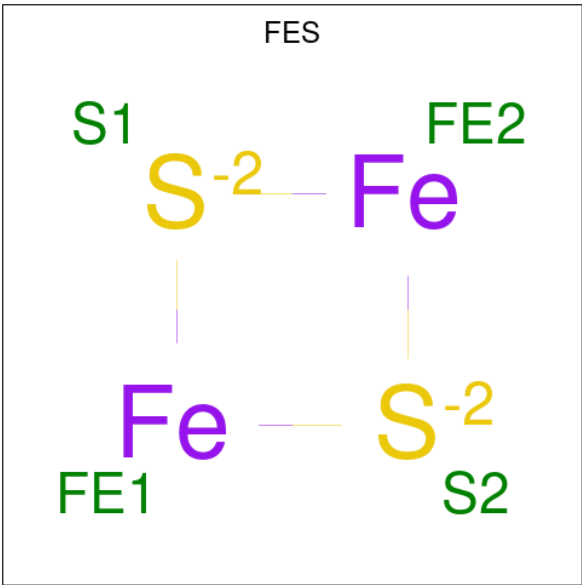
Mol	Chain	Residues	Atoms			AltConf
45	1B	1	Total	Fe	S	0
			8	4	4	
45	1F	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	

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



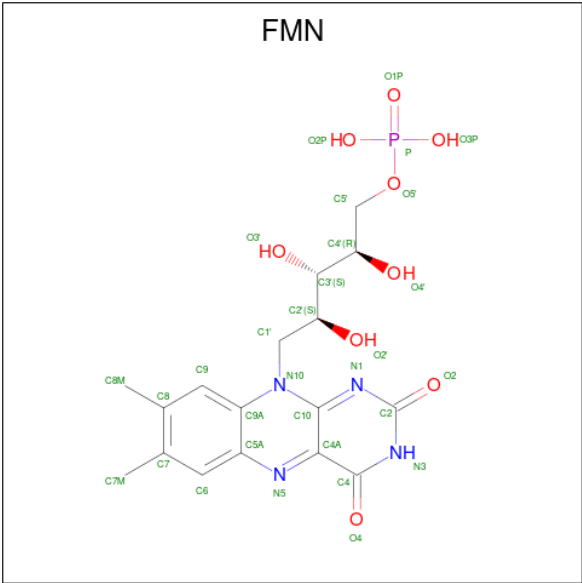
Mol	Chain	Residues	Atoms					AltConf
46	1B	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1f	1	Total	C	N	O	P	0
			25	15	1	8	1	
46	1q	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



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

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).

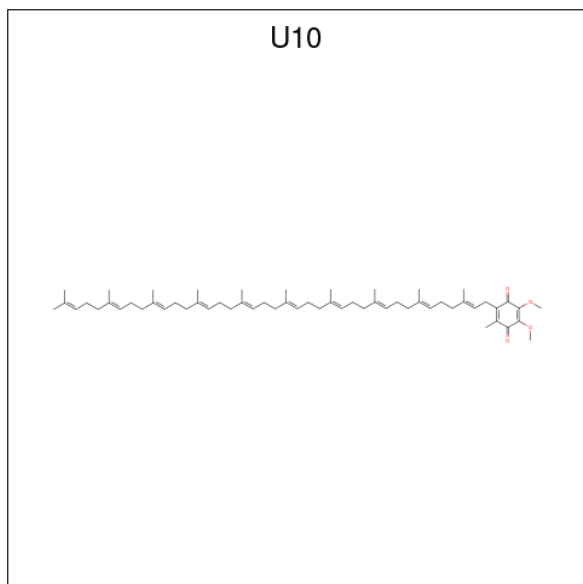


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

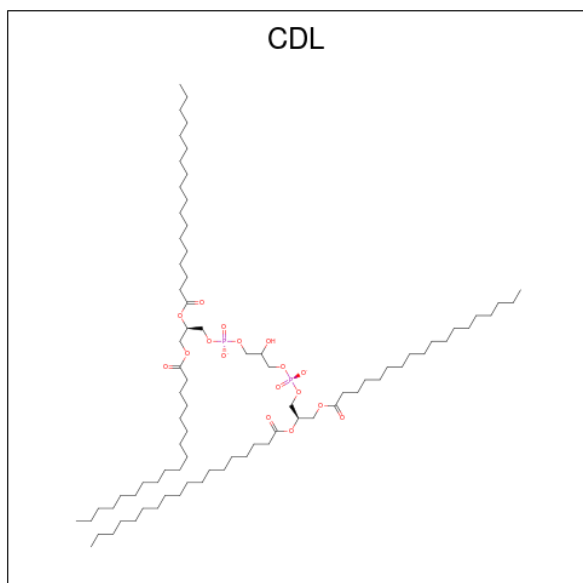
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

- Molecule 50 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$) (labeled as "Ligand of Interest" by depositor).



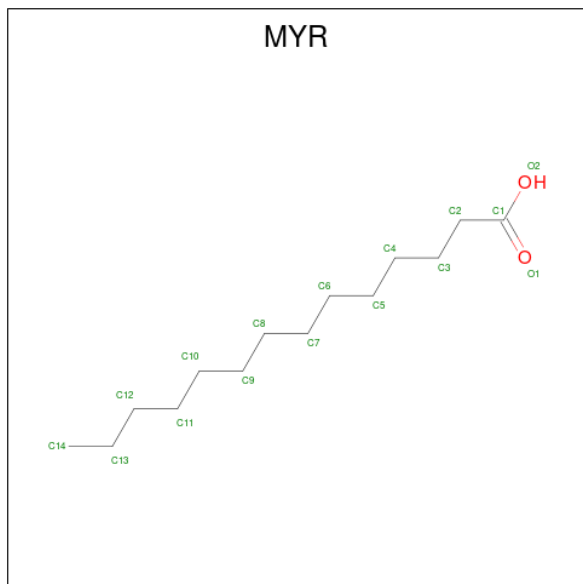
Mol	Chain	Residues	Atoms			AltConf
50	1H	1	Total	C	O	0
			63	59	4	

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



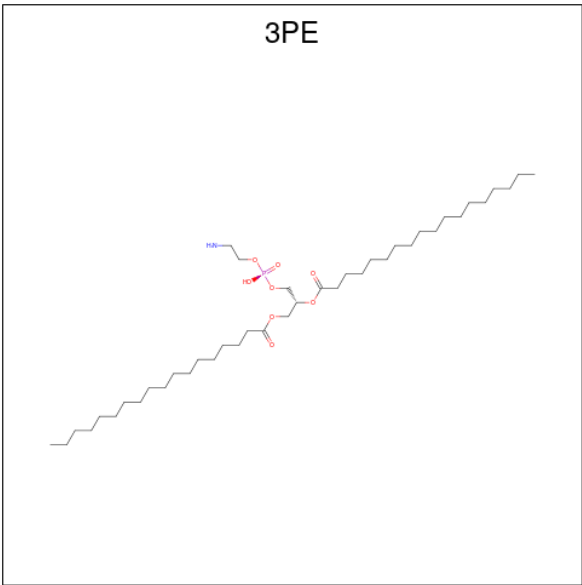
Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total	C	O	P	0
			51	32	17	2	
51	1O	1	Total	C	O	P	0
			67	48	17	2	
51	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



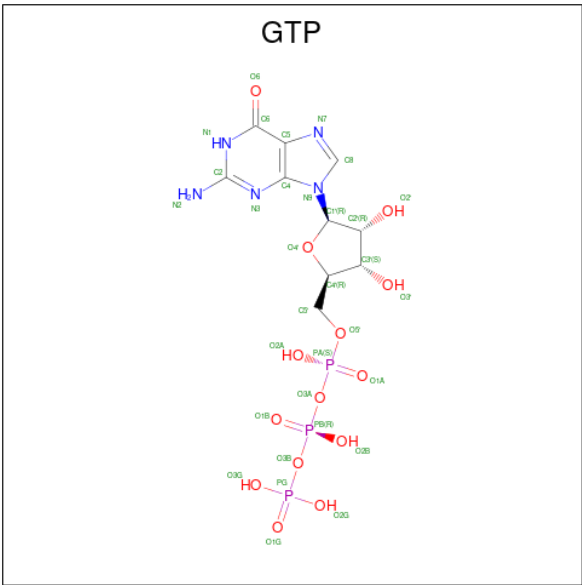
Mol	Chain	Residues	Atoms			AltConf
52	1L	1	Total	C	O	0
			15	14	1	

- Molecule 53 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
53	1M	1	Total	C	N	O	P	0
			38	28	1	8	1	
53	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

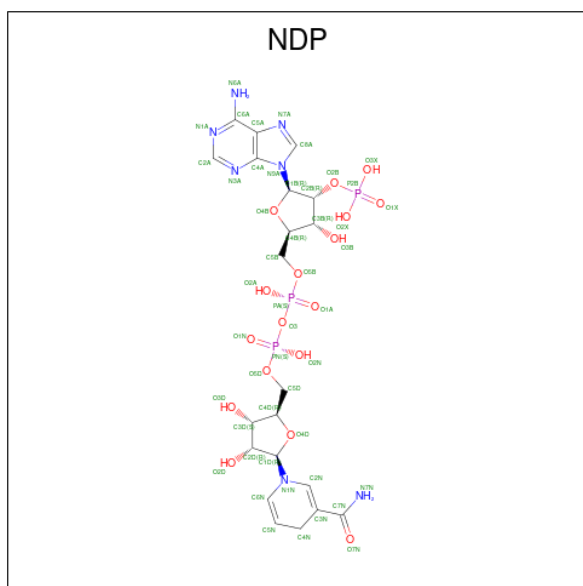


Mol	Chain	Residues	Atoms					AltConf
54	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
55	1O	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

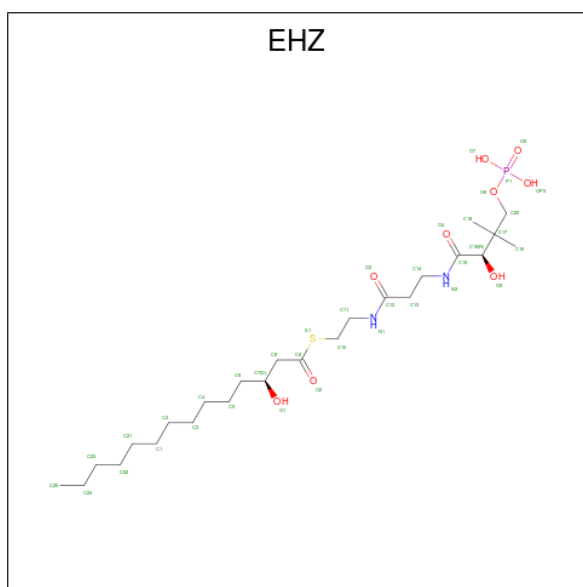


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
57	1R	1	Total	Zn	0
			1	1	

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).

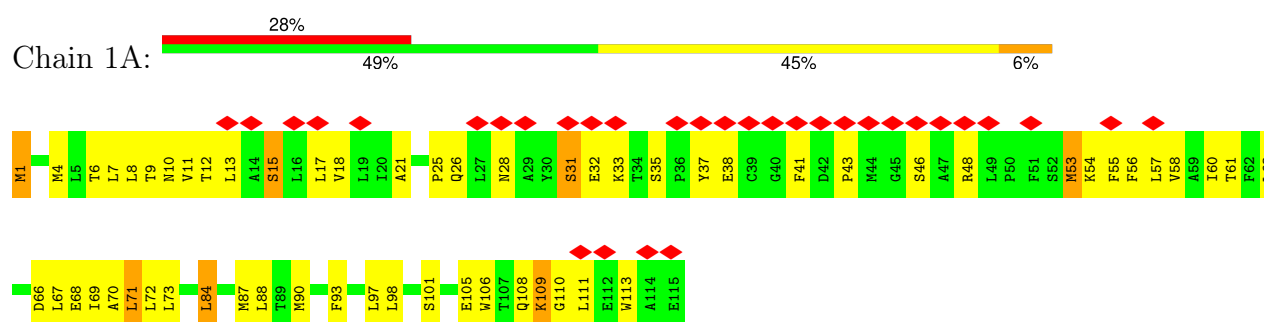


Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total 37	C 25	N 2	O 8	P 1	S 1	0
58	1n	1	Total 37	C 25	N 2	O 8	P 1	S 1	0

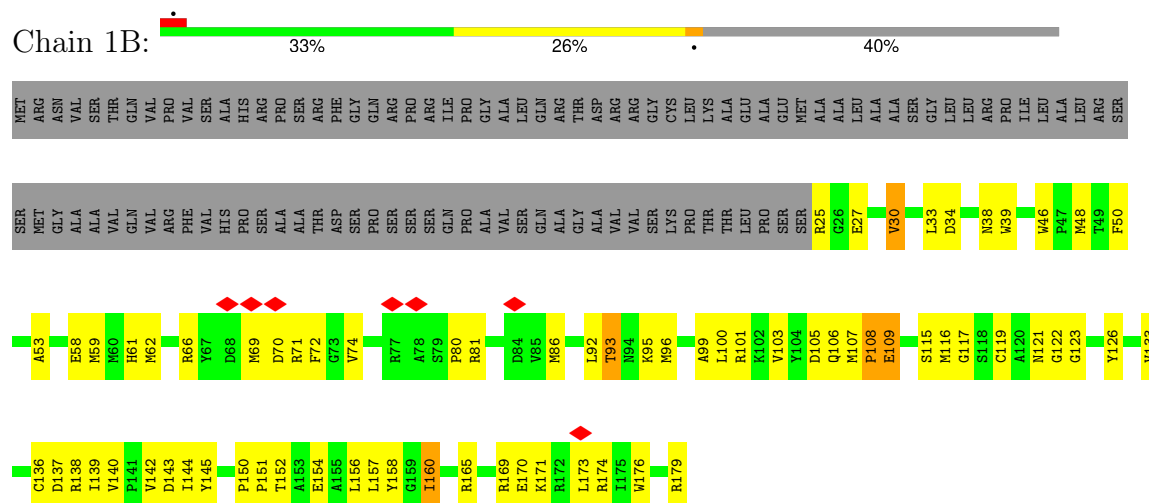
3 Residue-property plots [i](#)

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

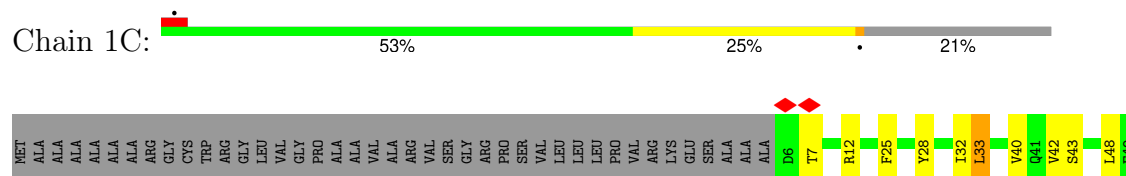
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

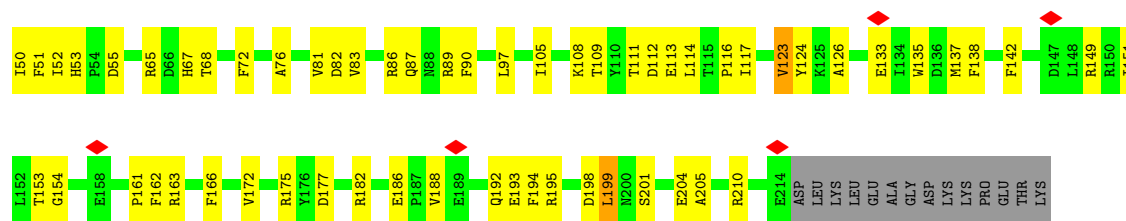


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

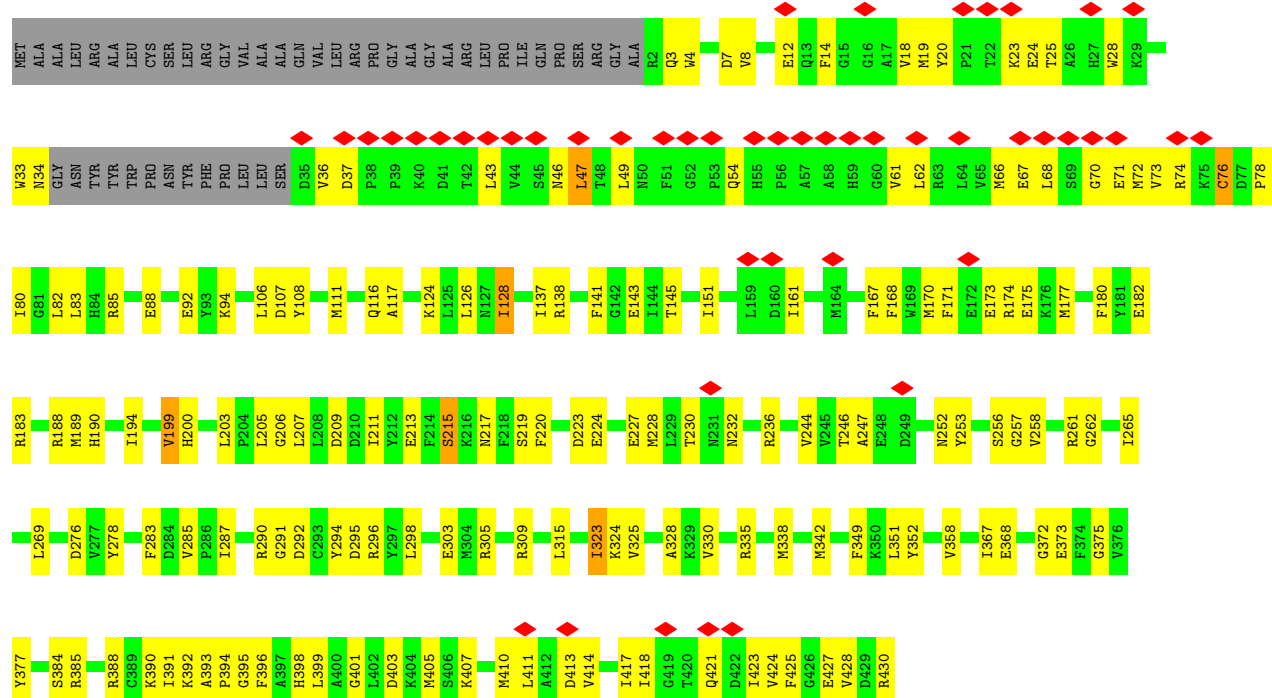


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

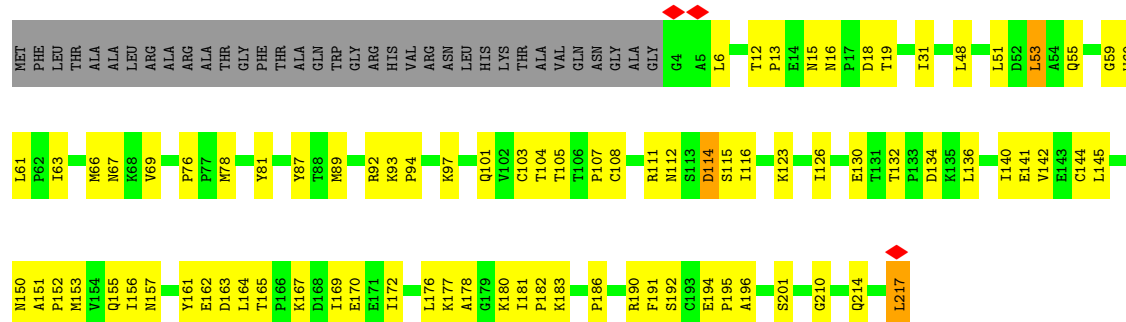




- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

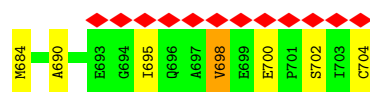


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

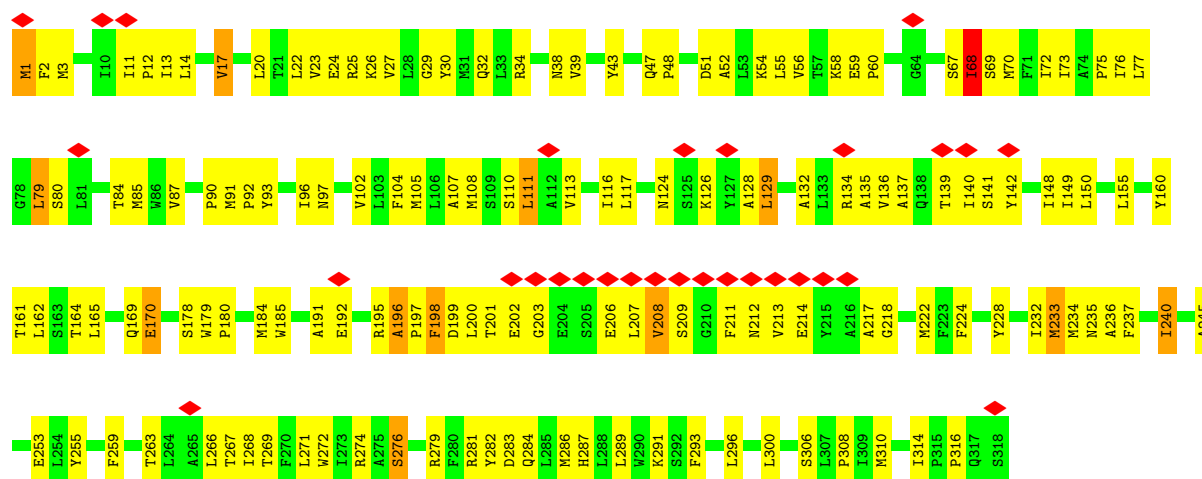


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial





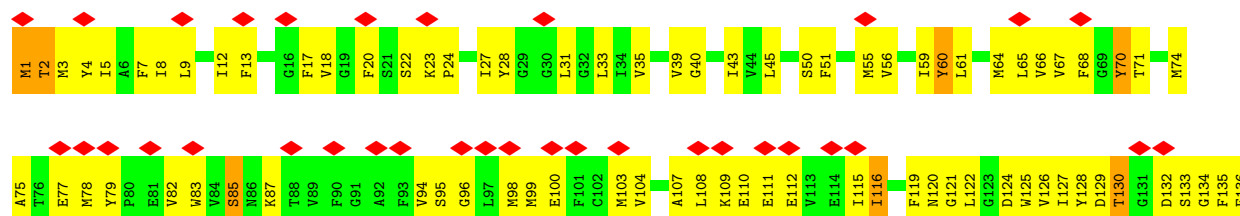
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

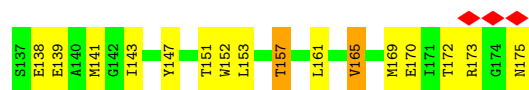


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

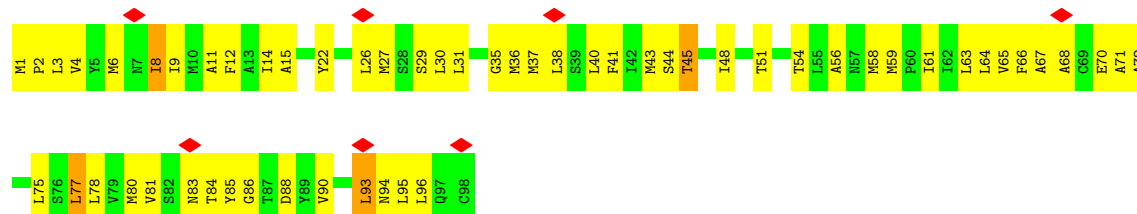
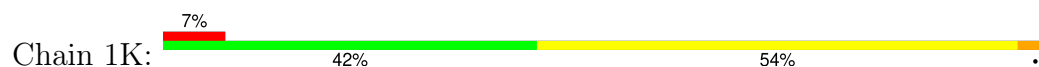


• Molecule 10: NADH-ubiquinone oxidoreductase chain 6

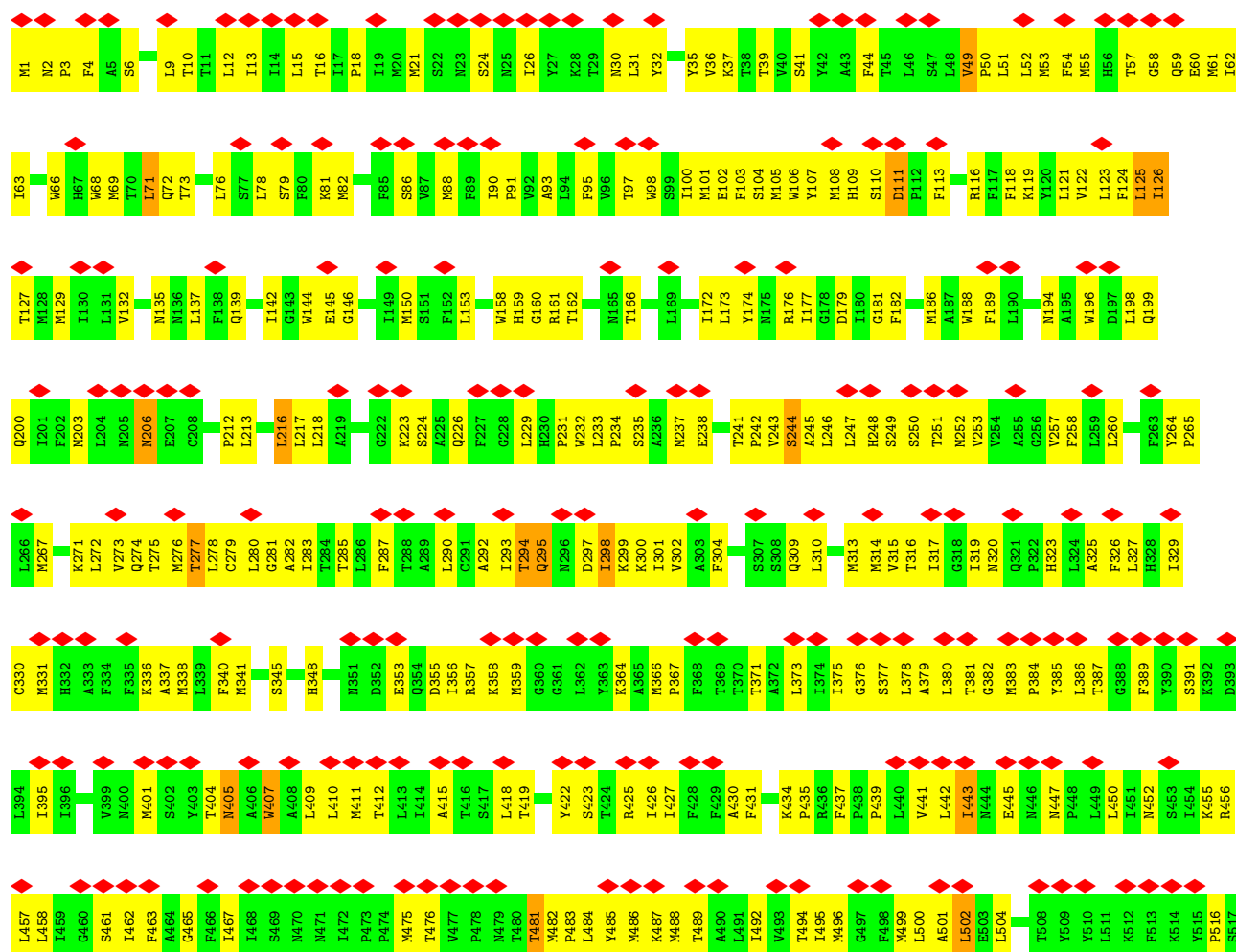


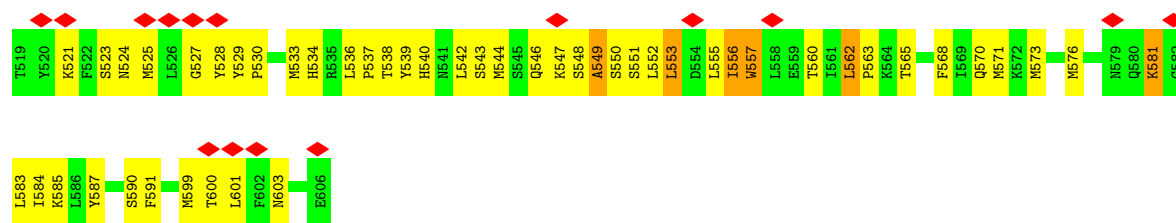


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

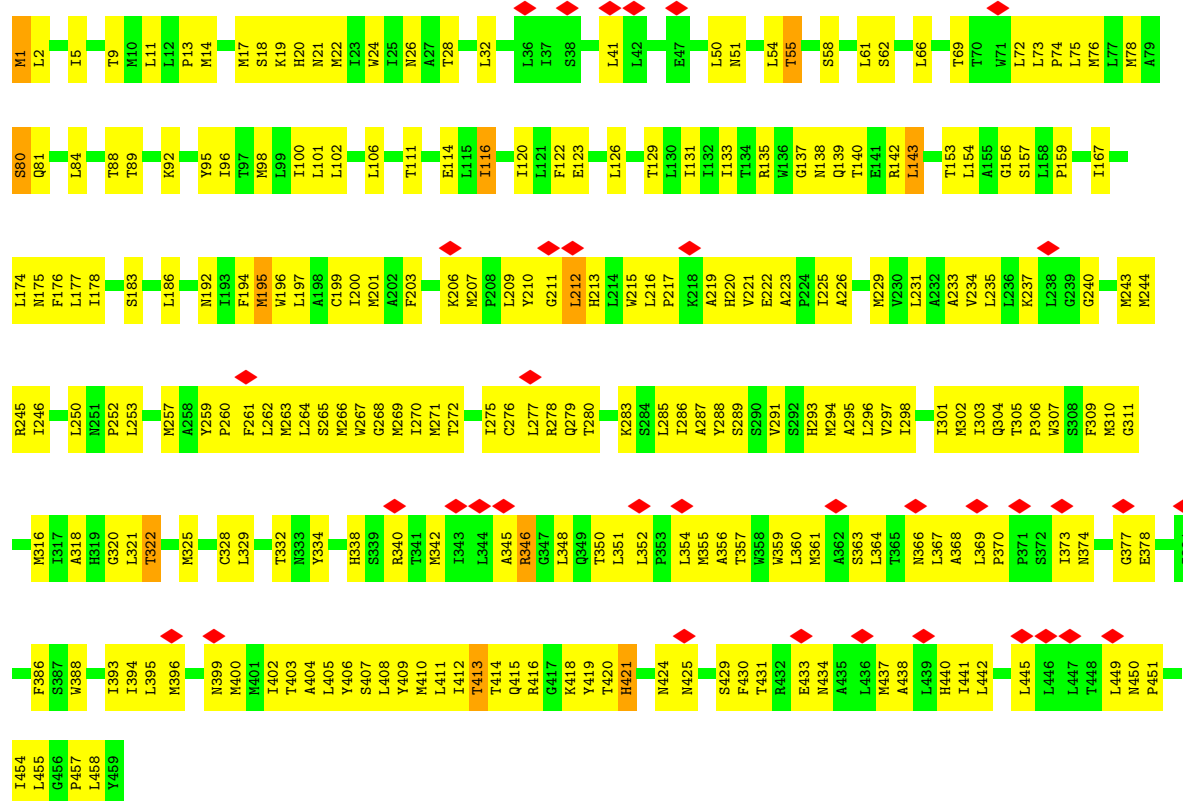


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

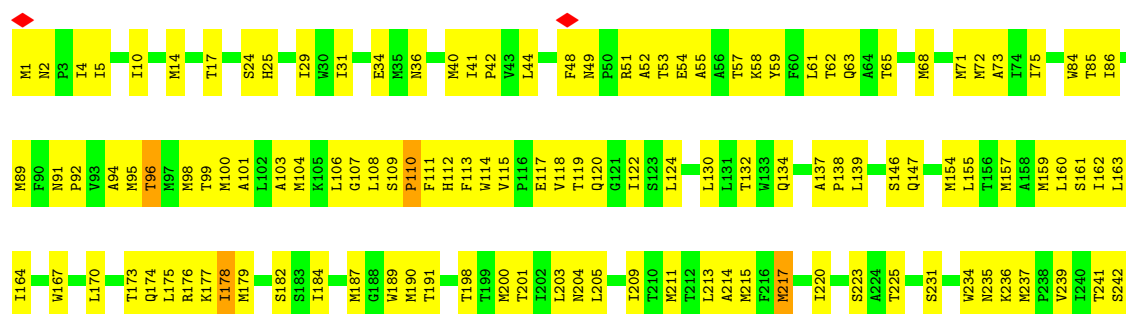




• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

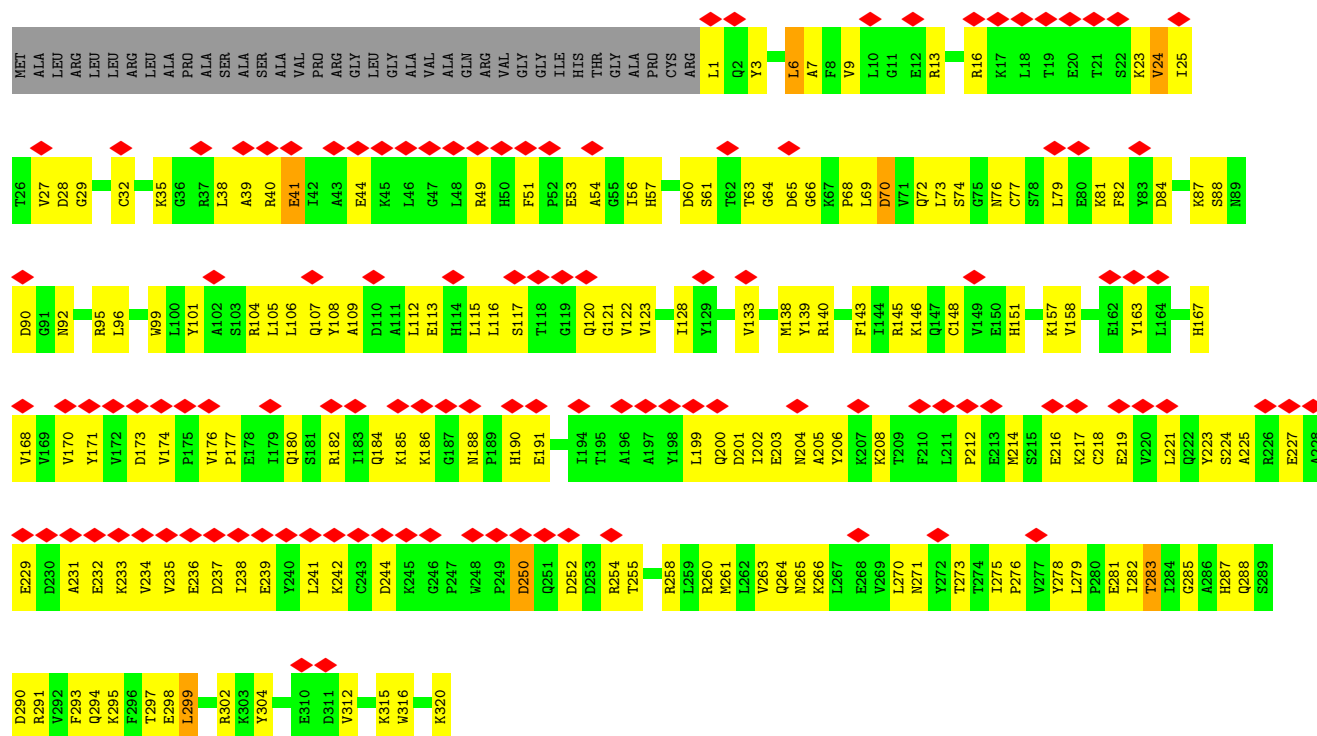
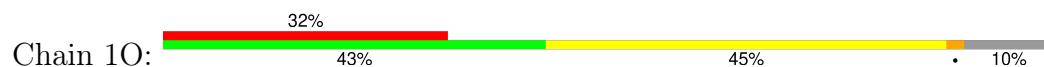


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

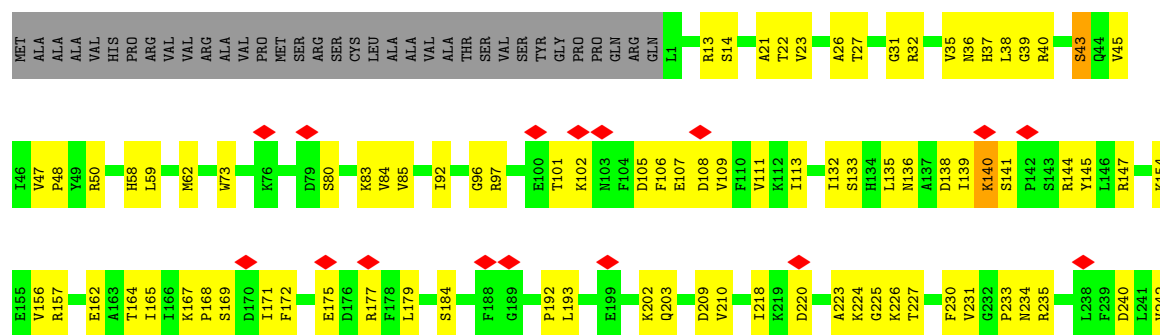


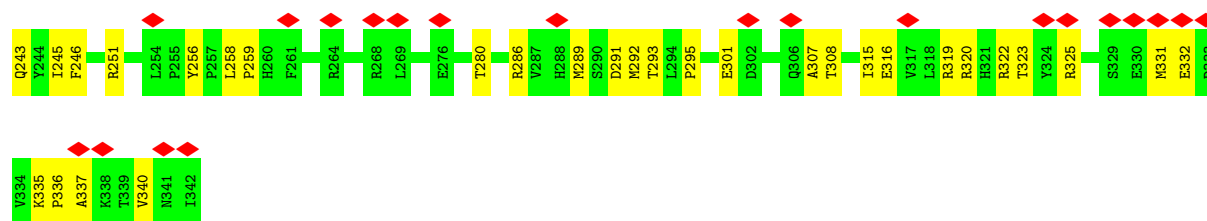


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

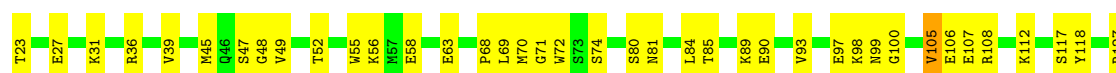
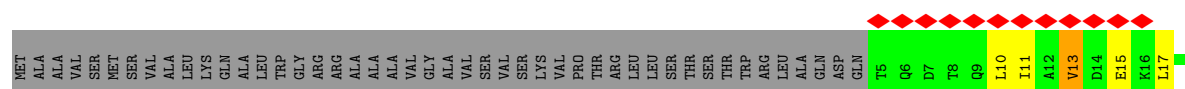


- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

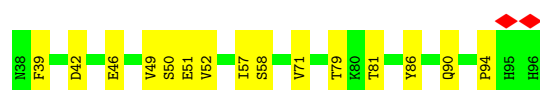
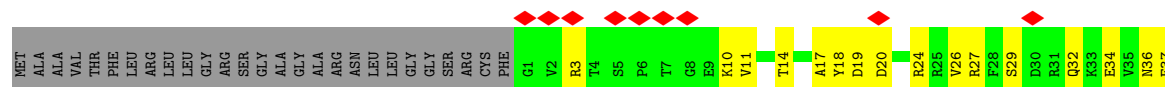




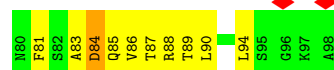
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



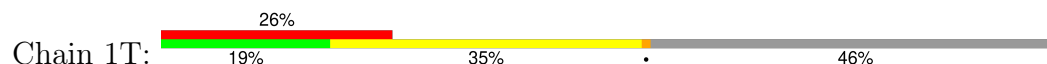
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

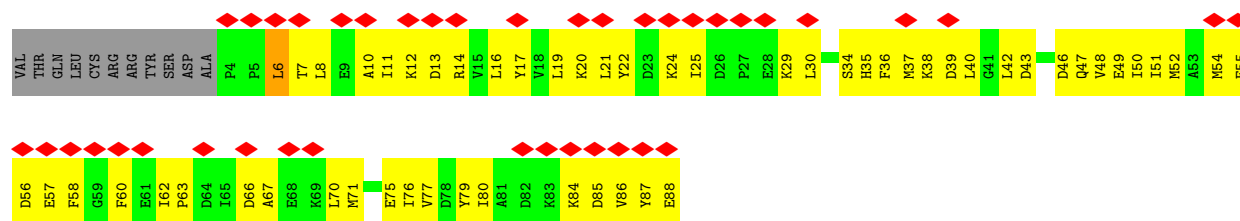


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

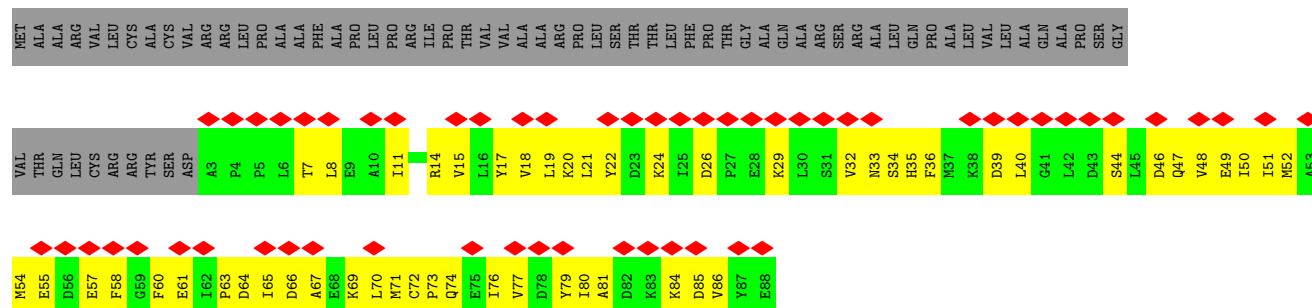
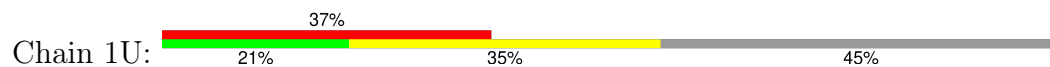


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1





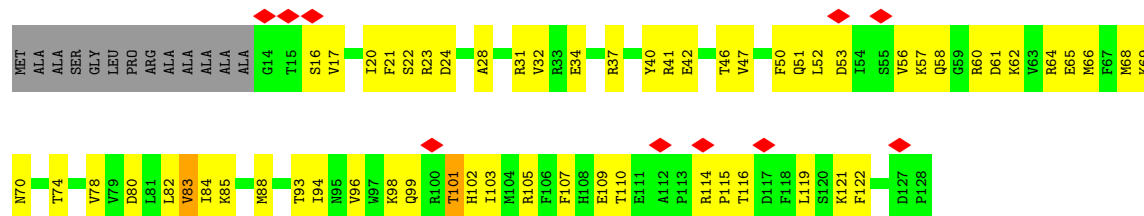
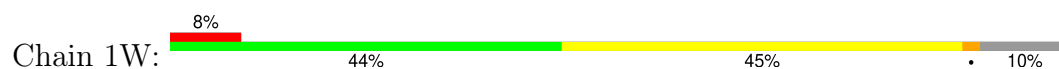
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



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

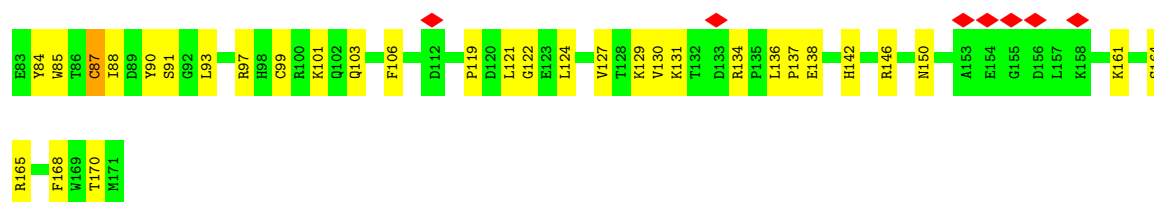


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

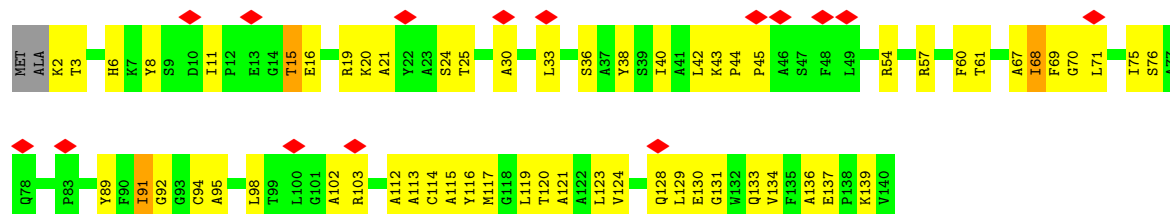


• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8





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



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



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



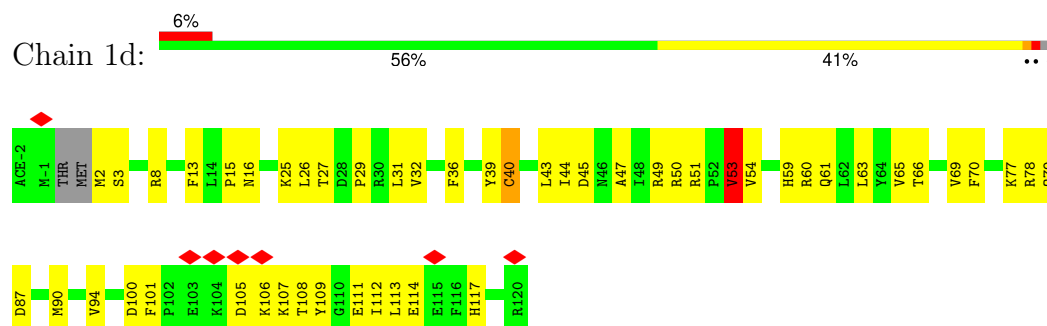
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



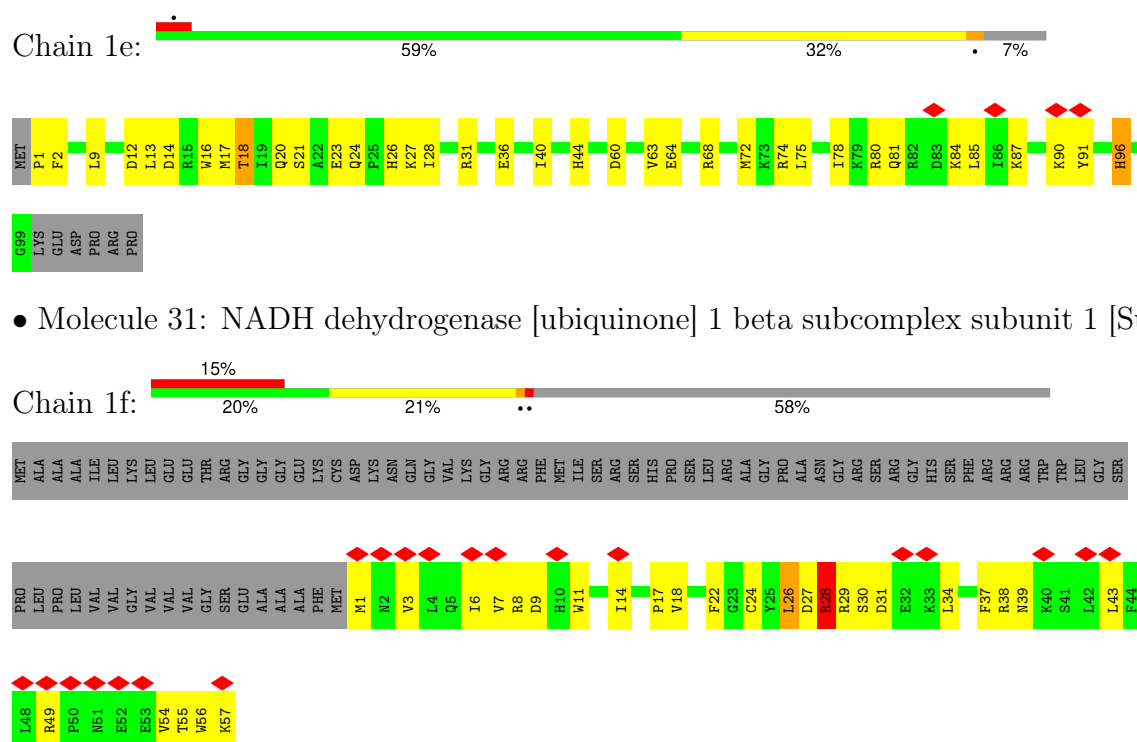
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



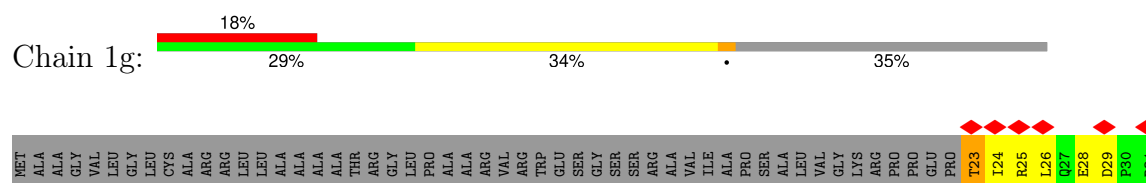
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

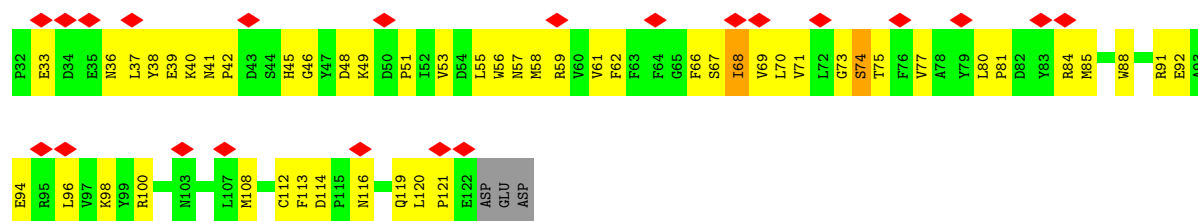


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

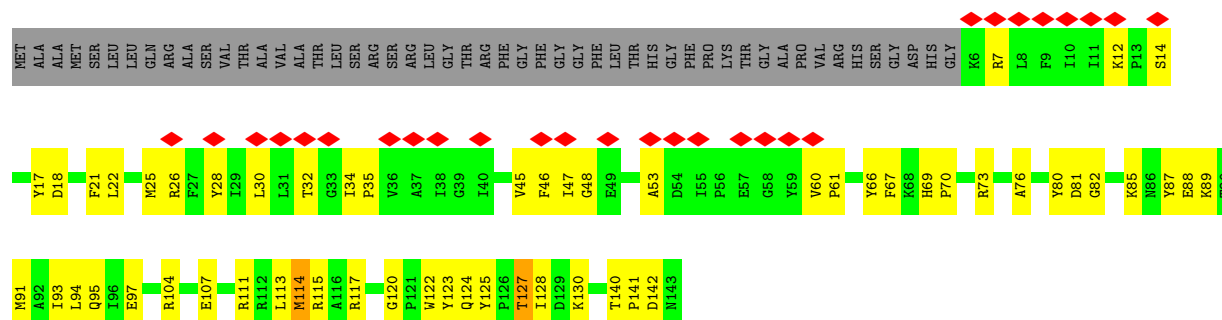


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

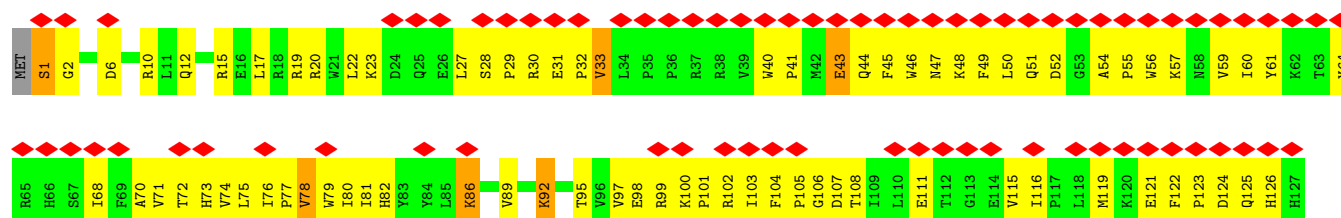




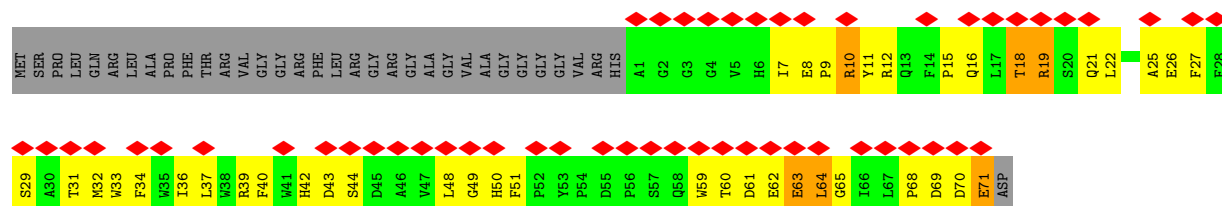
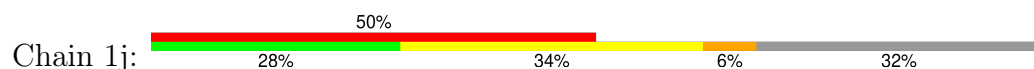
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

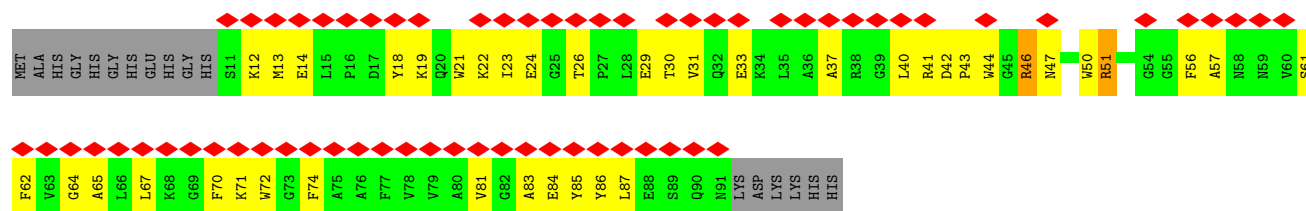


- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

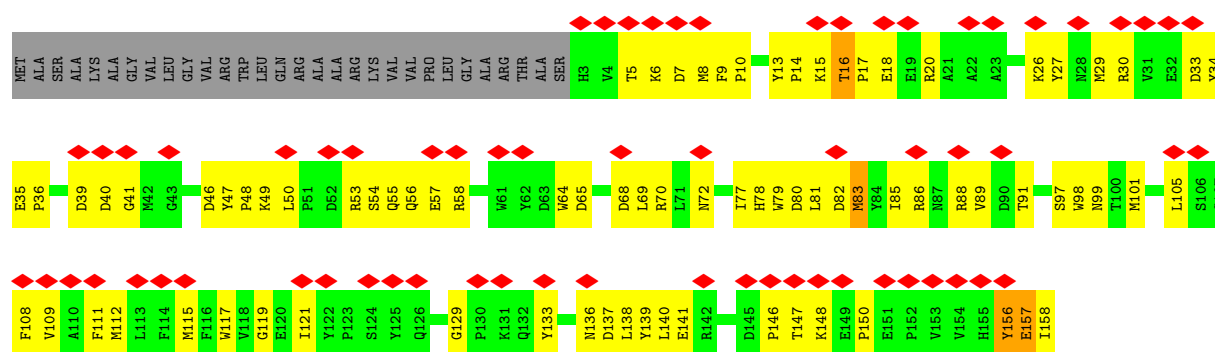
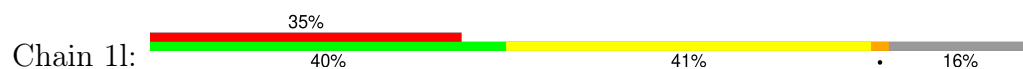


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

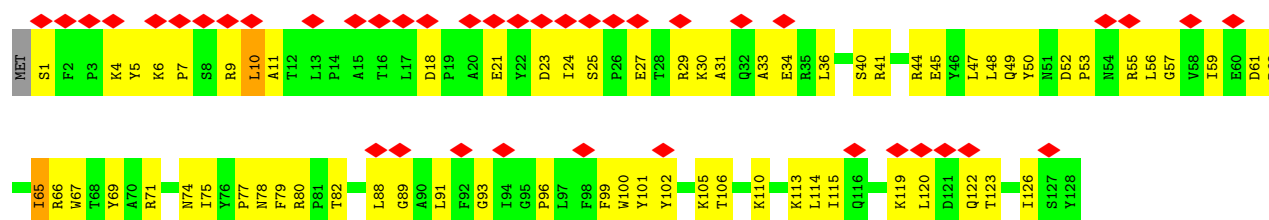




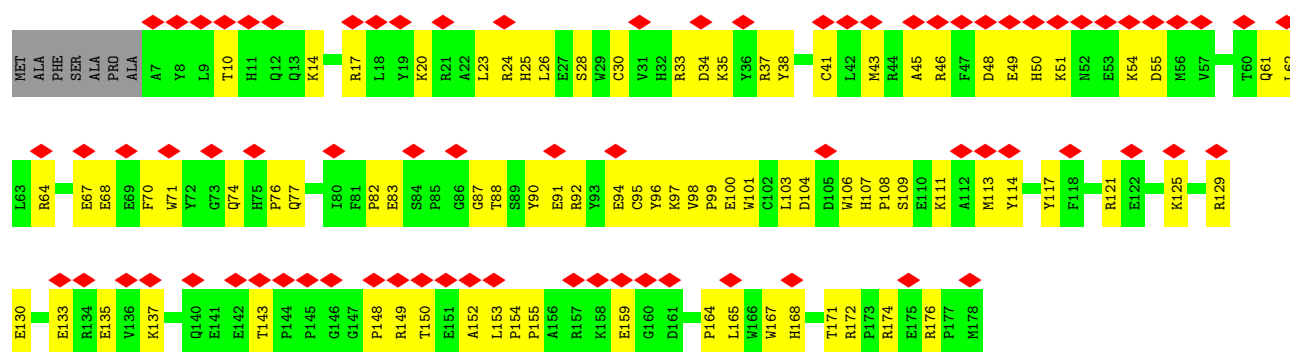
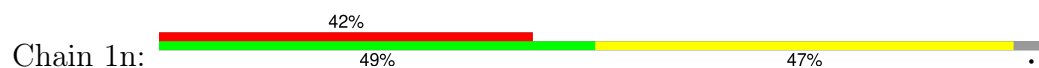
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



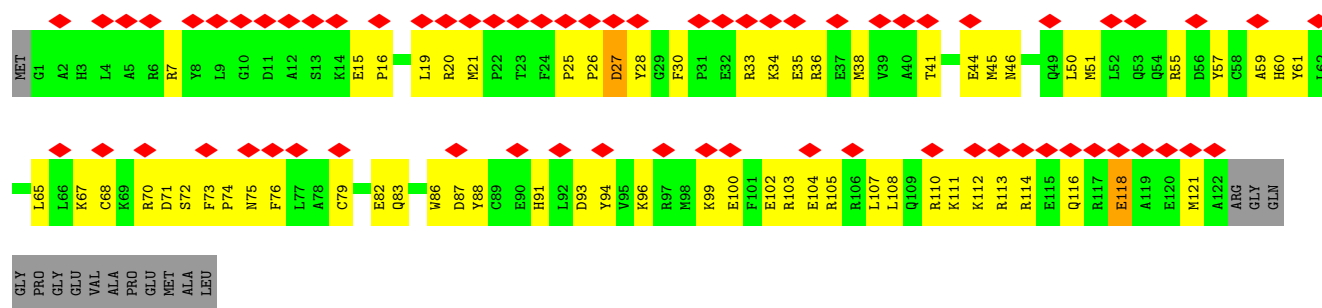
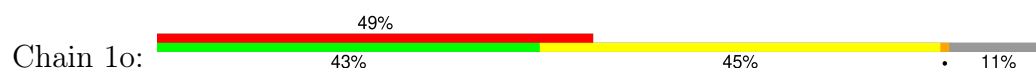
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



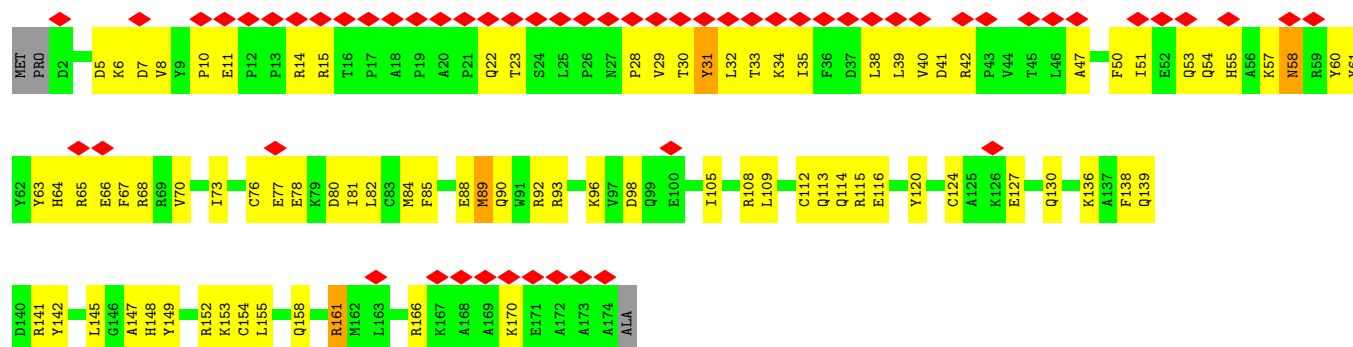
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



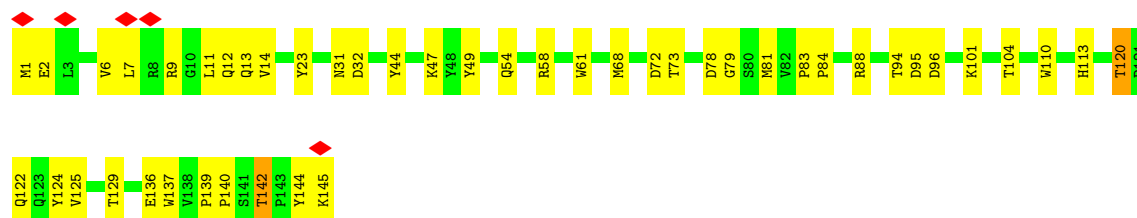
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



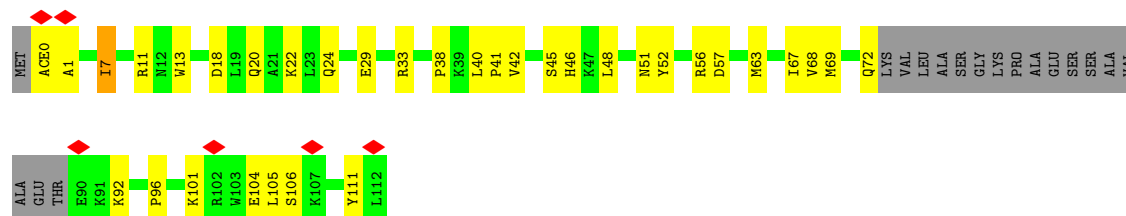
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



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



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



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

PRO	VAL	ALA	GLU	VAL	GLU	VAL	LEU	ALA	MET
ALA	ALA	PRO	ARG	ASP	ARG	LYS	VAL	GLN	ALA
ALA	GLU	GLU	ALA	ARG	GLY	THR	PHE	GLU	ALA
ALA	LYS	GLY	GLY	ALA	GLY	SER	PHE	GLY	LEU
ALA	GLY	PRO	PRO	PRO	PRO	PRO	ARG	THR	LEU
E31	GLU	ALA	ALA	LYS	LYS	GLY	LYS	PRO	GLN
P32	LEU	LEU	SER	ALA	ALA	GLY	VAL	LEU	ARG
F33	LEU	GLU	ALA	ALA	SER	SER	LEU	ALA	GLN
D34	GLY	GLU	ALA	PRO	PRO	LYS	SER	THR	GLY
N35	ARG	ALA	ALA	GLY	ALA	ALA	PHE	ALA	ALA
S36	PRO	PRO	ALA	SER	GLU	GLU	SER	ALA	ARG
Q42	PRO	LEU	THR	ARG	ALA	ALA	GLN	PRO	ARG
E45	GLN	ALA	ALA	GLY	GLY	ARG	GLY	LEU	LEU
D53	PRO	ALA	LEU	ALA	ALA	ALA	SER	GLN	VAL
L54	LYS	ARG	LEU	ALA	GLY	ALA	ALA	GLN	LEU
L58	VAL	VAL	PRO	ARG	GLY	ALA	ALA	SER	GLY
S59	ASP	ALA	PRO	THR	SER	PRO	GLN	THR	GLY
K60	GLY	ALA	ALA	GLY	GLN	ALA	ALA	SER	VAL
F61	GLN	THR	THR	THR	THR	THR	ALA	ALA	PHE
R62	ASP	GLU	GLU	PRO	GLY	VAL	ARG	PRO	ARG
P66	GLY	GLY	GLY	SER	GLY	VAL	GLY	PRO	GLY
R70	ALA	GLY	GLY	LYS	ALA	ALA	ALA	LEU	ALA
Q71	GLU	ARG	ARG	ILE	LYS	GLU	GLY	ALA	PRO
S72	LYS	PRO	LEU	PRO	ARG	ALA	ALA	ARG	VAL
F73	ALA	GLY	GLY	SER	THR	PRO	THR	GLY	SER
R74	LEU	GLU	GLU	GLY	GLY	GLY	SER	LEU	LEU
H75	ARG	VAL	ARG	GLU	GLU	PRO	SER	THR	SER
	PRO	ALA	ARG	ALA	ALA	ASP	SER	LEU	ALA
	PRO	PHE	LEU	LYS	THR	ARG	ASP	PHE	PRO
	GLY	SER	SER	SER	GLU	PRO	GLU	THR	ASN
	THR	ARG	ALA	ALA	GLN	ARG	GLU	ASP	ASN
	ALA	ALA	PRO	PRO	LEU	ALA	SER	THR	GLY
	ASP	VAL	GLN	LYS	GLN	ASP	SER	GLY	ASN
	ILE	GLN	GLY	GLY	GLY	ASP	SER	PRO	ASN
	ALA	VAL	ALA	ALA	ALA	ALA	ASP	GLY	GLY
	GLY	ALA	SER	GLU	SER	GLU	SER	ASP	LYS
	ASP	ALA	GLY	ALA	GLY	ALA	GLU	THR	ARG
	ALA	ALA	PRO	VAL	VAL	GLU	SER	LEU	ARG
	PRO	LEU	LEU	LYS	THR	ARG	ASP	ASP	SER
	GLY	PHE	SER	THR	LYS	PRO	ASP	THR	PRO
	GLY	SER	SER	SER	GLY	ARG	GLU	ASP	ASN
	THR	ARG	ALA	GLN	ALA	GLY	GLU	ARG	LYS
	ALA	ALA	PRO	PRO	GLY	LYS	GLY	GLY	VAL
	GLY	ALA	ALA	ASP	PRO	GLY	GLY	ARG	VAL
	ARG	LEU	PRO	THR	THR	LYS	GLY	PRO	LYS
	ASP	GLY	GLY	THR	LYS	GLY	GLY	ARG	VAL
	ALA	GLN	SER	LYS	GLY	GLY	SER	PHE	ALA
	THR	GLN	THR	THR	THR	GLY	GLU	THR	THR
	GLN	ALA	ALA	GLY	GLY	GLY	VAL	ARG	VAL
	PRO	GLY	GLY	SER	SER	PRO	ARG	LYS	ALA
	THR	GLY	THR	THR	THR	PRO	PRO	THR	ALA

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	46000	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	1.011	Depositor
Minimum map value	-0.198	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	556.0, 556.0, 556.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: EHZ, FME, CDL, ZN, FES, U10, MYR, GTP, PC1, MG, ACE, 3PE, FMN, NDP, SF4, SAC, K

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	0.28	0/930	0.46	0/1271
2	1B	0.21	0/1273	0.39	0/1722
3	1C	0.16	0/1791	0.29	0/2439
4	1D	0.20	0/3545	0.35	0/4806
5	1E	0.15	0/1698	0.34	0/2311
6	1F	0.62	7/3401 (0.2%)	0.83	10/4595 (0.2%)
7	1G	0.21	1/5451 (0.0%)	0.31	1/7387 (0.0%)
8	1H	0.25	0/2566	0.42	0/3509
9	1I	0.25	0/1443	0.33	0/1952
10	1J	0.24	0/1364	0.46	0/1850
11	1K	0.35	1/751 (0.1%)	0.50	0/1018
12	1L	0.28	1/4939 (0.0%)	0.46	0/6718
13	1M	0.22	1/3713 (0.0%)	0.41	0/5063
14	1N	0.38	1/2765 (0.0%)	0.45	2/3758 (0.1%)
15	1O	0.18	0/2650	0.40	0/3588
16	1P	0.17	0/2828	0.31	0/3834
17	1Q	0.20	0/1070	0.36	0/1446
18	1R	0.17	0/755	0.31	0/1018
19	1S	0.13	0/711	0.29	0/956
20	1T	0.29	0/701	0.50	0/946
20	1U	0.19	0/706	0.42	0/954
21	1V	0.27	0/946	0.47	0/1281
22	1W	0.19	0/995	0.40	0/1340
23	1X	0.27	1/1436 (0.1%)	0.31	0/1938
24	1Y	0.27	0/1037	0.44	0/1404
25	1Z	0.25	1/1199 (0.1%)	0.31	0/1617
26	1a	0.18	0/577	0.31	0/777
27	1b	0.27	0/664	0.38	0/912
28	1c	0.21	0/430	0.50	0/581
29	1d	0.20	0/1024	0.46	0/1383
30	1e	0.15	0/836	0.33	0/1118
31	1f	0.19	0/499	0.58	1/673 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.16	0/858	0.44	0/1165
33	1h	0.15	0/1184	0.33	0/1603
34	1i	0.21	0/1131	0.46	0/1541
35	1j	0.44	1/627 (0.2%)	0.47	0/858
36	1k	0.23	0/668	0.44	0/903
37	1l	0.17	0/1365	0.39	0/1867
38	1m	0.22	0/1092	0.39	0/1481
39	1n	0.14	0/1549	0.34	0/2098
40	1o	0.14	0/1069	0.36	0/1430
41	1p	0.13	0/1481	0.30	0/1997
42	1q	0.37	1/1253 (0.1%)	0.46	1/1704 (0.1%)
43	1r	0.21	0/782	0.37	0/1057
44	1s	0.95	5/394 (1.3%)	1.21	7/533 (1.3%)
All	All	0.27	21/68147 (0.0%)	0.43	22/92402 (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
2	1B	0	2
6	1F	0	2
8	1H	0	1
21	1V	0	1
31	1f	0	1
All	All	0	7

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1F	207	PRO	CG-CD	-23.91	0.69	1.50
14	1N	323	MET	SD-CE	-14.93	1.42	1.79
12	1L	90	ILE	CA-CB	13.37	1.61	1.54
6	1F	206	LYS	C-N	13.09	1.48	1.33
44	1s	32	PRO	CG-CD	-11.18	1.12	1.50
6	1F	207	PRO	CB-CG	10.37	2.01	1.49
6	1F	207	PRO	CA-CB	-10.32	1.39	1.54
42	1q	139	PRO	CA-C	9.80	1.58	1.52
6	1F	206	LYS	CA-CB	9.64	1.63	1.53
6	1F	207	PRO	C-N	9.54	1.46	1.33
23	1X	87	CYS	CB-SG	-8.63	1.52	1.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	1s	32	PRO	N-CA	-7.48	1.37	1.47
44	1s	32	PRO	N-CD	6.89	1.57	1.47
11	1K	8	ILE	CG1-CD1	-6.73	1.25	1.51
44	1s	31	GLU	C-N	6.60	1.49	1.33
25	1Z	120	MET	SD-CE	-6.10	1.64	1.79
35	1j	71	GLU	CD-OE1	-5.70	1.14	1.25
13	1M	212	LEU	CG-CD1	-5.42	1.34	1.52
44	1s	32	PRO	CB-CG	5.39	1.76	1.49
7	1G	21	GLU	CD-OE2	-5.11	1.15	1.25
6	1F	206	LYS	CA-C	5.09	1.58	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	1F	207	PRO	CB-CG-CD	-33.15	0.04	106.10
6	1F	207	PRO	CA-N-CD	-29.18	71.15	112.00
44	1s	32	PRO	CA-N-CD	-19.83	84.24	112.00
6	1F	207	PRO	N-CA-CB	-17.24	86.35	103.08
6	1F	207	PRO	CA-CB-CG	-12.52	80.72	104.50
6	1F	207	PRO	N-CD-CG	-10.55	87.37	103.20
42	1q	139	PRO	O-C-N	10.35	126.02	121.15
6	1F	206	LYS	C-N-CD	9.25	162.92	125.00
6	1F	207	PRO	O-C-N	-7.84	112.20	121.46
6	1F	206	LYS	CA-C-O	-7.83	110.47	120.80
44	1s	31	GLU	C-N-CD	7.75	156.80	125.00
44	1s	32	PRO	CA-CB-CG	-6.97	91.25	104.50
44	1s	32	PRO	N-CD-CG	-6.67	93.20	103.20
14	1N	323	MET	CA-CB-CG	6.47	127.04	114.10
31	1f	28	ARG	CA-CB-CG	6.25	126.61	114.10
6	1F	206	LYS	CA-C-N	-5.88	114.32	120.38
6	1F	206	LYS	C-N-CA	-5.88	114.32	120.38
14	1N	323	MET	N-CA-CB	-5.87	100.57	110.49
44	1s	32	PRO	CB-CG-CD	-5.58	88.26	106.10
7	1G	631	VAL	N-CA-C	-5.32	108.32	113.53
44	1s	31	GLU	CA-C-N	-5.27	113.25	119.84
44	1s	31	GLU	C-N-CA	-5.27	113.25	119.84

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1B	108	PRO	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	1B	109	GLU	Peptide
6	1F	206	LYS	Peptide
6	1F	207	PRO	Mainchain
8	1H	196	ALA	Peptide
21	1V	113	TRP	Peptide
31	1f	28	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	78	0
2	1B	1242	0	1248	64	0
3	1C	1740	0	1691	58	0
4	1D	3452	0	3389	158	0
5	1E	1658	0	1662	70	0
6	1F	3325	0	3288	138	0
7	1G	5362	0	5388	198	0
8	1H	2504	0	2602	182	0
9	1I	1412	0	1366	72	0
10	1J	1339	0	1337	125	0
11	1K	750	0	798	74	0
12	1L	4818	0	4954	360	0
13	1M	3632	0	3836	261	0
14	1N	2712	0	2873	208	0
15	1O	2590	0	2556	168	0
16	1P	2751	0	2776	100	0
17	1Q	1047	0	1042	42	0
18	1R	741	0	704	19	0
19	1S	700	0	719	29	0
20	1T	689	0	687	79	0
20	1U	694	0	691	69	0
21	1V	927	0	972	72	0
22	1W	971	0	975	66	0
23	1X	1398	0	1378	54	0
24	1Y	1016	0	1020	56	0
25	1Z	1168	0	1161	65	0
26	1a	562	0	557	25	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	1b	643	0	645	41	0
28	1c	417	0	425	27	0
29	1d	996	0	990	55	0
30	1e	816	0	823	37	0
31	1f	487	0	496	35	0
32	1g	835	0	795	58	0
33	1h	1151	0	1164	66	0
34	1i	1100	0	1106	93	0
35	1j	601	0	546	51	0
36	1k	649	0	626	64	0
37	1l	1310	0	1204	104	0
38	1m	1062	0	1075	89	0
39	1n	1495	0	1434	86	0
40	1o	1045	0	1018	69	0
41	1p	1449	0	1416	84	0
42	1q	1212	0	1172	39	0
43	1r	767	0	791	33	0
44	1s	382	0	351	20	0
45	1B	8	0	0	0	0
45	1F	8	0	0	3	0
45	1G	16	0	0	0	0
45	1I	16	0	0	1	0
46	1B	34	0	42	2	0
46	1L	46	0	66	5	0
46	1M	35	0	44	1	0
46	1d	39	0	49	4	0
46	1f	25	0	21	3	0
46	1q	48	0	68	1	0
47	1E	4	0	0	0	0
47	1G	4	0	0	1	0
48	1F	31	0	19	1	0
49	1G	1	0	0	0	0
50	1H	63	0	90	8	0
51	1H	51	0	46	2	0
51	1O	67	0	78	3	0
51	1a	61	0	65	4	0
52	1L	15	0	27	2	0
53	1M	38	0	48	4	0
53	1Y	35	0	42	7	0
54	1O	32	0	12	1	0
55	1O	1	0	0	0	0
56	1P	48	0	26	8	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
57	1R	1	0	0	0	0
58	1W	37	0	0	2	0
58	1n	37	0	0	4	0
All	All	67334	0	67440	3326	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 25.

All (3326) 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)
44:1s:32:PRO:CG	44:1s:32:PRO:CB	1.76	1.33
27:1b:78:GLU:HA	27:1b:81:LYS:NZ	1.57	1.17
21:1V:97:LYS:HA	21:1V:97:LYS:HE3	1.25	1.14
16:1P:162:GLU:HB2	16:1P:224:LYS:HG3	1.26	1.12
13:1M:408:LEU:HA	13:1M:411:LEU:HD12	1.14	1.12
13:1M:310:MET:HG2	13:1M:455:LEU:HB3	1.33	1.11
21:1V:94:LEU:HB3	21:1V:95:ARG:HH22	1.11	1.11
34:1i:41:PRO:HA	34:1i:44:GLN:NE2	1.65	1.10
11:1K:9:ILE:HG13	11:1K:43:MET:HE1	1.22	1.10
22:1W:114:ARG:HE	22:1W:115:PRO:HD2	1.17	1.07
13:1M:209:LEU:HB3	13:1M:212:LEU:CD1	1.86	1.05
20:1T:6:LEU:HD12	20:1T:86:VAL:HG21	1.34	1.05
37:1l:111:PHE:HB3	37:1l:115:MET:HE1	1.37	1.05
10:1J:127:ILE:HA	25:1Z:120:MET:CE	1.86	1.05
20:1U:54:MET:HE1	20:1U:76:ILE:HD13	1.34	1.04
2:1B:50:PHE:CZ	2:1B:103:VAL:HG21	1.93	1.02
1:1A:10:ASN:HD22	8:1H:84:THR:CG2	1.70	1.02
16:1P:292:MET:HE3	16:1P:292:MET:H	1.24	1.02
10:1J:95:SER:HA	10:1J:98:MET:HE3	1.37	1.01
35:1j:29:SER:O	35:1j:32:MET:HE3	1.59	1.01
34:1i:45:PHE:O	34:1i:48:LYS:NZ	1.93	1.00
13:1M:209:LEU:CB	13:1M:212:LEU:HD11	1.91	0.98
27:1b:78:GLU:HA	27:1b:81:LYS:HZ1	1.11	0.98
10:1J:127:ILE:HA	25:1Z:120:MET:HE3	1.42	0.98
28:1c:17:VAL:HG23	29:1d:59:HIS:CD2	1.99	0.98
10:1J:95:SER:CA	10:1J:98:MET:HE3	1.93	0.98
24:1Y:117:MET:HE3	24:1Y:117:MET:H	1.28	0.98
35:1j:68:PRO:HD2	35:1j:71:GLU:OE1	1.65	0.97
21:1V:94:LEU:HB3	21:1V:95:ARG:NH2	1.79	0.97
36:1k:19:LYS:HE2	36:1k:19:LYS:N	1.79	0.97

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:284:ILE:HD12	7:1G:294:THR:HG21	1.47	0.96
37:1l:41:GLY:N	38:1m:80:ARG:HH21	1.63	0.95
12:1L:337:ALA:O	12:1L:341:MET:HE1	1.67	0.95
37:1l:129:GLY:HA2	40:1o:21:MET:HE1	1.49	0.94
22:1W:65:GLU:OE1	22:1W:69:LYS:NZ	2.00	0.94
8:1H:253:GLU:N	8:1H:253:GLU:OE2	1.98	0.94
10:1J:172:THR:HA	11:1K:80:MET:HE2	1.48	0.93
4:1D:71:GLU:HB3	4:1D:72:MET:HE2	1.46	0.93
8:1H:58:LYS:HD2	8:1H:217:ALA:HB2	1.50	0.93
40:1o:73:PHE:HD1	40:1o:74:PRO:HA	1.34	0.92
7:1G:673:MET:HE3	7:1G:679:ARG:HA	1.52	0.92
22:1W:50:PHE:HE1	22:1W:96:VAL:HG22	1.35	0.92
12:1L:150:MET:HA	12:1L:150:MET:HE3	1.50	0.91
14:1N:2:ASN:HB3	14:1N:5:ILE:HD13	1.52	0.91
16:1P:292:MET:H	16:1P:292:MET:CE	1.84	0.91
17:1Q:69:LEU:HG	17:1Q:70:MET:HE2	1.52	0.90
12:1L:181:GLY:H	12:1L:218:LEU:HD12	1.37	0.90
3:1C:194:PHE:O	17:1Q:81:ASN:ND2	2.05	0.89
13:1M:434:ASN:HB3	33:1h:21:PHE:CE2	2.08	0.89
14:1N:187:MET:HA	14:1N:187:MET:HE3	1.55	0.89
12:1L:486:MET:HE3	12:1L:486:MET:H	1.36	0.88
14:1N:95:MET:HE3	14:1N:95:MET:O	1.74	0.88
1:1A:10:ASN:HD22	8:1H:84:THR:HG23	1.38	0.88
31:1f:56:TRP:O	31:1f:57:LYS:HE3	1.73	0.88
4:1D:19:MET:HE3	14:1N:295:ARG:HD3	1.56	0.87
9:1I:15:LYS:HE2	9:1I:15:LYS:HA	1.56	0.87
13:1M:209:LEU:HB3	13:1M:212:LEU:HD11	0.95	0.87
18:1R:46:GLU:N	18:1R:46:GLU:OE2	2.07	0.87
4:1D:111:MET:HE3	4:1D:189:MET:HG3	1.54	0.87
37:1l:41:GLY:N	38:1m:80:ARG:NH2	2.21	0.86
1:1A:9:THR:HG21	8:1H:3:MET:HE1	1.57	0.86
12:1L:237:MET:HE3	12:1L:244:SER:HB3	1.56	0.86
12:1L:415:ALA:O	12:1L:419:THR:HG22	1.74	0.86
6:1F:347:ILE:HG22	6:1F:376:MET:HE2	1.56	0.86
13:1M:266:MET:HA	13:1M:269:MET:HE1	1.58	0.86
1:1A:10:ASN:HD22	8:1H:84:THR:HG22	1.41	0.86
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.58	0.85
21:1V:97:LYS:HE3	21:1V:97:LYS:CA	2.05	0.85
22:1W:80:ASP:O	22:1W:83:VAL:HG12	1.75	0.85
7:1G:55:CYS:HB3	47:1G:804:FES:S2	2.16	0.85
10:1J:60:TYR:HB3	10:1J:64:MET:HE1	1.57	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:482:MET:HE1	12:1L:487:LYS:HB2	1.58	0.85
8:1H:310:MET:HE1	27:1b:31:LEU:HB2	1.59	0.85
20:1U:24:LYS:CD	36:1k:41:ARG:HH21	1.89	0.85
40:1o:118:GLU:O	40:1o:121:MET:HE3	1.77	0.85
34:1i:71:VAL:HA	34:1i:75:LEU:HB3	1.58	0.85
12:1L:88:MET:HE2	12:1L:88:MET:O	1.77	0.85
21:1V:37:ILE:HG23	21:1V:99:TRP:HZ3	1.41	0.85
28:1c:17:VAL:HG23	29:1d:59:HIS:CG	2.12	0.85
10:1J:78:MET:HE1	10:1J:79:TYR:CD1	2.11	0.84
14:1N:89:MET:HE2	14:1N:98:MET:HE1	1.57	0.84
4:1D:20:TYR:HE2	12:1L:571:MET:HG2	1.39	0.84
7:1G:21:GLU:OE2	7:1G:22:PRO:O	1.94	0.84
34:1i:41:PRO:HA	34:1i:44:GLN:HE21	1.41	0.84
12:1L:573:MET:HE2	12:1L:573:MET:O	1.77	0.84
40:1o:73:PHE:CD1	40:1o:74:PRO:HA	2.12	0.84
13:1M:72:LEU:HG	13:1M:76:MET:HE1	1.59	0.83
9:1I:9:GLU:N	9:1I:9:GLU:OE2	2.10	0.83
14:1N:323:MET:H	14:1N:323:MET:HE2	1.42	0.83
35:1j:70:ASP:OD1	35:1j:71:GLU:OE2	1.96	0.83
13:1M:364:LEU:HB3	13:1M:369:LEU:HD23	1.61	0.83
28:1c:1:LYS:HZ3	28:1c:3:TYR:HD1	1.25	0.83
12:1L:68:TRP:C	12:1L:69:MET:HE2	2.04	0.83
13:1M:32:LEU:HD23	13:1M:74:PRO:HG2	1.60	0.83
21:1V:36:GLN:OE1	21:1V:36:GLN:N	2.11	0.83
21:1V:97:LYS:HE2	21:1V:99:TRP:CE3	2.13	0.83
29:1d:25:LYS:HG2	29:1d:27:THR:HG22	1.61	0.83
36:1k:18:TYR:HD2	36:1k:19:LYS:HZ3	1.26	0.83
2:1B:50:PHE:CE1	2:1B:103:VAL:HG21	2.14	0.83
15:1O:3:TYR:O	15:1O:261:MET:HE1	1.78	0.82
13:1M:176:PHE:CE2	13:1M:245:ARG:HG3	2.14	0.82
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.59	0.82
11:1K:37:MET:HE3	11:1K:67:ALA:HA	1.61	0.82
12:1L:378:LEU:HG	12:1L:383:MET:CE	2.10	0.82
20:1T:29:LYS:NZ	20:1T:40:LEU:HA	1.94	0.82
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.62	0.82
13:1M:360:LEU:O	13:1M:364:LEU:HD23	1.79	0.82
38:1m:80:ARG:NE	38:1m:82:THR:OG1	2.12	0.82
10:1J:24:PRO:HG3	10:1J:83:TRP:CZ3	2.13	0.82
20:1T:34:SER:HB3	20:1T:40:LEU:HD11	1.61	0.82
4:1D:71:GLU:HB3	4:1D:72:MET:CE	2.08	0.82
11:1K:9:ILE:HG13	11:1K:43:MET:CE	2.07	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:18:TYR:O	36:1k:22:LYS:NZ	2.14	0.81
21:1V:37:ILE:HG23	21:1V:99:TRP:CZ3	2.15	0.81
22:1W:114:ARG:NE	22:1W:115:PRO:HD2	1.96	0.81
37:1l:40:ASP:C	38:1m:80:ARG:HH21	1.89	0.81
43:1r:29:GLU:OE2	43:1r:29:GLU:N	2.10	0.81
13:1M:21:ASN:C	13:1M:22:MET:HE2	2.05	0.81
14:1N:318:GLU:OE1	14:1N:318:GLU:N	2.15	0.80
13:1M:434:ASN:HB3	33:1h:21:PHE:HE2	1.42	0.80
34:1i:74:VAL:O	34:1i:78:VAL:HG23	1.81	0.80
36:1k:12:LYS:HD2	36:1k:13:MET:N	1.97	0.80
16:1P:335:LYS:HZ2	16:1P:336:PRO:HB2	1.46	0.80
12:1L:203:MET:HE1	41:1p:109:LEU:HG	1.64	0.80
12:1L:119:LYS:O	12:1L:123:LEU:HD12	1.82	0.79
15:1O:61:SER:HA	15:1O:66:GLY:HA2	1.62	0.79
17:1Q:97:GLU:N	17:1Q:97:GLU:OE2	2.15	0.79
7:1G:41:CYS:SG	7:1G:52:CYS:CB	2.71	0.79
27:1b:78:GLU:CA	27:1b:81:LYS:NZ	2.41	0.79
6:1F:28:ARG:NH1	44:1s:35:ASN:O	2.16	0.79
22:1W:34:GLU:OE1	22:1W:34:GLU:N	2.16	0.79
1:1A:10:ASN:ND2	8:1H:84:THR:CG2	2.45	0.79
7:1G:41:CYS:H	7:1G:52:CYS:HB2	1.47	0.79
16:1P:335:LYS:HD3	16:1P:336:PRO:O	1.83	0.79
21:1V:97:LYS:HE2	21:1V:99:TRP:CZ3	2.18	0.78
37:1l:156:TYR:HA	40:1o:35:GLU:HA	1.65	0.78
12:1L:341:MET:HE3	12:1L:341:MET:H	1.47	0.78
20:1T:71:MET:O	20:1T:71:MET:HE3	1.83	0.78
20:1T:76:ILE:O	20:1T:80:ILE:HD13	1.84	0.78
24:1Y:11:ILE:HD11	24:1Y:20:LYS:HG2	1.64	0.78
34:1i:30:ARG:HD2	34:1i:31:GLU:HG2	1.65	0.78
12:1L:492:ILE:O	12:1L:496:MET:HE1	1.84	0.78
36:1k:12:LYS:HD2	36:1k:14:GLU:H	1.48	0.78
16:1P:335:LYS:HZ2	16:1P:336:PRO:CB	1.95	0.78
11:1K:94:ASN:ND2	12:1L:583:LEU:HD23	1.99	0.78
40:1o:38:MET:HE1	40:1o:57:TYR:HA	1.66	0.78
1:1A:90:MET:HA	1:1A:90:MET:HE3	1.64	0.77
8:1H:23:VAL:HG21	26:1a:9:ILE:CD1	2.14	0.77
12:1L:181:GLY:N	12:1L:218:LEU:HD12	1.98	0.77
22:1W:42:GLU:OE2	22:1W:42:GLU:N	2.15	0.77
7:1G:41:CYS:SG	7:1G:52:CYS:HB2	2.23	0.77
22:1W:96:VAL:HG12	22:1W:96:VAL:O	1.83	0.77
14:1N:313:MET:HE3	15:1O:99:TRP:CZ3	2.18	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:96:MET:HE2	2:1B:96:MET:O	1.85	0.77
9:1I:67:LEU:CD1	9:1I:154:LEU:HB3	2.15	0.77
13:1M:197:LEU:HB3	13:1M:201:MET:HE1	1.67	0.77
12:1L:15:LEU:HD12	12:1L:126:ILE:HG23	1.67	0.77
37:1I:27:TYR:HB3	37:1I:29:MET:HE1	1.67	0.77
14:1N:236:LYS:HB2	14:1N:311:MET:HE1	1.66	0.77
17:1Q:11:ILE:HG22	22:1W:23:ARG:HH21	1.46	0.77
37:1I:112:MET:O	37:1I:112:MET:HE3	1.84	0.77
20:1T:8:LEU:HD12	20:1T:86:VAL:CG1	2.14	0.77
12:1L:199:GLN:O	12:1L:203:MET:HG3	1.83	0.76
20:1T:52:MET:HA	20:1T:55:GLU:OE1	1.85	0.76
6:1F:317:MET:HE1	6:1F:322:LEU:HD11	1.67	0.76
27:1b:42:ILE:HG22	27:1b:46:ARG:HH12	1.50	0.76
4:1D:398:HIS:HB3	4:1D:421:GLN:NE2	2.00	0.76
14:1N:118:VAL:O	14:1N:122:ILE:HG12	1.85	0.76
34:1i:92:LYS:O	34:1i:95:THR:HG23	1.86	0.76
9:1I:148:LEU:HD23	17:1Q:70:MET:HE1	1.66	0.76
38:1m:80:ARG:HG2	38:1m:82:THR:H	1.50	0.76
13:1M:167:ILE:HD11	13:1M:195:MET:HE1	1.68	0.76
14:1N:342:ALA:HB3	46:1d:201:PC1:H3D2	1.67	0.76
20:1T:29:LYS:HZ1	20:1T:40:LEU:HA	1.49	0.76
20:1T:84:LYS:HG2	20:1T:84:LYS:O	1.86	0.76
25:1Z:121:MET:C	25:1Z:121:MET:SD	2.68	0.76
34:1i:92:LYS:HB2	34:1i:95:THR:CG2	2.16	0.76
42:1q:84:PRO:HD3	42:1q:113:HIS:HD2	1.50	0.76
20:1U:71:MET:HE2	20:1U:71:MET:HA	1.67	0.75
44:1s:34:ASP:OD1	44:1s:34:ASP:O	2.04	0.75
13:1M:176:PHE:CZ	13:1M:245:ARG:HG3	2.22	0.75
6:1F:68:ARG:O	6:1F:224:ASN:ND2	2.19	0.75
39:1n:61:GLN:HA	39:1n:64:ARG:HD2	1.68	0.75
1:1A:9:THR:CG2	8:1H:3:MET:HE1	2.16	0.75
7:1G:215:PHE:HB3	9:1I:104:ARG:HD2	1.69	0.75
20:1U:26:ASP:H	20:1U:29:LYS:HE2	1.51	0.75
35:1j:71:GLU:OE2	35:1j:71:GLU:N	2.19	0.75
37:1I:27:TYR:HB3	37:1I:29:MET:CE	2.16	0.75
2:1B:117:GLY:O	2:1B:121:ASN:ND2	2.19	0.75
10:1J:3:MET:HE2	10:1J:3:MET:HA	1.68	0.75
12:1L:295:GLN:HB3	12:1L:301:ILE:HD11	1.67	0.75
14:1N:200:MET:HE3	14:1N:200:MET:HA	1.68	0.75
12:1L:200:GLN:HA	12:1L:203:MET:SD	2.26	0.75
12:1L:542:LEU:O	13:1M:278:ARG:NH1	2.19	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:89:MET:CE	14:1N:98:MET:HE1	2.17	0.75
29:1d:106:LYS:HZ1	41:1p:78:GLU:H	1.33	0.75
8:1H:25:ARG:NH1	50:1H:701:U10:H152	2.02	0.74
8:1H:224:PHE:CE2	8:1H:228:TYR:CE2	2.76	0.74
11:1K:37:MET:HE3	11:1K:67:ALA:CA	2.15	0.74
21:1V:41:ALA:HB2	21:1V:99:TRP:CE3	2.21	0.74
42:1q:11:LEU:O	42:1q:14:VAL:HG22	1.87	0.74
16:1P:162:GLU:HB2	16:1P:224:LYS:CG	2.12	0.74
29:1d:107:LYS:HZ3	29:1d:111:GLU:HB2	1.53	0.74
3:1C:68:THR:HA	21:1V:82:GLN:HE21	1.53	0.74
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.69	0.74
23:1X:134:ARG:O	27:1b:57:ARG:NH2	2.20	0.74
29:1d:112:ILE:HG22	29:1d:114:GLU:H	1.51	0.74
20:1U:24:LYS:CE	36:1k:41:ARG:HH21	2.01	0.74
13:1M:410:MET:HE3	13:1M:410:MET:H	1.51	0.74
27:1b:78:GLU:CA	27:1b:81:LYS:HZ1	1.96	0.74
8:1H:26:LYS:HE3	26:1a:5:ILE:HA	1.68	0.74
13:1M:114:GLU:OE1	23:1X:168:PHE:HB3	1.88	0.74
14:1N:159:MET:HA	14:1N:159:MET:HE2	1.68	0.74
24:1Y:117:MET:H	24:1Y:117:MET:CE	2.00	0.74
25:1Z:120:MET:HB3	25:1Z:123:GLU:HG2	1.67	0.74
1:1A:10:ASN:ND2	8:1H:84:THR:HG22	2.02	0.73
7:1G:533:THR:HA	7:1G:556:MET:HE1	1.70	0.73
8:1H:117:LEU:HD13	8:1H:136:VAL:HG11	1.70	0.73
17:1Q:107:GLU:N	17:1Q:107:GLU:OE2	2.20	0.73
34:1i:100:LYS:HZ2	34:1i:101:PRO:HD2	1.52	0.73
37:1l:105:LEU:O	37:1l:109:VAL:HG22	1.88	0.73
4:1D:20:TYR:CE2	12:1L:571:MET:HG2	2.23	0.73
7:1G:54:MET:HE1	7:1G:94:MET:HE3	1.70	0.73
8:1H:235:ASN:HB3	8:1H:266:LEU:HB3	1.70	0.73
15:1O:290:ASP:OD1	15:1O:294:GLN:NE2	2.21	0.73
16:1P:21:ALA:HB3	16:1P:45:VAL:HG12	1.69	0.73
24:1Y:120:THR:O	24:1Y:124:VAL:HG13	1.89	0.73
7:1G:147:LYS:NZ	7:1G:704:CYS:O	2.21	0.72
9:1I:44:GLU:OE1	26:1a:1:MET:HE1	1.88	0.72
24:1Y:117:MET:HE3	24:1Y:117:MET:N	2.04	0.72
7:1G:103:LEU:O	18:1R:86:TYR:OH	2.05	0.72
12:1L:359:MET:HB3	12:1L:430:ALA:HA	1.72	0.72
14:1N:159:MET:HE1	14:1N:282:MET:HG3	1.71	0.72
8:1H:25:ARG:HH22	8:1H:47:GLN:HE21	1.36	0.72
14:1N:309:ASN:HB3	15:1O:282:ILE:HD12	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:90:MET:HE1	33:1h:107:GLU:HA	1.71	0.72
51:1H:702:CDL:H722	51:1H:702:CDL:H521	1.71	0.72
11:1K:94:ASN:ND2	12:1L:581:LYS:O	2.23	0.72
12:1L:486:MET:H	12:1L:486:MET:CE	2.01	0.72
7:1G:19:MET:HA	7:1G:19:MET:HE3	1.71	0.72
8:1H:224:PHE:CE2	8:1H:228:TYR:CD2	2.77	0.72
13:1M:237:LYS:HD2	13:1M:316:MET:HG3	1.72	0.72
12:1L:150:MET:HA	12:1L:150:MET:CE	2.20	0.72
32:1g:49:LYS:HE2	32:1g:49:LYS:HA	1.69	0.72
2:1B:96:MET:HE1	2:1B:100:LEU:HB2	1.72	0.72
10:1J:126:VAL:HG13	25:1Z:122:GLY:HA3	1.70	0.72
24:1Y:11:ILE:HD11	24:1Y:20:LYS:CG	2.19	0.72
37:1l:26:LYS:NZ	37:1l:46:ASP:OD2	2.23	0.72
10:1J:94:VAL:O	10:1J:98:MET:HG3	1.90	0.71
12:1L:53:MET:SD	12:1L:53:MET:N	2.58	0.71
27:1b:79:TRP:CZ3	27:1b:80:LEU:HD13	2.25	0.71
4:1D:393:ALA:HB3	4:1D:396:PHE:HB2	1.71	0.71
12:1L:341:MET:H	12:1L:341:MET:CE	2.02	0.71
24:1Y:11:ILE:CD1	24:1Y:20:LYS:HG2	2.20	0.71
29:1d:106:LYS:HE3	41:1p:77:GLU:HB3	1.72	0.71
13:1M:386:PHE:HB2	13:1M:393:ILE:HD11	1.72	0.71
17:1Q:27:GLU:O	17:1Q:31:LYS:NZ	2.23	0.71
21:1V:57:MET:CE	21:1V:70:GLN:HG2	2.21	0.71
12:1L:295:GLN:OE1	39:1n:77:GLN:NE2	2.23	0.71
15:1O:69:LEU:HB2	15:1O:74:SER:HB2	1.72	0.71
20:1T:12:LYS:HE2	20:1T:77:VAL:HG21	1.71	0.71
23:1X:122:GLY:HA3	27:1b:77:LEU:HD21	1.73	0.71
29:1d:111:GLU:HG3	32:1g:119:GLN:HB3	1.73	0.71
12:1L:18:PRO:HG3	12:1L:39:THR:HG21	1.72	0.71
13:1M:286:ILE:HD12	13:1M:286:ILE:H	1.55	0.71
20:1T:6:LEU:HD12	20:1T:86:VAL:CG2	2.16	0.71
25:1Z:97:ILE:O	30:1e:81:GLN:NE2	2.23	0.71
33:1h:53:ALA:HB2	41:1p:61:TYR:CE1	2.24	0.71
8:1H:23:VAL:HG21	26:1a:9:ILE:HD13	1.72	0.71
14:1N:89:MET:HE2	14:1N:98:MET:CE	2.20	0.71
20:1T:8:LEU:HD12	20:1T:86:VAL:HG12	1.71	0.71
42:1q:142:THR:HG22	42:1q:144:TYR:H	1.56	0.71
4:1D:33:TRP:HE1	15:1O:276:PRO:HD2	1.55	0.71
6:1F:262:VAL:HG11	6:1F:284:ALA:HB1	1.73	0.71
21:1V:97:LYS:CE	21:1V:99:TRP:CZ3	2.74	0.71
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:71:THR:HG22	11:1K:27:MET:HG3	1.72	0.71
13:1M:367:LEU:CD2	13:1M:404:ALA:HA	2.21	0.71
21:1V:97:LYS:HA	21:1V:97:LYS:CE	2.07	0.71
31:1f:54:VAL:HG21	31:1f:57:LYS:HD2	1.72	0.71
36:1k:29:GLU:OE2	36:1k:30:THR:HG23	1.90	0.71
8:1H:67:SER:O	8:1H:69:SER:N	2.24	0.70
20:1U:15:VAL:HG23	20:1U:54:MET:SD	2.31	0.70
13:1M:244:MET:HE1	13:1M:316:MET:HE1	1.71	0.70
4:1D:68:LEU:HD13	4:1D:70:GLY:C	2.16	0.70
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.74	0.70
10:1J:126:VAL:HG12	25:1Z:120:MET:HE2	1.72	0.70
20:1T:36:PHE:HB2	20:1T:71:MET:HE1	1.73	0.70
12:1L:272:LEU:O	12:1L:276:MET:HE3	1.92	0.70
43:1r:72:GLN:OE1	43:1r:72:GLN:N	2.21	0.70
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.73	0.70
4:1D:74:ARG:CZ	4:1D:74:ARG:HA	2.21	0.70
11:1K:9:ILE:CG1	11:1K:43:MET:HE1	2.13	0.70
21:1V:94:LEU:HA	21:1V:97:LYS:HD2	1.74	0.70
9:1I:15:LYS:NZ	25:1Z:33:TYR:CD2	2.53	0.70
10:1J:78:MET:CE	10:1J:79:TYR:CD1	2.75	0.69
12:1L:37:LYS:HZ2	12:1L:102:GLU:HG2	1.57	0.69
31:1f:22:PHE:CE1	31:1f:26:LEU:HD23	2.27	0.69
1:1A:9:THR:HG21	8:1H:3:MET:CE	2.21	0.69
8:1H:224:PHE:HE2	8:1H:228:TYR:CE2	2.10	0.69
13:1M:400:MET:HE2	13:1M:400:MET:O	1.92	0.69
16:1P:92:ILE:HD11	16:1P:218:ILE:HD11	1.73	0.69
21:1V:65:LYS:NZ	21:1V:66:LYS:HG3	2.07	0.69
12:1L:160:GLY:H	39:1n:95:CYS:HB3	1.56	0.69
13:1M:272:THR:HA	13:1M:275:ILE:HD12	1.74	0.69
20:1U:69:LYS:O	34:1i:2:GLY:N	2.26	0.69
8:1H:117:LEU:HD11	10:1J:68:PHE:HE2	1.58	0.69
15:1O:285:GLY:HA2	32:1g:26:LEU:HD11	1.73	0.69
37:1l:69:LEU:HD11	37:1l:85:ILE:HB	1.74	0.69
3:1C:32:ILE:HG22	3:1C:33:LEU:HG	1.74	0.69
6:1F:82:MET:SD	6:1F:129:MET:HE3	2.32	0.69
14:1N:160:LEU:O	14:1N:164:ILE:HD13	1.93	0.69
6:1F:212:ASP:OD1	6:1F:212:ASP:N	2.25	0.69
34:1i:10:ARG:HE	39:1n:155:PRO:HA	1.56	0.69
9:1I:15:LYS:NZ	25:1Z:33:TYR:CE2	2.60	0.69
10:1J:95:SER:HA	10:1J:98:MET:CE	2.17	0.69
12:1L:272:LEU:C	12:1L:276:MET:HE3	2.18	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:76:MET:O	13:1M:80:SER:OG	2.09	0.69
13:1M:176:PHE:CZ	13:1M:245:ARG:HA	2.28	0.69
21:1V:93:MET:O	21:1V:97:LYS:HD2	1.92	0.69
20:1T:79:TYR:HD1	20:1T:80:ILE:HD12	1.57	0.69
11:1K:37:MET:HE3	11:1K:67:ALA:CB	2.23	0.69
8:1H:20:LEU:HD23	8:1H:228:TYR:HD1	1.57	0.68
12:1L:247:LEU:HA	12:1L:251:THR:OG1	1.93	0.68
19:1S:19:ARG:NH2	19:1S:73:GLU:OE2	2.22	0.68
34:1i:92:LYS:HB2	34:1i:95:THR:HG21	1.74	0.68
40:1o:20:ARG:HH21	40:1o:21:MET:HB3	1.58	0.68
2:1B:30:VAL:HG22	2:1B:173:LEU:HB3	1.75	0.68
3:1C:204:GLU:OE1	3:1C:210:ARG:NH1	2.27	0.68
10:1J:55:MET:HE2	10:1J:55:MET:HA	1.74	0.68
14:1N:337:LEU:O	14:1N:340:THR:OG1	2.12	0.68
12:1L:60:GLU:HB2	34:1i:99:ARG:HD2	1.75	0.68
15:1O:101:TYR:HE1	15:1O:128:ILE:HG23	1.59	0.68
16:1P:292:MET:HE3	16:1P:292:MET:N	2.05	0.68
16:1P:335:LYS:HG2	16:1P:336:PRO:HD2	1.74	0.68
19:1S:18:ILE:HD13	19:1S:50:LEU:HD11	1.75	0.68
40:1o:102:GLU:HG3	40:1o:105:ARG:HE	1.57	0.68
4:1D:92:GLU:C	4:1D:92:GLU:OE1	2.36	0.68
5:1E:103:CYS:HB3	5:1E:108:CYS:SG	2.34	0.68
7:1G:672:TYR:HB3	7:1G:684:MET:CE	2.24	0.68
7:1G:704:CYS:O	9:1I:104:ARG:NH2	2.26	0.68
14:1N:68:MET:HA	14:1N:68:MET:HE3	1.75	0.68
16:1P:96:GLY:HA3	56:1P:501:NDP:H3D	1.75	0.68
23:1X:15:GLN:HE21	23:1X:67:LEU:HD11	1.59	0.68
40:1o:51:MET:N	40:1o:51:MET:SD	2.59	0.68
3:1C:205:ALA:HA	7:1G:122:MET:HE2	1.74	0.68
14:1N:325:LEU:O	14:1N:329:MET:N	2.24	0.68
41:1p:10:PRO:HD2	41:1p:108:ARG:HG2	1.76	0.68
3:1C:133:GLU:OE2	4:1D:390:LYS:NZ	2.27	0.68
10:1J:172:THR:HA	11:1K:80:MET:CE	2.24	0.68
7:1G:594:ARG:NH1	22:1W:122:PHE:O	2.27	0.67
37:1l:50:LEU:HB2	37:1l:78:HIS:HD2	1.57	0.67
12:1L:292:ALA:HB1	12:1L:301:ILE:HG23	1.75	0.67
20:1U:60:PHE:HZ	20:1U:80:ILE:HG12	1.59	0.67
13:1M:207:MET:HE1	13:1M:240:GLY:N	2.10	0.67
20:1T:48:VAL:O	20:1T:51:ILE:HD12	1.94	0.67
20:1U:8:LEU:HB2	20:1U:86:VAL:HG21	1.75	0.67
27:1b:24:ILE:HA	27:1b:27:LEU:HD12	1.76	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:71:GLU:OE2	8:1H:134:ARG:NH2	2.27	0.67
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.75	0.67
6:1F:365:CYS:HB2	45:1F:502:SF4:S2	2.35	0.67
8:1H:196:ALA:HB3	8:1H:274:ARG:HG2	1.77	0.67
12:1L:302:VAL:HG23	12:1L:340:PHE:HE1	1.58	0.67
24:1Y:30:ALA:HA	24:1Y:33:LEU:HD12	1.76	0.67
31:1f:28:ARG:O	31:1f:28:ARG:HD2	1.95	0.67
41:1p:31:TYR:HA	41:1p:34:LYS:HB2	1.77	0.67
12:1L:302:VAL:O	12:1L:336:LYS:NZ	2.28	0.67
20:1U:84:LYS:HD2	20:1U:84:LYS:O	1.95	0.67
41:1p:80:ASP:O	41:1p:84:MET:HG3	1.95	0.67
22:1W:57:LYS:O	22:1W:57:LYS:NZ	2.27	0.67
12:1L:316:THR:HA	12:1L:319:ILE:HG22	1.77	0.67
13:1M:285:LEU:HD12	13:1M:342:MET:HE1	1.77	0.67
10:1J:175:ASN:H	14:1N:48:PHE:HD1	1.41	0.67
13:1M:325:MET:HE3	13:1M:437:MET:HE3	1.77	0.67
21:1V:97:LYS:HD3	21:1V:99:TRP:CH2	2.30	0.67
38:1m:49:GLN:HB2	38:1m:55:ARG:HD3	1.76	0.67
1:1A:10:ASN:ND2	8:1H:84:THR:HG23	2.09	0.67
8:1H:281:ARG:HB3	8:1H:284:GLN:HG3	1.76	0.67
20:1T:11:ILE:HG22	20:1T:77:VAL:HG22	1.77	0.67
6:1F:347:ILE:HG22	6:1F:376:MET:CE	2.22	0.66
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.28	0.66
16:1P:37:HIS:HA	16:1P:40:ARG:HD2	1.77	0.66
20:1T:52:MET:HG3	20:1T:55:GLU:OE1	1.95	0.66
34:1i:104:PHE:HB3	34:1i:107:ASP:HB2	1.77	0.66
12:1L:241:THR:HG23	12:1L:299:LYS:HD3	1.77	0.66
15:1O:13:ARG:HB2	15:1O:16:ARG:HD2	1.77	0.66
15:1O:109:ALA:HA	15:1O:112:LEU:HD12	1.77	0.66
38:1m:33:ALA:O	39:1n:149:ARG:NH1	2.29	0.66
10:1J:77:GLU:N	10:1J:77:GLU:OE2	2.27	0.66
37:1l:39:ASP:C	38:1m:80:ARG:NH2	2.54	0.66
20:1U:8:LEU:HD21	20:1U:77:VAL:HG13	1.77	0.66
35:1j:29:SER:HA	35:1j:32:MET:HG3	1.77	0.66
4:1D:427:GLU:OE1	4:1D:427:GLU:O	2.14	0.66
14:1N:155:LEU:HD12	14:1N:278:MET:HE3	1.77	0.66
6:1F:42:TRP:H	6:1F:236:ARG:HH22	1.44	0.66
15:1O:54:ALA:HB3	15:1O:104:ARG:HD2	1.77	0.66
17:1Q:90:GLU:OE1	17:1Q:90:GLU:N	2.27	0.66
19:1S:57:CYS:SG	19:1S:58:SER:N	2.68	0.66
4:1D:342:MET:HE1	7:1G:103:LEU:HA	1.78	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:549:ALA:HB1	13:1M:271:MET:HE1	1.78	0.66
15:1O:108:TYR:HD1	15:1O:128:ILE:HD12	1.61	0.66
34:1i:41:PRO:HA	34:1i:44:GLN:CD	2.21	0.66
41:1p:92:ARG:NH2	41:1p:149:TYR:O	2.28	0.66
1:1A:35:SER:O	2:1B:81:ARG:NH2	2.29	0.66
5:1E:6:LEU:O	5:1E:92:ARG:NH2	2.28	0.66
7:1G:80:LEU:HB3	7:1G:83:SER:HB3	1.78	0.66
8:1H:213:VAL:HG23	8:1H:214:GLU:H	1.61	0.66
13:1M:280:THR:OG1	38:1m:71:ARG:NH1	2.29	0.66
4:1D:227:GLU:HB2	25:1Z:25:LEU:HD21	1.77	0.66
7:1G:283:MET:HE3	7:1G:293:TYR:CD1	2.31	0.66
12:1L:326:PHE:HA	12:1L:329:ILE:HD12	1.78	0.66
14:1N:100:MET:O	14:1N:104:MET:HG3	1.95	0.66
20:1T:8:LEU:CD1	20:1T:86:VAL:HG12	2.26	0.65
1:1A:108:GLN:O	1:1A:110:GLY:N	2.29	0.65
4:1D:421:GLN:HB3	4:1D:423:ILE:HG13	1.79	0.65
13:1M:409:TYR:O	13:1M:413:THR:OG1	2.14	0.65
37:1l:30:ARG:NH1	38:1m:31:ALA:O	2.26	0.65
5:1E:162:GLU:OE1	6:1F:108:ARG:NH2	2.28	0.65
8:1H:54:LYS:HZ3	8:1H:55:LEU:HD21	1.60	0.65
34:1i:98:GLU:O	41:1p:14:ARG:NH2	2.27	0.65
35:1j:71:GLU:H	35:1j:71:GLU:CD	2.02	0.65
37:1l:56:GLN:HA	37:1l:70:ARG:HH21	1.61	0.65
4:1D:393:ALA:HA	4:1D:427:GLU:OE2	1.96	0.65
8:1H:85:MET:HG2	8:1H:233:MET:SD	2.36	0.65
8:1H:134:ARG:HH11	8:1H:282:TYR:HD2	1.43	0.65
21:1V:97:LYS:NZ	21:1V:99:TRP:CZ3	2.64	0.65
37:1l:16:THR:OG1	37:1l:18:GLU:OE2	2.14	0.65
4:1D:391:ILE:HB	4:1D:430:ARG:HD3	1.78	0.65
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.30	0.65
7:1G:74:MET:N	7:1G:74:MET:SD	2.68	0.65
7:1G:372:GLU:HA	7:1G:398:SER:HB2	1.77	0.65
14:1N:323:MET:HE2	14:1N:323:MET:N	2.10	0.65
15:1O:41:GLU:HG2	15:1O:231:ALA:CB	2.27	0.65
20:1U:24:LYS:HE2	36:1k:43:PRO:HB3	1.79	0.65
3:1C:87:GLN:OE1	3:1C:87:GLN:N	2.22	0.65
10:1J:130:THR:HG22	25:1Z:121:MET:HB2	1.79	0.65
14:1N:5:ILE:H	14:1N:5:ILE:HD12	1.61	0.65
14:1N:211:MET:HE3	14:1N:211:MET:HA	1.79	0.65
15:1O:49:ARG:O	15:1O:123:VAL:N	2.28	0.65
6:1F:207:PRO:HB2	6:1F:208:PRO:CD	2.27	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:170:GLU:OE1	23:1X:97:ARG:NH1	2.30	0.65
21:1V:35:GLY:HA2	21:1V:44:ARG:HH21	1.61	0.65
27:1b:23:ALA:O	27:1b:27:LEU:HD12	1.95	0.65
37:1l:39:ASP:O	38:1m:80:ARG:NH2	2.29	0.65
10:1J:45:LEU:HD23	10:1J:50:SER:HA	1.77	0.65
12:1L:521:LYS:HG2	39:1n:76:PRO:HB3	1.79	0.65
13:1M:418:LYS:NZ	13:1M:419:TYR:O	2.29	0.65
23:1X:129:LYS:HB2	27:1b:58:ASP:HB2	1.78	0.65
25:1Z:79:LYS:HA	25:1Z:79:LYS:HE2	1.78	0.65
40:1o:67:LYS:HA	40:1o:70:ARG:HG2	1.78	0.65
34:1i:52:ASP:HB2	34:1i:57:LYS:HG2	1.79	0.65
1:1A:67:LEU:HD12	11:1K:65:VAL:HA	1.79	0.65
6:1F:254:LYS:HZ2	6:1F:332:ALA:HB3	1.61	0.65
12:1L:88:MET:HE2	12:1L:88:MET:C	2.22	0.65
13:1M:457:PRO:O	32:1g:84:ARG:NH2	2.29	0.65
35:1j:31:THR:HA	35:1j:34:PHE:CE2	2.32	0.65
13:1M:352:LEU:HB3	13:1M:355:MET:HB2	1.78	0.64
13:1M:361:MET:HA	13:1M:364:LEU:HB2	1.80	0.64
15:1O:113:GLU:OE1	15:1O:263:VAL:HG23	1.97	0.64
22:1W:99:GLN:N	22:1W:99:GLN:OE1	2.30	0.64
38:1m:44:ARG:NH2	39:1n:143:THR:OG1	2.31	0.64
7:1G:375:ASP:N	7:1G:375:ASP:OD1	2.29	0.64
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.14	0.64
41:1p:84:MET:HE2	41:1p:84:MET:O	1.97	0.64
4:1D:403:ASP:OD1	4:1D:407:LYS:NZ	2.30	0.64
11:1K:40:LEU:HD22	14:1N:71:MET:HG3	1.78	0.64
15:1O:250:ASP:OD1	15:1O:250:ASP:N	2.26	0.64
33:1h:53:ALA:HB2	41:1p:61:TYR:CZ	2.32	0.64
2:1B:137:ASP:OD2	2:1B:145:TYR:OH	2.15	0.64
7:1G:41:CYS:SG	7:1G:52:CYS:HB3	2.37	0.64
12:1L:16:THR:HG22	12:1L:126:ILE:HG21	1.79	0.64
29:1d:109:TYR:OH	41:1p:152:ARG:NH1	2.31	0.64
7:1G:564:ALA:O	7:1G:569:LYS:NZ	2.31	0.64
7:1G:672:TYR:HB3	7:1G:684:MET:HE2	1.80	0.64
12:1L:386:LEU:HG	12:1L:387:THR:N	2.12	0.64
12:1L:442:LEU:HA	35:1j:9:PRO:HB3	1.80	0.64
13:1M:412:ILE:HA	13:1M:416:ARG:HB2	1.80	0.64
20:1T:52:MET:HE1	22:1W:37:ARG:HA	1.79	0.64
31:1f:28:ARG:HA	31:1f:31:ASP:OD2	1.97	0.64
15:1O:24:VAL:HB	15:1O:115:LEU:HD21	1.80	0.64
22:1W:47:VAL:HA	22:1W:52:LEU:HD23	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:97:VAL:HG23	41:1p:115:ARG:HE	1.62	0.64
37:1l:156:TYR:HB2	40:1o:33:ARG:HE	1.61	0.64
38:1m:23:ASP:OD1	39:1n:64:ARG:NH2	2.31	0.64
10:1J:124:ASP:OD2	11:1K:2:PRO:HB2	1.97	0.64
11:1K:30:LEU:HD23	11:1K:75:LEU:HD23	1.79	0.64
20:1U:54:MET:CE	20:1U:76:ILE:HD13	2.19	0.64
4:1D:335:ARG:NH2	9:1I:123:GLN:O	2.30	0.64
37:1l:36:PRO:HA	37:1l:48:PRO:HA	1.80	0.64
2:1B:34:ASP:HB2	2:1B:173:LEU:HB2	1.80	0.63
5:1E:196:ALA:H	6:1F:264:HIS:HB3	1.63	0.63
12:1L:24:SER:O	33:1h:26:ARG:NH1	2.31	0.63
13:1M:237:LYS:NZ	13:1M:316:MET:O	2.31	0.63
21:1V:57:MET:HE3	21:1V:70:GLN:HG2	1.80	0.63
6:1F:317:MET:HA	6:1F:317:MET:HE3	1.79	0.63
12:1L:422:TYR:HA	12:1L:425:ARG:HB2	1.78	0.63
13:1M:356:ALA:HA	13:1M:359:TRP:HD1	1.63	0.63
38:1m:30:LYS:NZ	38:1m:34:GLU:OE1	2.28	0.63
15:1O:35:LYS:NZ	15:1O:53:GLU:OE1	2.27	0.63
1:1A:8:LEU:O	1:1A:12:THR:HG23	1.98	0.63
7:1G:276:ARG:NH1	7:1G:680:ALA:O	2.32	0.63
11:1K:94:ASN:HD21	12:1L:583:LEU:HD23	1.64	0.63
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.33	0.63
12:1L:380:LEU:HD21	12:1L:423:SER:OG	1.98	0.63
13:1M:357:THR:O	13:1M:360:LEU:N	2.30	0.63
24:1Y:113:ALA:O	24:1Y:117:MET:HE1	1.97	0.63
41:1p:6:LYS:HD2	41:1p:11:GLU:H	1.63	0.63
19:1S:85:GLN:HA	19:1S:88:ARG:HE	1.63	0.63
7:1G:433:ALA:O	7:1G:476:ASN:ND2	2.31	0.63
12:1L:295:GLN:NE2	12:1L:523:SER:O	2.30	0.63
15:1O:115:LEU:HD12	15:1O:116:LEU:HD22	1.81	0.63
13:1M:72:LEU:HD12	13:1M:75:LEU:HD12	1.81	0.63
13:1M:318:ALA:O	13:1M:322:THR:OG1	2.17	0.63
14:1N:258:SER:HB2	14:1N:336:VAL:HG22	1.80	0.63
20:1T:36:PHE:HB3	20:1T:42:LEU:HD12	1.80	0.63
37:1l:17:PRO:HA	37:1l:20:ARG:HG2	1.81	0.63
40:1o:26:PRO:HA	40:1o:103:ARG:HH12	1.63	0.63
1:1A:93:PHE:HE2	1:1A:97:LEU:HD22	1.64	0.63
3:1C:135:TRP:HE1	22:1W:88:MET:HE1	1.64	0.63
8:1H:54:LYS:NZ	8:1H:55:LEU:HD21	2.14	0.63
9:1I:15:LYS:CE	25:1Z:33:TYR:CE2	2.82	0.63
13:1M:325:MET:CE	13:1M:437:MET:HE3	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:81:LYS:NZ	15:1O:90:ASP:OD2	2.32	0.63
1:1A:87:MET:HE3	1:1A:88:LEU:N	2.14	0.62
6:1F:250:ASN:ND2	6:1F:320:ASP:OD1	2.32	0.62
10:1J:5:ILE:HG22	10:1J:9:LEU:HG	1.80	0.62
12:1L:249:SER:HB2	12:1L:340:PHE:CD2	2.34	0.62
26:1a:1:MET:HE2	51:1a:101:CDL:HB21	1.79	0.62
32:1g:85:MET:N	32:1g:85:MET:SD	2.71	0.62
35:1j:29:SER:O	35:1j:32:MET:CE	2.43	0.62
2:1B:96:MET:HB3	4:1D:82:LEU:HD22	1.81	0.62
4:1D:261:ARG:NH2	4:1D:368:GLU:OE2	2.32	0.62
5:1E:107:PRO:HG3	6:1F:335:ILE:HD13	1.81	0.62
5:1E:114:ASP:OD2	5:1E:114:ASP:N	2.33	0.62
7:1G:54:MET:HE1	7:1G:94:MET:HB2	1.80	0.62
7:1G:284:ILE:HD11	7:1G:299:ALA:HA	1.80	0.62
8:1H:24:GLU:OE1	8:1H:271:LEU:HD13	1.99	0.62
13:1M:260:PRO:HG3	46:1M:501:PC1:H251	1.81	0.62
13:1M:306:PRO:O	13:1M:310:MET:HE2	1.99	0.62
21:1V:97:LYS:HE2	21:1V:99:TRP:CH2	2.33	0.62
34:1i:33:VAL:O	39:1n:113:MET:HG2	1.99	0.62
34:1i:100:LYS:NZ	41:1p:15:ARG:O	2.31	0.62
37:1l:6:LYS:HA	37:1l:9:PHE:HB2	1.81	0.62
39:1n:50:HIS:NE2	58:1n:201:EHZ:S1	2.67	0.62
5:1E:153:MET:HB3	5:1E:162:GLU:HA	1.79	0.62
7:1G:257:ASP:OD2	7:1G:579:ARG:NH2	2.31	0.62
34:1i:76:ILE:HG22	34:1i:77:PRO:HD3	1.81	0.62
2:1B:139:ILE:HG22	2:1B:140:VAL:HG13	1.80	0.62
5:1E:165:THR:HG22	5:1E:167:LYS:HD3	1.80	0.62
12:1L:37:LYS:NZ	12:1L:102:GLU:HG2	2.15	0.62
37:1l:8:MET:HA	37:1l:26:LYS:HG3	1.80	0.62
1:1A:25:PRO:HB2	8:1H:60:PRO:HD3	1.82	0.62
7:1G:283:MET:HE3	7:1G:293:TYR:CE1	2.34	0.62
31:1f:56:TRP:NE1	33:1h:88:GLU:OE1	2.32	0.62
37:1l:17:PRO:HA	37:1l:20:ARG:CG	2.29	0.62
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.80	0.62
13:1M:221:VAL:HG12	13:1M:340:ARG:HH21	1.65	0.62
15:1O:104:ARG:NH1	54:1O:401:GTP:N7	2.48	0.62
6:1F:45:THR:HA	6:1F:48:ILE:HD12	1.81	0.62
7:1G:536:ASP:OD1	7:1G:536:ASP:N	2.22	0.62
10:1J:95:SER:CB	10:1J:98:MET:HE3	2.29	0.62
13:1M:263:MET:HA	13:1M:266:MET:HB2	1.80	0.62
22:1W:50:PHE:CE1	22:1W:96:VAL:HG22	2.27	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:116:GLN:NE2	4:1D:276:ASP:OD2	2.33	0.62
7:1G:48:VAL:HG23	17:1Q:118:TYR:HD1	1.65	0.62
10:1J:17:PHE:HA	10:1J:20:PHE:HE2	1.64	0.62
13:1M:143:LEU:HD11	14:1N:303:THR:HG21	1.80	0.62
12:1L:533:MET:C	12:1L:533:MET:HE3	2.25	0.61
20:1U:24:LYS:HE3	36:1k:41:ARG:HH21	1.65	0.61
33:1h:21:PHE:HE1	33:1h:25:MET:SD	2.23	0.61
35:1j:68:PRO:CD	35:1j:71:GLU:OE1	2.45	0.61
39:1n:49:GLU:OE1	39:1n:50:HIS:ND1	2.33	0.61
20:1T:37:MET:HB2	20:1T:38:LYS:HE3	1.82	0.61
14:1N:59:TYR:CE2	14:1N:63:GLN:HG3	2.35	0.61
14:1N:190:MET:HG2	14:1N:204:ASN:HB3	1.82	0.61
15:1O:81:LYS:HD2	15:1O:92:ASN:HB3	1.80	0.61
20:1T:50:ILE:HD12	20:1T:50:ILE:H	1.65	0.61
29:1d:31:LEU:HD11	29:1d:69:VAL:HG23	1.82	0.61
38:1m:9:ARG:H	38:1m:9:ARG:HD2	1.65	0.61
12:1L:539:TYR:HB2	37:1l:89:VAL:HG11	1.82	0.61
16:1P:335:LYS:NZ	16:1P:336:PRO:HB2	2.14	0.61
5:1E:141:GLU:C	5:1E:141:GLU:OE2	2.44	0.61
9:1I:132:VAL:HG21	9:1I:165:ILE:HG21	1.82	0.61
12:1L:455:LYS:HA	12:1L:458:LEU:HD23	1.81	0.61
12:1L:483:PRO:C	12:1L:486:MET:HE1	2.26	0.61
15:1O:214:MET:SD	15:1O:218:CYS:HB2	2.41	0.61
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.19	0.61
6:1F:129:MET:HE1	6:1F:221:THR:HB	1.82	0.61
12:1L:88:MET:HE1	12:1L:330:CYS:SG	2.41	0.61
16:1P:293:THR:HG22	16:1P:295:PRO:HD3	1.83	0.61
25:1Z:20:ASP:N	25:1Z:20:ASP:OD1	2.33	0.61
32:1g:68:ILE:HD12	32:1g:69:VAL:H	1.65	0.61
13:1M:367:LEU:HD22	13:1M:404:ALA:HA	1.82	0.61
25:1Z:69:ILE:HA	25:1Z:72:MET:HG3	1.83	0.61
26:1a:49:GLU:OE1	26:1a:52:ARG:NH1	2.33	0.61
6:1F:78:LYS:NZ	48:1F:501:FMN:O1P	2.34	0.61
8:1H:207:LEU:O	8:1H:209:SER:N	2.27	0.61
12:1L:224:SER:HB3	12:1L:310:LEU:HD12	1.83	0.61
20:1T:51:ILE:HD12	20:1T:52:MET:N	2.16	0.61
8:1H:195:ARG:HG3	8:1H:196:ALA:H	1.65	0.61
32:1g:70:LEU:O	32:1g:74:SER:OG	2.17	0.61
35:1j:10:ARG:HD2	35:1j:15:PRO:HA	1.82	0.61
1:1A:54:LYS:NZ	4:1D:70:GLY:HA3	2.16	0.61
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:29:HIS:HB3	23:1X:119:PRO:HD2	1.82	0.61
36:1k:42:ASP:O	36:1k:46:ARG:NH2	2.33	0.61
7:1G:256:GLU:O	17:1Q:112:LYS:NZ	2.34	0.60
12:1L:331:MET:HE2	12:1L:331:MET:N	2.15	0.60
14:1N:270:MET:HE3	14:1N:279:PRO:HG3	1.83	0.60
15:1O:229:GLU:N	15:1O:229:GLU:OE2	2.33	0.60
21:1V:97:LYS:HE2	21:1V:99:TRP:CD2	2.35	0.60
24:1Y:115:ALA:O	24:1Y:119:LEU:HD23	2.01	0.60
41:1p:158:GLN:HA	41:1p:161:ARG:HE	1.66	0.60
8:1H:90:PRO:HG3	8:1H:162:LEU:HB3	1.83	0.60
10:1J:4:TYR:HH	10:1J:7:PHE:HD2	1.50	0.60
12:1L:135:ASN:O	12:1L:198:LEU:N	2.29	0.60
12:1L:181:GLY:H	12:1L:218:LEU:CD1	2.12	0.60
12:1L:341:MET:HE3	12:1L:341:MET:N	2.16	0.60
13:1M:303:ILE:HG23	13:1M:305:THR:HG23	1.82	0.60
15:1O:73:LEU:HD13	15:1O:299:LEU:HD11	1.82	0.60
23:1X:48:GLU:OE1	23:1X:134:ARG:NH1	2.33	0.60
24:1Y:11:ILE:HG13	24:1Y:20:LYS:HD3	1.82	0.60
53:1Y:201:3PE:O14	53:1Y:201:3PE:N	2.28	0.60
31:1f:14:ILE:O	31:1f:18:VAL:HG12	2.00	0.60
2:1B:86:MET:HG3	2:1B:107:MET:CE	2.32	0.60
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.81	0.60
10:1J:28:TYR:CE1	10:1J:82:VAL:HG23	2.36	0.60
13:1M:216:LEU:HD11	13:1M:287:ALA:O	2.02	0.60
20:1U:24:LYS:HE3	36:1k:41:ARG:HE	1.65	0.60
35:1j:50:HIS:ND1	35:1j:50:HIS:O	2.32	0.60
3:1C:116:PRO:C	3:1C:117:ILE:HD13	2.26	0.60
12:1L:79:SER:O	12:1L:139:GLN:NE2	2.34	0.60
16:1P:136:ASN:OD1	16:1P:292:MET:HE1	2.01	0.60
21:1V:97:LYS:CE	21:1V:99:TRP:CH2	2.83	0.60
12:1L:584:ILE:HD11	14:1N:58:LYS:HD2	1.83	0.60
13:1M:329:LEU:HB3	13:1M:359:TRP:CZ3	2.36	0.60
14:1N:308:THR:HG22	14:1N:310:ASN:H	1.67	0.60
23:1X:142:HIS:ND1	25:1Z:114:THR:OG1	2.34	0.60
32:1g:41:ASN:HD21	32:1g:51:PRO:HB3	1.65	0.60
39:1n:135:GLU:HB2	39:1n:164:PRO:HA	1.83	0.60
40:1o:74:PRO:HD3	41:1p:28:PRO:HD3	1.82	0.60
8:1H:24:GLU:OE1	8:1H:24:GLU:HA	2.02	0.60
16:1P:315:ILE:HG12	16:1P:331:MET:HG2	1.82	0.60
21:1V:53:GLU:OE2	43:1r:92:LYS:NZ	2.34	0.60
21:1V:63:ASP:OD1	21:1V:65:LYS:HE3	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:81:VAL:HA	36:1k:84:GLU:HB2	1.83	0.60
6:1F:123:LEU:HD23	6:1F:162:ILE:HG22	1.83	0.60
12:1L:309:GLN:O	12:1L:313:MET:HE1	2.02	0.60
14:1N:236:LYS:CB	14:1N:311:MET:HE1	2.30	0.60
16:1P:40:ARG:NH1	22:1W:110:THR:O	2.35	0.60
27:1b:78:GLU:HA	27:1b:81:LYS:HZ3	1.60	0.60
40:1o:50:LEU:O	40:1o:55:ARG:NE	2.27	0.60
1:1A:68:GLU:HG3	1:1A:98:LEU:HD13	1.83	0.60
4:1D:298:LEU:HB3	9:1I:5:VAL:HG21	1.83	0.60
5:1E:12:THR:HG23	5:1E:15:ASN:H	1.65	0.60
6:1F:321:ALA:O	6:1F:324:GLN:NE2	2.35	0.60
8:1H:77:LEU:HD11	8:1H:111:LEU:HD23	1.82	0.60
12:1L:177:ILE:O	12:1L:218:LEU:HD11	2.02	0.60
13:1M:2:LEU:HA	13:1M:5:ILE:HB	1.84	0.60
14:1N:95:MET:HE2	14:1N:99:THR:OG1	2.01	0.60
15:1O:287:HIS:ND1	32:1g:28:GLU:OE2	2.29	0.60
18:1R:52:VAL:HG21	18:1R:57:ILE:HD12	1.83	0.60
20:1U:54:MET:HA	20:1U:57:GLU:HB3	1.82	0.60
22:1W:61:ASP:HA	22:1W:64:ARG:HB3	1.82	0.60
40:1o:57:TYR:O	40:1o:60:HIS:ND1	2.35	0.60
1:1A:46:SER:HB3	4:1D:47:LEU:HD11	1.84	0.60
1:1A:93:PHE:CE2	1:1A:97:LEU:HD22	2.37	0.60
14:1N:109:SER:HB3	14:1N:157:MET:HE2	1.82	0.60
20:1T:70:LEU:HG	20:1T:75:GLU:HB3	1.83	0.60
5:1E:78:MET:O	5:1E:78:MET:HE3	2.02	0.60
11:1K:41:PHE:O	11:1K:45:THR:OG1	2.18	0.60
17:1Q:15:GLU:OE2	17:1Q:15:GLU:N	2.30	0.60
28:1c:1:LYS:NZ	28:1c:3:TYR:HD1	1.97	0.60
30:1e:21:SER:N	30:1e:36:GLU:OE2	2.35	0.60
32:1g:58:MET:HE3	32:1g:59:ARG:N	2.17	0.60
42:1q:144:TYR:CE2	42:1q:145:LYS:HG3	2.37	0.60
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.34	0.59
20:1U:60:PHE:CZ	20:1U:80:ILE:HG12	2.36	0.59
6:1F:15:LEU:HD13	6:1F:271:GLU:HB2	1.84	0.59
12:1L:32:TYR:HA	12:1L:35:TYR:HB3	1.84	0.59
13:1M:137:GLY:HA3	13:1M:142:ARG:HD2	1.84	0.59
13:1M:221:VAL:HG13	13:1M:283:LYS:HB2	1.83	0.59
20:1T:17:TYR:CE1	20:1T:21:LEU:HD21	2.37	0.59
30:1e:85:LEU:HD21	30:1e:91:TYR:HB3	1.83	0.59
35:1j:64:LEU:HD12	40:1o:99:LYS:HZ2	1.67	0.59
2:1B:61:HIS:ND1	4:1D:175:GLU:OE2	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:19:LYS:NZ	31:1f:8:ARG:O	2.35	0.59
28:1c:19:LEU:O	28:1c:23:THR:HG22	2.02	0.59
36:1k:70:PHE:CE1	36:1k:74:PHE:HB2	2.37	0.59
8:1H:113:VAL:HG21	8:1H:139:THR:HG21	1.83	0.59
12:1L:172:ILE:O	12:1L:176:ARG:HG2	2.02	0.59
16:1P:235:ARG:NH2	16:1P:293:THR:OG1	2.36	0.59
20:1U:24:LYS:HE3	36:1k:41:ARG:NE	2.17	0.59
7:1G:582:GLN:OE1	7:1G:620:ARG:NH2	2.35	0.59
12:1L:161:ARG:NH1	12:1L:238:GLU:OE1	2.35	0.59
12:1L:405:ASN:HD22	37:1l:119:GLY:HA3	1.67	0.59
15:1O:279:LEU:HB2	15:1O:282:ILE:HG22	1.83	0.59
34:1i:54:ALA:HB3	34:1i:57:LYS:HD3	1.84	0.59
1:1A:87:MET:HE3	1:1A:87:MET:C	2.28	0.59
7:1G:45:ARG:NH1	7:1G:261:GLU:OE1	2.36	0.59
13:1M:211:GLY:H	13:1M:213:HIS:CE1	2.20	0.59
13:1M:271:MET:O	13:1M:271:MET:HE3	2.01	0.59
14:1N:103:ALA:O	14:1N:107:GLY:N	2.30	0.59
16:1P:32:ARG:NH1	16:1P:175:GLU:OE2	2.35	0.59
20:1T:12:LYS:CE	20:1T:77:VAL:HG21	2.31	0.59
34:1i:32:PRO:HB3	39:1n:114:TYR:HE1	1.67	0.59
37:1l:10:PRO:HB2	38:1m:74:ASN:HD22	1.67	0.59
8:1H:23:VAL:HG21	26:1a:9:ILE:HD11	1.84	0.59
10:1J:122:LEU:CD1	10:1J:126:VAL:HG21	2.32	0.59
12:1L:550:SER:HB2	13:1M:275:ILE:HG23	1.84	0.59
20:1U:24:LYS:HE3	36:1k:41:ARG:NH2	2.16	0.59
31:1f:54:VAL:HG21	31:1f:57:LYS:CE	2.32	0.59
41:1p:51:ILE:O	41:1p:55:HIS:ND1	2.34	0.59
1:1A:105:GLU:OE2	1:1A:111:LEU:HD22	2.03	0.59
7:1G:235:GLY:O	7:1G:581:GLN:NE2	2.35	0.59
15:1O:254:ARG:HH12	15:1O:255:THR:HG22	1.67	0.59
24:1Y:11:ILE:HD12	24:1Y:16:GLU:HB2	1.84	0.59
29:1d:107:LYS:NZ	29:1d:111:GLU:HB2	2.17	0.59
6:1F:207:PRO:HB2	6:1F:208:PRO:HD3	1.85	0.59
7:1G:66:VAL:HB	7:1G:71:MET:HG3	1.85	0.59
8:1H:117:LEU:HD11	10:1J:68:PHE:CE2	2.36	0.59
12:1L:378:LEU:HG	12:1L:383:MET:HE2	1.83	0.59
12:1L:486:MET:HE3	12:1L:486:MET:N	2.14	0.59
20:1T:22:TYR:OH	20:1T:49:GLU:HB2	2.02	0.59
23:1X:43:MET:HE1	27:1b:52:TYR:CE1	2.37	0.59
24:1Y:89:TYR:HB3	24:1Y:121:ALA:HB1	1.85	0.59
28:1c:45:ARG:NH2	29:1d:16:ASN:OD1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:43:MET:HE2	58:1n:201:EHZ:C2	2.33	0.59
39:1n:104:ASP:OD2	39:1n:125:LYS:NZ	2.36	0.59
2:1B:144:ILE:HA	9:1I:142:GLU:HA	1.84	0.59
7:1G:285:ARG:NH1	7:1G:289:GLY:O	2.36	0.59
8:1H:1:FME:HE2	26:1a:29:PHE:HE2	1.68	0.59
8:1H:141:SER:HB3	8:1H:289:LEU:HD11	1.85	0.59
11:1K:71:ALA:O	11:1K:75:LEU:HG	2.03	0.59
12:1L:176:ARG:HH21	12:1L:179:ASP:CG	2.11	0.59
20:1T:36:PHE:HD1	20:1T:40:LEU:HD13	1.68	0.59
20:1T:54:MET:HG3	20:1T:76:ILE:HG12	1.85	0.59
20:1U:61:GLU:HG2	39:1n:83:GLU:HG2	1.85	0.59
34:1i:71:VAL:HG13	34:1i:72:THR:HG23	1.84	0.59
37:1l:20:ARG:HH21	37:1l:36:PRO:CD	2.15	0.59
3:1C:28:TYR:OH	3:1C:67:HIS:NE2	2.36	0.58
10:1J:82:VAL:HG12	10:1J:85:SER:HB3	1.85	0.58
10:1J:120:ASN:ND2	30:1e:72:MET:SD	2.76	0.58
11:1K:8:ILE:HD13	11:1K:43:MET:HE2	1.84	0.58
12:1L:373:LEU:O	12:1L:377:SER:OG	2.19	0.58
13:1M:407:SER:HA	13:1M:410:MET:HE1	1.85	0.58
20:1T:48:VAL:O	20:1T:51:ILE:CD1	2.50	0.58
34:1i:106:GLY:N	34:1i:116:ILE:O	2.33	0.58
40:1o:36:ARG:NH2	40:1o:93:ASP:OD2	2.36	0.58
40:1o:79:CYS:O	40:1o:83:GLN:NE2	2.34	0.58
4:1D:67:GLU:O	4:1D:74:ARG:N	2.25	0.58
5:1E:183:LYS:NZ	5:1E:186:PRO:O	2.36	0.58
6:1F:294:LEU:O	6:1F:339:ARG:NH2	2.36	0.58
8:1H:142:TYR:CD2	8:1H:191:ALA:HB1	2.38	0.58
10:1J:68:PHE:HA	10:1J:71:THR:HG23	1.84	0.58
13:1M:22:MET:HE2	13:1M:22:MET:N	2.18	0.58
32:1g:112:CYS:HB2	41:1p:141:ARG:HD2	1.85	0.58
13:1M:367:LEU:HD11	13:1M:408:LEU:HD21	1.85	0.58
25:1Z:121:MET:SD	25:1Z:121:MET:O	2.61	0.58
33:1h:114:MET:SD	33:1h:120:GLY:HA3	2.43	0.58
7:1G:248:MET:H	7:1G:248:MET:HE2	1.67	0.58
7:1G:543:ILE:HB	7:1G:557:ALA:HA	1.85	0.58
11:1K:56:ALA:HA	30:1e:17:MET:HE2	1.84	0.58
12:1L:49:VAL:HG13	12:1L:50:PRO:HD3	1.85	0.58
13:1M:167:ILE:CD1	13:1M:195:MET:HE1	2.31	0.58
15:1O:180:GLN:O	15:1O:184:GLN:NE2	2.37	0.58
22:1W:93:THR:HG22	22:1W:103:ILE:HD11	1.84	0.58
37:1l:8:MET:HE2	38:1m:66:ARG:HH11	1.68	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:60:ILE:HD11	11:1K:72:ALA:HA	1.85	0.58
5:1E:13:PRO:O	5:1E:16:ASN:ND2	2.36	0.58
6:1F:214:GLY:HA3	6:1F:220:THR:HG22	1.85	0.58
8:1H:91:MET:O	8:1H:93:TYR:N	2.36	0.58
25:1Z:86:MET:O	25:1Z:90:ASN:ND2	2.36	0.58
34:1i:10:ARG:NH2	39:1n:153:LEU:HD12	2.19	0.58
37:1l:18:GLU:OE2	37:1l:18:GLU:N	2.26	0.58
40:1o:36:ARG:HH21	40:1o:57:TYR:HB2	1.69	0.58
5:1E:104:THR:O	5:1E:104:THR:HG22	2.02	0.58
11:1K:8:ILE:CD1	11:1K:43:MET:CE	2.82	0.58
13:1M:263:MET:SD	13:1M:263:MET:N	2.75	0.58
15:1O:41:GLU:CG	15:1O:231:ALA:HB1	2.33	0.58
40:1o:113:ARG:HA	40:1o:116:GLN:HB2	1.84	0.58
14:1N:236:LYS:HB2	14:1N:311:MET:CE	2.32	0.58
16:1P:177:ARG:NH2	56:1P:501:NDP:O2N	2.37	0.58
16:1P:258:LEU:HD13	16:1P:259:PRO:O	2.04	0.58
20:1U:24:LYS:HG3	36:1k:41:ARG:NH2	2.18	0.58
3:1C:114:LEU:HD12	17:1Q:17:LEU:HD11	1.84	0.58
7:1G:8:LEU:HD23	7:1G:19:MET:HB3	1.86	0.58
9:1I:136:ASN:HD22	9:1I:161:TRP:HZ2	1.50	0.58
17:1Q:36:ARG:NE	17:1Q:106:GLU:OE1	2.37	0.58
40:1o:93:ASP:HA	40:1o:96:LYS:HD2	1.85	0.58
7:1G:475:GLN:HB2	7:1G:646:ASN:ND2	2.19	0.58
7:1G:632:ARG:NE	19:1S:57:CYS:SG	2.77	0.58
15:1O:227:GLU:O	15:1O:233:LYS:NZ	2.33	0.58
27:1b:39:ASN:N	27:1b:39:ASN:OD1	2.37	0.58
31:1f:54:VAL:HG21	31:1f:57:LYS:CD	2.33	0.58
32:1g:48:ASP:OD2	32:1g:48:ASP:N	2.35	0.58
37:1l:10:PRO:HG3	38:1m:66:ARG:HE	1.68	0.58
38:1m:80:ARG:CD	38:1m:82:THR:OG1	2.52	0.58
7:1G:672:TYR:CD1	7:1G:684:MET:HE1	2.38	0.58
15:1O:51:PHE:N	15:1O:123:VAL:O	2.31	0.58
15:1O:288:GLN:N	32:1g:28:GLU:OE1	2.33	0.58
30:1e:12:ASP:OD2	30:1e:16:TRP:HD1	1.87	0.58
12:1L:375:ILE:HG21	12:1L:462:ILE:HD11	1.86	0.57
35:1j:40:PHE:O	35:1j:44:SER:OG	2.17	0.57
6:1F:287:VAL:HG21	6:1F:294:LEU:HD12	1.86	0.57
8:1H:236:ALA:HA	8:1H:263:THR:HG22	1.86	0.57
33:1h:14:SER:HB2	39:1n:106:TRP:HA	1.86	0.57
37:1l:20:ARG:HH21	37:1l:36:PRO:HD2	1.69	0.57
6:1F:43:TYR:H	6:1F:236:ARG:HH12	1.53	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:377:ILE:HG22	7:1G:406:VAL:HA	1.85	0.57
11:1K:84:THR:HG23	11:1K:85:TYR:CD1	2.40	0.57
12:1L:118:PHE:HA	12:1L:121:LEU:HD13	1.86	0.57
12:1L:377:SER:O	12:1L:380:LEU:CD2	2.53	0.57
15:1O:53:GLU:OE2	15:1O:104:ARG:NH2	2.38	0.57
24:1Y:43:LYS:HB2	24:1Y:54:ARG:HH12	1.69	0.57
7:1G:380:VAL:HG22	7:1G:409:ILE:HD12	1.85	0.57
13:1M:367:LEU:CD2	13:1M:407:SER:HB2	2.34	0.57
20:1U:85:ASP:HB3	34:1i:22:LEU:HD11	1.86	0.57
31:1f:49:ARG:NH1	33:1h:60:VAL:HG22	2.20	0.57
41:1p:105:ILE:HD11	41:1p:130:GLN:HG3	1.86	0.57
10:1J:71:THR:HA	10:1J:75:ALA:HB3	1.87	0.57
10:1J:122:LEU:O	10:1J:122:LEU:HD13	2.05	0.57
12:1L:496:MET:CE	12:1L:496:MET:H	2.17	0.57
46:1L:702:PC1:H2B1	24:1Y:116:TYR:HE1	1.70	0.57
13:1M:135:ARG:NH1	14:1N:301:SER:O	2.37	0.57
22:1W:68:MET:HE2	22:1W:68:MET:HA	1.85	0.57
36:1k:22:LYS:HB2	36:1k:24:GLU:OE2	2.04	0.57
41:1p:84:MET:SD	41:1p:84:MET:C	2.88	0.57
44:1s:32:PRO:CD	44:1s:34:ASP:HB3	2.34	0.57
14:1N:25:HIS:HE2	30:1e:17:MET:HG2	1.68	0.57
14:1N:53:THR:OG1	14:1N:54:GLU:OE2	2.22	0.57
15:1O:38:LEU:HD21	15:1O:234:VAL:HG11	1.86	0.57
15:1O:105:LEU:HA	15:1O:128:ILE:HD11	1.86	0.57
16:1P:292:MET:N	16:1P:292:MET:SD	2.78	0.57
18:1R:51:GLU:HB3	18:1R:94:PRO:HG3	1.86	0.57
24:1Y:11:ILE:HD11	24:1Y:20:LYS:CD	2.34	0.57
25:1Z:98:MET:HE3	30:1e:78:ILE:HA	1.86	0.57
32:1g:112:CYS:HG	41:1p:142:TYR:HH	1.52	0.57
6:1F:435:LEU:HA	6:1F:438:GLN:HG2	1.84	0.57
8:1H:47:GLN:NE2	8:1H:51:ASP:OD1	2.37	0.57
10:1J:1:FME:O	10:1J:3:MET:N	2.36	0.57
2:1B:101:ARG:NH1	2:1B:105:ASP:OD1	2.37	0.57
14:1N:308:THR:HG23	15:1O:282:ILE:HG13	1.87	0.57
14:1N:317:PHE:CE2	15:1O:106:LEU:HD21	2.39	0.57
16:1P:202:LYS:NZ	16:1P:289:MET:O	2.36	0.57
2:1B:71:ARG:NH1	8:1H:38:ASN:OD1	2.38	0.57
4:1D:291:GLY:O	4:1D:296:ARG:NH1	2.37	0.57
7:1G:40:PHE:N	7:1G:52:CYS:SG	2.77	0.57
8:1H:137:ALA:HB3	8:1H:282:TYR:OH	2.04	0.57
9:1I:106:THR:OG1	9:1I:151:LYS:NZ	2.30	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:264:TYR:HA	12:1L:267:MET:HB3	1.86	0.57
25:1Z:50:MET:HA	25:1Z:50:MET:HE3	1.85	0.57
35:1j:70:ASP:O	40:1o:114:ARG:NH1	2.38	0.57
41:1p:58:ASN:N	41:1p:58:ASN:OD1	2.38	0.57
4:1D:68:LEU:HD13	4:1D:70:GLY:O	2.04	0.57
12:1L:496:MET:SD	12:1L:496:MET:N	2.75	0.57
12:1L:548:SER:HA	12:1L:552:LEU:HB3	1.86	0.57
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.04	0.57
16:1P:38:LEU:O	16:1P:43:SER:OG	2.22	0.57
20:1T:12:LYS:HE2	20:1T:12:LYS:HA	1.87	0.57
2:1B:176:TRP:HA	2:1B:179:ARG:HD2	1.87	0.56
4:1D:224:GLU:HA	9:1I:36:MET:HE1	1.87	0.56
8:1H:58:LYS:CD	8:1H:217:ALA:HB2	2.31	0.56
12:1L:247:LEU:O	12:1L:252:MET:N	2.29	0.56
12:1L:313:MET:N	12:1L:313:MET:SD	2.78	0.56
12:1L:570:GLN:OE1	14:1N:167:TRP:NE1	2.24	0.56
14:1N:119:THR:HG22	14:1N:176:ARG:HB3	1.85	0.56
14:1N:160:LEU:O	14:1N:164:ILE:CD1	2.53	0.56
15:1O:84:ASP:OD1	15:1O:190:HIS:ND1	2.38	0.56
15:1O:260:ARG:HA	15:1O:263:VAL:HG22	1.87	0.56
20:1T:35:HIS:O	20:1T:39:ASP:N	2.37	0.56
29:1d:113:LEU:O	29:1d:113:LEU:HD13	2.05	0.56
33:1h:67:PHE:HB2	33:1h:73:ARG:HG2	1.86	0.56
39:1n:100:GLU:O	39:1n:121:ARG:NH2	2.38	0.56
7:1G:351:THR:HG22	7:1G:509:PRO:HG2	1.87	0.56
9:1I:67:LEU:HD12	9:1I:154:LEU:HB3	1.86	0.56
10:1J:60:TYR:O	10:1J:64:MET:HE2	2.05	0.56
12:1L:137:LEU:HB2	12:1L:186:MET:HE2	1.87	0.56
13:1M:192:ASN:HA	13:1M:195:MET:HB3	1.86	0.56
15:1O:3:TYR:O	15:1O:264:GLN:NE2	2.33	0.56
16:1P:335:LYS:NZ	16:1P:336:PRO:HD2	2.18	0.56
30:1e:81:GLN:HG2	30:1e:84:LYS:HE3	1.88	0.56
4:1D:33:TRP:CD1	15:1O:275:ILE:HG23	2.41	0.56
4:1D:46:ASN:HB3	4:1D:67:GLU:OE2	2.06	0.56
8:1H:90:PRO:HD3	8:1H:162:LEU:HD13	1.85	0.56
10:1J:115:ILE:HG13	10:1J:116:ILE:HG12	1.86	0.56
15:1O:115:LEU:HD23	15:1O:121:GLY:HA2	1.87	0.56
17:1Q:10:LEU:HG	22:1W:16:SER:HB2	1.87	0.56
34:1i:108:THR:HA	34:1i:115:VAL:HA	1.86	0.56
35:1j:68:PRO:O	35:1j:71:GLU:OE1	2.23	0.56
37:1l:10:PRO:O	38:1m:74:ASN:ND2	2.38	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:48:ASP:OD1	39:1n:51:LYS:NZ	2.34	0.56
39:1n:133:GLU:O	39:1n:137:LYS:HG2	2.05	0.56
42:1q:68:MET:HE1	42:1q:81:MET:HB3	1.87	0.56
1:1A:58:VAL:HA	1:1A:61:THR:OG1	2.06	0.56
8:1H:184:MET:HE1	8:1H:300:LEU:HD12	1.88	0.56
9:1I:42:PHE:HD2	43:1r:7:ILE:HG13	1.71	0.56
12:1L:283:ILE:HG12	37:1l:112:MET:SD	2.45	0.56
12:1L:387:THR:HA	12:1L:465:GLY:HA3	1.86	0.56
21:1V:84:GLU:C	21:1V:84:GLU:OE2	2.48	0.56
29:1d:107:LYS:HZ1	29:1d:112:ILE:N	2.03	0.56
31:1f:54:VAL:HG11	31:1f:57:LYS:HD2	1.85	0.56
39:1n:23:LEU:HA	39:1n:26:LEU:HD12	1.87	0.56
7:1G:475:GLN:HB2	7:1G:646:ASN:HD21	1.70	0.56
12:1L:295:GLN:HE22	12:1L:524:ASN:HA	1.70	0.56
13:1M:75:LEU:HD13	13:1M:440:HIS:CD2	2.40	0.56
14:1N:321:LYS:HB3	14:1N:323:MET:HE1	1.88	0.56
15:1O:77:CYS:HB3	15:1O:95:ARG:HE	1.69	0.56
20:1U:18:VAL:HA	20:1U:21:LEU:HB3	1.87	0.56
23:1X:165:ARG:O	33:1h:104:ARG:NH1	2.38	0.56
24:1Y:11:ILE:HG13	24:1Y:11:ILE:O	2.04	0.56
32:1g:53:VAL:HA	32:1g:56:TRP:HB2	1.86	0.56
6:1F:17:ASP:HA	6:1F:20:ARG:HG3	1.87	0.56
12:1L:61:MET:HG2	12:1L:82:MET:SD	2.45	0.56
16:1P:102:LYS:H	16:1P:102:LYS:HD3	1.70	0.56
16:1P:141:SER:O	16:1P:147:ARG:NH1	2.39	0.56
20:1U:18:VAL:HG21	20:1U:57:GLU:HG3	1.87	0.56
24:1Y:38:TYR:O	24:1Y:42:LEU:HD12	2.05	0.56
31:1f:37:PHE:HD2	33:1h:91:MET:HB3	1.69	0.56
37:1l:39:ASP:C	38:1m:80:ARG:HH22	2.13	0.56
38:1m:80:ARG:HG2	38:1m:82:THR:N	2.21	0.56
11:1K:37:MET:HE3	11:1K:67:ALA:HB1	1.87	0.56
12:1L:174:TYR:HD2	12:1L:229:LEU:HA	1.71	0.56
13:1M:348:LEU:H	13:1M:415:GLN:HA	1.71	0.56
34:1i:6:ASP:HA	39:1n:155:PRO:HG3	1.88	0.56
3:1C:199:LEU:HD11	4:1D:385:ARG:HD3	1.88	0.56
4:1D:401:GLY:O	4:1D:405:MET:HG3	2.06	0.56
12:1L:66:TRP:HE3	12:1L:78:LEU:HD22	1.71	0.56
24:1Y:21:ALA:O	24:1Y:25:THR:OG1	2.21	0.56
28:1c:26:PHE:O	28:1c:26:PHE:HD2	1.89	0.56
29:1d:8:ARG:NH2	46:1d:201:PC1:O14	2.39	0.56
34:1i:105:PRO:HA	34:1i:116:ILE:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:32:LEU:HD13	41:1p:35:ILE:HD11	1.87	0.56
8:1H:20:LEU:CD2	8:1H:228:TYR:HD1	2.18	0.56
15:1O:72:GLN:OE1	15:1O:76:ASN:ND2	2.39	0.56
20:1T:46:ASP:OD1	22:1W:64:ARG:NH2	2.39	0.56
20:1U:51:ILE:HD11	39:1n:20:LYS:HD3	1.86	0.56
22:1W:84:ILE:HD12	22:1W:85:LYS:N	2.21	0.56
29:1d:108:THR:OG1	41:1p:76:CYS:O	2.24	0.56
36:1k:12:LYS:HD2	36:1k:12:LYS:C	2.31	0.56
39:1n:46:ARG:O	39:1n:46:ARG:NH1	2.36	0.56
44:1s:32:PRO:HD3	44:1s:34:ASP:HB3	1.87	0.56
7:1G:356:THR:O	19:1S:55:ARG:NH2	2.39	0.56
7:1G:539:LYS:NZ	7:1G:540:ASP:H	2.04	0.56
12:1L:51:LEU:HD11	12:1L:91:PRO:HG3	1.87	0.56
13:1M:400:MET:HE2	13:1M:400:MET:C	2.31	0.56
19:1S:13:LEU:HB2	19:1S:68:TYR:HD2	1.71	0.56
27:1b:42:ILE:HG22	27:1b:46:ARG:NH1	2.19	0.56
41:1p:109:LEU:HD13	41:1p:127:GLU:HB3	1.87	0.56
4:1D:175:GLU:OE1	4:1D:188:ARG:NH1	2.39	0.55
8:1H:54:LYS:HD2	8:1H:55:LEU:N	2.22	0.55
8:1H:161:THR:HB	8:1H:164:THR:HG23	1.88	0.55
10:1J:17:PHE:CZ	11:1K:15:ALA:HB2	2.42	0.55
10:1J:82:VAL:HG22	10:1J:83:TRP:H	1.70	0.55
12:1L:135:ASN:ND2	12:1L:199:GLN:OE1	2.36	0.55
12:1L:488:MET:N	12:1L:488:MET:SD	2.79	0.55
23:1X:150:ASN:ND2	33:1h:124:GLN:OE1	2.37	0.55
30:1e:12:ASP:OD2	30:1e:12:ASP:C	2.47	0.55
1:1A:69:ILE:HG22	8:1H:148:ILE:HD11	1.87	0.55
2:1B:115:SER:OG	2:1B:136:CYS:SG	2.64	0.55
12:1L:69:MET:HB3	12:1L:71:LEU:HD23	1.88	0.55
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	1.88	0.55
13:1M:351:LEU:HD11	13:1M:419:TYR:HB3	1.88	0.55
14:1N:217:MET:HE3	14:1N:326:LEU:HB2	1.88	0.55
15:1O:32:CYS:SG	15:1O:186:LYS:NZ	2.64	0.55
20:1T:47:GLN:O	20:1T:51:ILE:HG13	2.06	0.55
20:1T:48:VAL:HA	20:1T:51:ILE:HD11	1.89	0.55
21:1V:97:LYS:CD	21:1V:99:TRP:CH2	2.89	0.55
22:1W:114:ARG:HD3	22:1W:115:PRO:O	2.06	0.55
24:1Y:128:GLN:OE1	53:1Y:201:3PE:H11	2.06	0.55
27:1b:78:GLU:CA	27:1b:81:LYS:HZ3	2.17	0.55
37:1l:55:GLN:NE2	37:1l:69:LEU:O	2.38	0.55
3:1C:42:VAL:HG22	3:1C:48:LEU:HD13	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:206:GLY:N	25:1Z:9:ASP:OD2	2.40	0.55
8:1H:141:SER:HB2	8:1H:289:LEU:HD21	1.87	0.55
10:1J:104:VAL:HG22	10:1J:108:LEU:HD23	1.87	0.55
12:1L:58:GLY:HA3	34:1i:102:ARG:HH22	1.71	0.55
13:1M:269:MET:HG2	13:1M:399:ASN:CG	2.31	0.55
13:1M:434:ASN:HB3	33:1h:21:PHE:CD2	2.41	0.55
14:1N:307:SER:OG	14:1N:308:THR:N	2.36	0.55
19:1S:30:GLN:NE2	19:1S:34:ASP:OD1	2.38	0.55
38:1m:115:ILE:HD12	38:1m:120:LEU:HD13	1.87	0.55
5:1E:181:ILE:HD12	5:1E:181:ILE:O	2.06	0.55
13:1M:11:LEU:HB3	13:1M:100:ILE:HD13	1.89	0.55
14:1N:40:MET:HE1	14:1N:130:LEU:HA	1.88	0.55
16:1P:258:LEU:HD22	16:1P:259:PRO:HD2	1.88	0.55
31:1f:54:VAL:HG21	31:1f:57:LYS:NZ	2.21	0.55
33:1h:111:ARG:HG2	33:1h:122:TRP:HZ2	1.70	0.55
13:1M:197:LEU:CB	13:1M:201:MET:HE1	2.36	0.55
16:1P:203:GLN:HG2	16:1P:231:VAL:HB	1.88	0.55
21:1V:95:ARG:NE	21:1V:95:ARG:HA	2.22	0.55
23:1X:129:LYS:HD3	27:1b:65:VAL:HG12	1.88	0.55
25:1Z:100:ASP:OD1	25:1Z:100:ASP:N	2.39	0.55
36:1k:64:GLY:HA2	36:1k:67:LEU:HB3	1.88	0.55
8:1H:283:ASP:OD1	8:1H:283:ASP:N	2.40	0.55
10:1J:103:MET:N	10:1J:103:MET:SD	2.80	0.55
12:1L:68:TRP:CD2	12:1L:69:MET:HE3	2.42	0.55
26:1a:2:TRP:NE1	51:1a:101:CDL:OB4	2.40	0.55
29:1d:25:LYS:HG2	29:1d:27:THR:CG2	2.36	0.55
29:1d:90:MET:HE1	33:1h:107:GLU:CA	2.35	0.55
38:1m:4:LYS:HE3	39:1n:68:GLU:HG2	1.88	0.55
7:1G:444:LYS:NZ	7:1G:480:SER:OG	2.30	0.55
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.89	0.55
13:1M:364:LEU:O	13:1M:368:ALA:N	2.40	0.55
16:1P:335:LYS:HD3	16:1P:336:PRO:N	2.21	0.55
28:1c:40:LEU:HA	28:1c:43:LYS:HE3	1.87	0.55
32:1g:37:LEU:HG	32:1g:46:GLY:HA2	1.88	0.55
35:1j:42:HIS:ND1	35:1j:43:ASP:OD1	2.35	0.55
35:1j:64:LEU:HD21	40:1o:102:GLU:HG2	1.87	0.55
2:1B:86:MET:HG3	2:1B:107:MET:HE2	1.89	0.55
6:1F:207:PRO:HB3	7:1G:72:PRO:HD3	1.88	0.55
8:1H:55:LEU:HD23	8:1H:58:LYS:HE3	1.88	0.55
13:1M:346:ARG:NH2	13:1M:420:THR:OG1	2.36	0.55
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.40	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:23:LYS:HA	15:1O:167:HIS:CD2	2.42	0.55
25:1Z:4:SER:OG	25:1Z:5:LYS:N	2.35	0.55
6:1F:68:ARG:HD2	6:1F:254:LYS:HD3	1.88	0.55
10:1J:129:ASP:OD1	10:1J:130:THR:N	2.39	0.55
10:1J:141:MET:HE1	30:1e:26:HIS:CG	2.42	0.55
12:1L:218:LEU:O	12:1L:218:LEU:HD22	2.06	0.55
12:1L:243:VAL:HA	12:1L:246:LEU:HG	1.89	0.55
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.41	0.55
13:1M:406:TYR:O	13:1M:409:TYR:N	2.39	0.55
15:1O:65:ASP:HA	28:1c:4:ILE:HG23	1.89	0.55
25:1Z:88:ARG:O	25:1Z:92:GLU:HG2	2.07	0.55
28:1c:23:THR:O	28:1c:27:LEU:HD22	2.06	0.55
30:1e:14:ASP:OD1	30:1e:14:ASP:N	2.40	0.55
36:1k:18:TYR:C	36:1k:19:LYS:HE2	2.30	0.55
36:1k:19:LYS:N	36:1k:19:LYS:CE	2.64	0.55
37:1l:85:ILE:HD12	37:1l:88:ARG:HB2	1.88	0.55
37:1l:108:PHE:HD1	37:1l:108:PHE:C	2.14	0.55
39:1n:150:THR:HG23	39:1n:152:ALA:H	1.72	0.55
42:1q:14:VAL:HA	42:1q:23:TYR:HD2	1.72	0.55
6:1F:175:VAL:O	44:1s:62:ARG:NH2	2.33	0.55
7:1G:365:ASN:N	7:1G:491:ASN:OD1	2.40	0.55
13:1M:129:THR:HG21	13:1M:235:LEU:HD11	1.89	0.55
19:1S:29:SER:O	19:1S:29:SER:OG	2.24	0.55
20:1T:11:ILE:HD11	20:1T:84:LYS:HZ1	1.71	0.55
23:1X:2:GLY:O	25:1Z:105:LYS:NZ	2.39	0.55
6:1F:317:MET:CE	6:1F:322:LEU:HD11	2.37	0.54
7:1G:212:PRO:HB3	7:1G:683:THR:HG21	1.89	0.54
7:1G:690:ALA:HB2	7:1G:698:VAL:HG11	1.88	0.54
14:1N:261:MET:HE2	14:1N:340:THR:HA	1.89	0.54
14:1N:270:MET:CE	14:1N:279:PRO:HG3	2.37	0.54
15:1O:298:GLU:OE1	15:1O:298:GLU:N	2.38	0.54
24:1Y:60:PHE:HB3	24:1Y:103:ARG:HH21	1.72	0.54
29:1d:107:LYS:NZ	29:1d:107:LYS:O	2.40	0.54
34:1i:77:PRO:O	34:1i:81:ILE:HD12	2.07	0.54
34:1i:98:GLU:HG3	41:1p:14:ARG:HH12	1.71	0.54
37:1l:14:PRO:HB2	37:1l:20:ARG:HD2	1.89	0.54
40:1o:107:LEU:O	40:1o:111:LYS:HD3	2.07	0.54
4:1D:290:ARG:N	4:1D:295:ASP:OD2	2.36	0.54
11:1K:95:LEU:HD21	14:1N:54:GLU:OE1	2.07	0.54
12:1L:158:TRP:HB2	12:1L:161:ARG:HB2	1.89	0.54
15:1O:168:VAL:HA	15:1O:218:CYS:HB3	1.88	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:174:VAL:HG22	15:1O:225:ALA:HB2	1.88	0.54
22:1W:74:THR:HG22	22:1W:74:THR:O	2.07	0.54
22:1W:78:VAL:O	22:1W:82:LEU:HD12	2.07	0.54
34:1i:41:PRO:CA	34:1i:44:GLN:NE2	2.54	0.54
37:1l:78:HIS:CE1	37:1l:80:ASP:HB2	2.42	0.54
4:1D:111:MET:HG2	4:1D:189:MET:O	2.07	0.54
7:1G:194:GLU:HG3	7:1G:389:PRO:HB3	1.90	0.54
10:1J:60:TYR:C	10:1J:64:MET:CE	2.80	0.54
12:1L:278:LEU:HA	12:1L:315:VAL:HG22	1.89	0.54
14:1N:163:LEU:HB3	14:1N:167:TRP:CZ3	2.41	0.54
15:1O:113:GLU:N	15:1O:113:GLU:OE2	2.40	0.54
20:1U:17:TYR:HA	20:1U:20:LYS:HE3	1.89	0.54
21:1V:93:MET:HE2	21:1V:98:PRO:HD3	1.88	0.54
35:1j:12:ARG:NH2	36:1k:47:ASN:OD1	2.33	0.54
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.21	0.54
8:1H:85:MET:SD	8:1H:233:MET:HE1	2.47	0.54
10:1J:4:TYR:OH	10:1J:7:PHE:HD2	1.91	0.54
13:1M:433:GLU:O	13:1M:437:MET:HG2	2.08	0.54
14:1N:237:MET:HA	14:1N:237:MET:HE2	1.89	0.54
16:1P:325:ARG:NH1	16:1P:325:ARG:O	2.41	0.54
24:1Y:68:ILE:HD13	24:1Y:95:ALA:C	2.33	0.54
24:1Y:139:LYS:HD2	24:1Y:139:LYS:N	2.22	0.54
28:1c:17:VAL:O	28:1c:21:LEU:HD12	2.08	0.54
30:1e:23:GLU:OE1	30:1e:27:LYS:NZ	2.38	0.54
3:1C:192:GLN:OE1	3:1C:195:ARG:NH2	2.41	0.54
6:1F:355:LYS:NZ	6:1F:370:ASP:OD1	2.40	0.54
8:1H:139:THR:OG1	8:1H:192:GLU:OE1	2.24	0.54
12:1L:172:ILE:HD12	12:1L:173:LEU:N	2.21	0.54
15:1O:227:GLU:HB3	15:1O:233:LYS:HZ3	1.72	0.54
15:1O:266:LYS:O	15:1O:270:LEU:HD23	2.07	0.54
16:1P:59:LEU:HA	16:1P:62:MET:SD	2.47	0.54
22:1W:101:THR:OG1	22:1W:105:ARG:NH2	2.41	0.54
25:1Z:123:GLU:HA	30:1e:75:LEU:HD21	1.90	0.54
29:1d:105:ASP:C	29:1d:105:ASP:OD2	2.51	0.54
32:1g:67:SER:O	32:1g:70:LEU:N	2.34	0.54
33:1h:113:LEU:HD13	33:1h:117:ARG:HE	1.73	0.54
34:1i:119:MET:HE1	40:1o:60:HIS:HB2	1.89	0.54
9:1I:113:MET:HE3	9:1I:149:TYR:CD2	2.42	0.54
12:1L:13:ILE:HD11	34:1i:77:PRO:HB3	1.90	0.54
13:1M:252:PRO:HG3	29:1d:117:HIS:CE1	2.43	0.54
13:1M:325:MET:HG3	13:1M:437:MET:CE	2.38	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:421:HIS:HB2	38:1m:50:TYR:CE1	2.42	0.54
14:1N:239:VAL:HG21	29:1d:47:ALA:HB1	1.90	0.54
15:1O:254:ARG:HH22	15:1O:255:THR:CG2	2.21	0.54
23:1X:161:LYS:N	29:1d:87:ASP:OD2	2.35	0.54
34:1i:60:ILE:O	34:1i:64:TYR:N	2.38	0.54
41:1p:39:LEU:HD12	41:1p:40:VAL:HG23	1.89	0.54
42:1q:32:ASP:OD2	42:1q:32:ASP:C	2.51	0.54
43:1r:11:ARG:NH1	43:1r:20:GLN:OE1	2.40	0.54
6:1F:89:ARG:NH1	6:1F:217:GLY:O	2.41	0.54
13:1M:259:TYR:HB3	13:1M:263:MET:HE1	1.89	0.54
15:1O:41:GLU:HG2	15:1O:231:ALA:HB2	1.88	0.54
21:1V:8:THR:O	21:1V:75:GLN:NE2	2.41	0.54
27:1b:30:ILE:HD12	27:1b:31:LEU:HD13	1.88	0.54
35:1j:27:PHE:O	35:1j:31:THR:OG1	2.15	0.54
35:1j:31:THR:HA	35:1j:34:PHE:HE2	1.73	0.54
2:1B:108:PRO:HB3	8:1H:59:GLU:O	2.08	0.54
4:1D:138:ARG:HG2	4:1D:194:ILE:HD12	1.90	0.54
8:1H:23:VAL:HG11	26:1a:12:MET:HE1	1.88	0.54
11:1K:59:MET:HE1	11:1K:63:LEU:HD12	1.89	0.54
12:1L:206:ASN:OD1	12:1L:206:ASN:N	2.40	0.54
12:1L:229:LEU:O	12:1L:232:TRP:NE1	2.40	0.54
13:1M:203:PHE:HA	13:1M:206:LYS:NZ	2.23	0.54
14:1N:265:MET:HE3	14:1N:265:MET:CA	2.34	0.54
14:1N:323:MET:H	14:1N:323:MET:CE	2.19	0.54
15:1O:25:ILE:HD11	15:1O:123:VAL:HG22	1.90	0.54
16:1P:210:VAL:HG22	16:1P:230:PHE:HD2	1.73	0.54
32:1g:94:GLU:HG2	41:1p:8:VAL:HG11	1.90	0.54
37:1l:77:ILE:HD11	38:1m:67:TRP:HB2	1.89	0.54
40:1o:110:ARG:HD3	40:1o:111:LYS:HD2	1.89	0.54
40:1o:118:GLU:HA	40:1o:121:MET:HG3	1.90	0.54
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.73	0.54
6:1F:361:GLN:HG3	7:1G:51:ASN:ND2	2.23	0.54
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.90	0.54
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	1.90	0.54
38:1m:69:TYR:HE1	38:1m:74:ASN:OD1	1.91	0.54
41:1p:54:GLN:HA	41:1p:57:LYS:HD3	1.90	0.54
1:1A:37:TYR:HE2	8:1H:208:VAL:HG11	1.72	0.54
2:1B:62:MET:HE1	2:1B:160:ILE:HD12	1.90	0.54
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.89	0.54
7:1G:347:GLU:HA	7:1G:459:GLN:HE22	1.73	0.54
11:1K:90:VAL:HG13	11:1K:90:VAL:O	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:17:TYR:O	20:1U:20:LYS:NZ	2.38	0.54
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	1.90	0.54
37:1l:16:THR:O	37:1l:20:ARG:HG2	2.08	0.54
4:1D:111:MET:CE	4:1D:189:MET:HG3	2.32	0.53
12:1L:51:LEU:O	12:1L:55:MET:HE3	2.09	0.53
13:1M:304:GLN:HE22	41:1p:148:HIS:H	1.56	0.53
20:1U:34:SER:H	20:1U:73:PRO:HD2	1.73	0.53
22:1W:70:ASN:O	58:1W:201:EHZ:N1	2.41	0.53
24:1Y:40:ILE:HD11	24:1Y:45:PRO:HB3	1.88	0.53
35:1j:48:LEU:HD22	35:1j:49:GLY:H	1.73	0.53
1:1A:31:SER:HB2	16:1P:320:ARG:HB2	1.90	0.53
10:1J:126:VAL:HA	25:1Z:121:MET:HE1	1.90	0.53
13:1M:449:LEU:HD23	13:1M:450:ASN:HB2	1.90	0.53
30:1e:60:ASP:HA	30:1e:63:VAL:HG12	1.90	0.53
4:1D:68:LEU:HA	4:1D:73:VAL:HA	1.89	0.53
7:1G:280:THR:OG1	42:1q:136:GLU:OE1	2.21	0.53
8:1H:29:GLY:O	8:1H:34:ARG:N	2.41	0.53
12:1L:79:SER:HB2	12:1L:135:ASN:HB3	1.90	0.53
13:1M:278:ARG:NH1	37:1l:83:MET:HE3	2.22	0.53
21:1V:97:LYS:HG3	21:1V:99:TRP:CZ2	2.42	0.53
34:1i:30:ARG:HD2	34:1i:31:GLU:N	2.23	0.53
5:1E:126:ILE:HG23	5:1E:130:GLU:HG2	1.90	0.53
12:1L:249:SER:OG	12:1L:250:SER:N	2.40	0.53
13:1M:186:LEU:HB3	13:1M:253:LEU:HD23	1.90	0.53
13:1M:269:MET:HB3	13:1M:295:ALA:HB3	1.91	0.53
15:1O:216:GLU:OE2	15:1O:216:GLU:N	2.30	0.53
31:1f:27:ASP:N	31:1f:27:ASP:OD1	2.41	0.53
36:1k:61:SER:O	36:1k:65:ALA:N	2.40	0.53
38:1m:99:PHE:CD2	38:1m:99:PHE:C	2.86	0.53
39:1n:159:GLU:OE2	39:1n:159:GLU:N	2.41	0.53
44:1s:45:GLU:OE1	44:1s:45:GLU:N	2.38	0.53
10:1J:56:VAL:O	10:1J:60:TYR:HB2	2.09	0.53
13:1M:199:CYS:HB3	13:1M:246:ILE:HG12	1.89	0.53
13:1M:229:MET:HE3	13:1M:328:CYS:SG	2.49	0.53
17:1Q:27:GLU:HG3	17:1Q:31:LYS:HZ1	1.73	0.53
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.08	0.53
35:1j:69:ASP:OD1	40:1o:113:ARG:NH1	2.28	0.53
36:1k:40:LEU:HD21	39:1n:45:ALA:HB2	1.90	0.53
38:1m:44:ARG:HE	39:1n:148:PRO:HG3	1.74	0.53
10:1J:170:GLU:HA	10:1J:170:GLU:OE2	2.09	0.53
12:1L:573:MET:HE2	12:1L:573:MET:C	2.32	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:270:ILE:HG12	13:1M:399:ASN:HB2	1.90	0.53
13:1M:311:GLY:HA2	13:1M:377:GLY:HA2	1.90	0.53
15:1O:221:LEU:HD21	15:1O:241:LEU:HD11	1.91	0.53
20:1T:22:TYR:CE1	20:1T:50:ILE:HG13	2.44	0.53
31:1f:49:ARG:HH12	33:1h:60:VAL:HG22	1.73	0.53
1:1A:53:MET:HE1	1:1A:56:PHE:HA	1.90	0.53
4:1D:19:MET:HE3	14:1N:295:ARG:CD	2.35	0.53
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.91	0.53
6:1F:292:ASP:O	6:1F:339:ARG:NH2	2.37	0.53
6:1F:338:ASP:OD1	6:1F:341:THR:OG1	2.27	0.53
16:1P:335:LYS:CD	16:1P:336:PRO:O	2.55	0.53
21:1V:94:LEU:HA	21:1V:97:LYS:CD	2.38	0.53
21:1V:94:LEU:O	21:1V:97:LYS:HG2	2.08	0.53
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.29	0.53
7:1G:201:ASP:HA	17:1Q:45:MET:CE	2.39	0.53
12:1L:524:ASN:HD22	39:1n:76:PRO:HB2	1.74	0.53
40:1o:104:GLU:HA	40:1o:107:LEU:HD12	1.90	0.53
3:1C:182:ARG:HD2	22:1W:101:THR:HA	1.91	0.53
5:1E:63:ILE:O	5:1E:67:ASN:ND2	2.41	0.53
5:1E:145:LEU:HD12	5:1E:153:MET:HE1	1.89	0.53
6:1F:337:MET:HG2	6:1F:341:THR:HG21	1.90	0.53
7:1G:243:ARG:H	7:1G:248:MET:HE1	1.74	0.53
13:1M:355:MET:HE1	13:1M:434:ASN:OD1	2.09	0.53
13:1M:438:ALA:O	13:1M:442:LEU:HG	2.08	0.53
14:1N:320:THR:OG1	15:1O:265:ASN:HB2	2.08	0.53
15:1O:82:PHE:C	15:1O:82:PHE:CD2	2.86	0.53
20:1T:79:TYR:CD1	20:1T:80:ILE:HD12	2.43	0.53
30:1e:96:HIS:H	30:1e:96:HIS:CD2	2.27	0.53
36:1k:12:LYS:CD	36:1k:14:GLU:H	2.18	0.53
2:1B:92:LEU:HD22	2:1B:133:VAL:HG11	1.91	0.53
4:1D:395:GLY:HA2	4:1D:398:HIS:HB2	1.91	0.53
8:1H:117:LEU:HB2	8:1H:132:ALA:HB1	1.90	0.53
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.22	0.53
12:1L:455:LYS:HZ2	12:1L:456:ARG:HH21	1.57	0.53
13:1M:216:LEU:C	13:1M:216:LEU:HD13	2.34	0.53
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.91	0.53
15:1O:27:VAL:HG22	15:1O:170:VAL:HB	1.91	0.53
20:1T:57:GLU:OE1	20:1T:58:PHE:N	2.42	0.53
22:1W:114:ARG:HD3	22:1W:114:ARG:C	2.34	0.53
25:1Z:28:ARG:NH2	43:1r:13:TRP:O	2.41	0.53
29:1d:94:VAL:HA	29:1d:101:PHE:HE2	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:61:PRO:HG3	41:1p:63:TYR:CD2	2.44	0.53
33:1h:127:THR:OG1	33:1h:128:ILE:N	2.41	0.53
43:1r:105:LEU:HD21	43:1r:111:TYR:HE2	1.73	0.53
7:1G:102:PRO:HG3	7:1G:151:THR:HG22	1.92	0.52
8:1H:54:LYS:HZ3	8:1H:55:LEU:CD2	2.22	0.52
12:1L:599:MET:O	12:1L:601:LEU:N	2.41	0.52
13:1M:424:ASN:HD21	38:1m:56:LEU:HA	1.74	0.52
28:1c:29:ILE:HD12	28:1c:30:TYR:N	2.23	0.52
41:1p:38:LEU:CD1	41:1p:42:ARG:HB2	2.38	0.52
2:1B:116:MET:HE2	2:1B:156:LEU:CD2	2.39	0.52
8:1H:25:ARG:HH22	8:1H:47:GLN:NE2	2.03	0.52
8:1H:233:MET:O	8:1H:236:ALA:N	2.43	0.52
9:1I:18:THR:HG22	25:1Z:32:GLY:HA3	1.91	0.52
10:1J:27:ILE:HG23	10:1J:28:TYR:HD2	1.74	0.52
12:1L:55:MET:N	12:1L:55:MET:HE2	2.25	0.52
12:1L:337:ALA:HA	12:1L:340:PHE:CD2	2.45	0.52
12:1L:383:MET:SD	12:1L:386:LEU:HD22	2.50	0.52
15:1O:28:ASP:N	15:1O:170:VAL:O	2.42	0.52
15:1O:219:GLU:HG2	15:1O:241:LEU:HD22	1.92	0.52
15:1O:252:ASP:C	15:1O:252:ASP:OD2	2.53	0.52
20:1U:24:LYS:CG	36:1k:41:ARG:HH21	2.21	0.52
20:1U:58:PHE:CB	20:1U:60:PHE:HE2	2.22	0.52
24:1Y:68:ILE:HD12	24:1Y:69:PHE:N	2.23	0.52
28:1c:38:ASP:OD2	29:1d:77:LYS:NZ	2.40	0.52
36:1k:29:GLU:CD	36:1k:30:THR:HG23	2.33	0.52
37:1l:20:ARG:NH2	37:1l:36:PRO:HD2	2.25	0.52
42:1q:68:MET:HE3	42:1q:81:MET:SD	2.50	0.52
43:1r:57:ASP:OD1	43:1r:57:ASP:N	2.38	0.52
12:1L:562:LEU:HB3	12:1L:563:PRO:HD3	1.91	0.52
13:1M:203:PHE:HD1	13:1M:206:LYS:HZ1	1.57	0.52
13:1M:367:LEU:HD21	13:1M:407:SER:HB2	1.90	0.52
14:1N:54:GLU:H	14:1N:54:GLU:CD	2.17	0.52
41:1p:73:ILE:HG23	41:1p:155:LEU:HD22	1.90	0.52
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.42	0.52
4:1D:168:PHE:CE1	8:1H:32:GLN:NE2	2.77	0.52
6:1F:347:ILE:CG2	6:1F:376:MET:HE2	2.36	0.52
12:1L:15:LEU:HD11	12:1L:125:LEU:HB3	1.91	0.52
12:1L:119:LYS:HG3	12:1L:123:LEU:CD1	2.39	0.52
14:1N:313:MET:HG2	15:1O:270:LEU:HD11	1.92	0.52
15:1O:173:ASP:HB3	15:1O:224:SER:HA	1.92	0.52
17:1Q:80:SER:OG	17:1Q:81:ASN:OD1	2.28	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1b:20:ALA:O	27:1b:24:ILE:HD12	2.10	0.52
34:1i:10:ARG:NE	39:1n:155:PRO:HA	2.23	0.52
40:1o:27:ASP:N	40:1o:27:ASP:OD1	2.41	0.52
42:1q:144:TYR:CD2	42:1q:145:LYS:N	2.77	0.52
4:1D:211:ILE:HG22	4:1D:315:LEU:HD11	1.91	0.52
10:1J:33:LEU:HD21	11:1K:38:LEU:HD11	1.91	0.52
14:1N:24:SER:HB3	30:1e:1:PRO:HG3	1.92	0.52
19:1S:34:ASP:HB2	19:1S:83:ALA:HB2	1.92	0.52
21:1V:76:ILE:O	21:1V:80:ILE:HD12	2.10	0.52
37:1l:14:PRO:HD3	37:1l:46:ASP:HA	1.91	0.52
37:1l:30:ARG:HH11	38:1m:34:GLU:HG2	1.75	0.52
37:1l:108:PHE:C	37:1l:108:PHE:CD1	2.87	0.52
1:1A:33:LYS:HE2	2:1B:109:GLU:HG2	1.91	0.52
2:1B:39:TRP:NE1	46:1q:201:PC1:H32	2.25	0.52
7:1G:12:PHE:O	7:1G:78:ASN:HA	2.09	0.52
12:1L:447:ASN:OD1	12:1L:450:LEU:N	2.38	0.52
13:1M:210:TYR:O	13:1M:264:LEU:HD11	2.09	0.52
13:1M:289:SER:O	13:1M:293:HIS:ND1	2.31	0.52
15:1O:76:ASN:HB3	15:1O:95:ARG:HD2	1.91	0.52
15:1O:82:PHE:HE2	15:1O:143:PHE:HE2	1.58	0.52
16:1P:96:GLY:O	56:1P:501:NDP:H8A	2.09	0.52
20:1U:24:LYS:HD2	36:1k:41:ARG:HH21	1.71	0.52
21:1V:32:ASP:C	21:1V:32:ASP:OD2	2.52	0.52
21:1V:56:GLY:HA2	21:1V:59:LYS:HE3	1.91	0.52
22:1W:114:ARG:HD3	22:1W:115:PRO:N	2.23	0.52
24:1Y:92:GLY:HA2	24:1Y:95:ALA:HB3	1.92	0.52
37:1l:13:TYR:HD1	37:1l:15:LYS:HD3	1.75	0.52
39:1n:20:LYS:O	39:1n:24:ARG:HG2	2.09	0.52
1:1A:111:LEU:HD22	1:1A:111:LEU:H	1.74	0.52
3:1C:198:ASP:OD1	3:1C:198:ASP:N	2.42	0.52
7:1G:148:THR:OG1	7:1G:148:THR:O	2.27	0.52
7:1G:306:MET:HE2	7:1G:306:MET:N	2.24	0.52
13:1M:123:GLU:C	13:1M:123:GLU:OE1	2.53	0.52
14:1N:159:MET:CE	14:1N:282:MET:HG3	2.38	0.52
28:1c:24:SER:HA	28:1c:27:LEU:HD23	1.90	0.52
10:1J:78:MET:CE	10:1J:79:TYR:HD1	2.22	0.52
12:1L:386:LEU:HG	12:1L:387:THR:H	1.74	0.52
15:1O:57:HIS:CD2	15:1O:68:PRO:HB3	2.44	0.52
16:1P:169:SER:HB3	16:1P:231:VAL:HG12	1.91	0.52
20:1T:11:ILE:CD1	20:1T:84:LYS:HZ1	2.22	0.52
20:1T:51:ILE:HB	20:1T:62:ILE:HD11	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:55:GLU:HB3	20:1T:62:ILE:HG12	1.90	0.52
21:1V:57:MET:HE3	21:1V:70:GLN:NE2	2.24	0.52
25:1Z:137:THR:OG1	25:1Z:138:TYR:N	2.43	0.52
1:1A:72:LEU:HA	10:1J:147:TYR:OH	2.10	0.52
3:1C:40:VAL:HG22	43:1r:69:MET:HE3	1.91	0.52
12:1L:68:TRP:O	12:1L:69:MET:HE2	2.10	0.52
12:1L:280:LEU:HA	12:1L:283:ILE:HD12	1.92	0.52
12:1L:366:MET:HE3	12:1L:445:GLU:HG2	1.91	0.52
13:1M:278:ARG:CZ	37:1l:83:MET:HE3	2.39	0.52
15:1O:214:MET:HE3	15:1O:214:MET:C	2.34	0.52
16:1P:335:LYS:HZ2	16:1P:336:PRO:CG	2.22	0.52
34:1i:29:PRO:HD2	34:1i:30:ARG:HH21	1.75	0.52
34:1i:44:GLN:OE1	34:1i:44:GLN:N	2.41	0.52
41:1p:29:VAL:O	41:1p:33:THR:HG23	2.10	0.52
6:1F:277:LYS:HE2	6:1F:291:TRP:CE2	2.45	0.52
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.92	0.52
8:1H:142:TYR:CD1	8:1H:289:LEU:HD22	2.45	0.52
12:1L:245:ALA:O	12:1L:246:LEU:HD23	2.10	0.52
12:1L:568:PHE:HE2	46:1L:702:PC1:H322	1.75	0.52
15:1O:41:GLU:HG2	15:1O:231:ALA:HB1	1.89	0.52
16:1P:157:ARG:NH1	16:1P:225:GLY:O	2.42	0.52
20:1U:24:LYS:CE	36:1k:41:ARG:NH2	2.69	0.52
37:1l:139:TYR:CG	37:1l:150:PRO:HB3	2.45	0.52
42:1q:44:TYR:HE2	42:1q:83:PRO:HB3	1.74	0.52
7:1G:201:ASP:HA	17:1Q:45:MET:HE2	1.91	0.51
7:1G:314:ASP:HB3	7:1G:520:LYS:HG2	1.92	0.51
9:1I:98:PRO:HA	9:1I:104:ARG:HB2	1.92	0.51
10:1J:60:TYR:OH	11:1K:37:MET:HB3	2.11	0.51
13:1M:303:ILE:HD11	13:1M:388:TRP:CD1	2.45	0.51
14:1N:189:TRP:CZ3	14:1N:282:MET:HE2	2.44	0.51
14:1N:313:MET:HE3	15:1O:99:TRP:CE3	2.44	0.51
14:1N:323:MET:HA	51:1O:403:CDL:C72	2.40	0.51
16:1P:335:LYS:HZ2	16:1P:336:PRO:CD	2.24	0.51
17:1Q:45:MET:HE2	17:1Q:45:MET:HA	1.92	0.51
22:1W:116:THR:C	22:1W:121:LYS:HZ1	2.17	0.51
27:1b:24:ILE:HA	27:1b:27:LEU:CD1	2.39	0.51
37:1l:14:PRO:HG2	37:1l:36:PRO:HG3	1.91	0.51
37:1l:20:ARG:HH11	37:1l:20:ARG:HG3	1.74	0.51
39:1n:43:MET:HE1	58:1n:201:EHZ:C5	2.40	0.51
8:1H:25:ARG:NH2	8:1H:47:GLN:HE21	2.07	0.51
12:1L:132:VAL:HA	12:1L:258:PHE:CE2	2.45	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:76:MET:SD	13:1M:76:MET:N	2.81	0.51
16:1P:139:ILE:H	16:1P:139:ILE:HD12	1.74	0.51
22:1W:34:GLU:HA	22:1W:37:ARG:HG3	1.92	0.51
32:1g:36:ASN:HD22	32:1g:39:GLU:CD	2.18	0.51
36:1k:23:ILE:O	36:1k:26:THR:OG1	2.25	0.51
38:1m:66:ARG:NE	38:1m:66:ARG:HA	2.25	0.51
13:1M:329:LEU:O	13:1M:332:THR:OG1	2.28	0.51
13:1M:357:THR:O	13:1M:361:MET:HE1	2.09	0.51
14:1N:120:GLN:OE1	14:1N:176:ARG:NH2	2.42	0.51
24:1Y:2:LYS:HG2	24:1Y:6:HIS:CE1	2.45	0.51
32:1g:68:ILE:HD12	32:1g:69:VAL:N	2.25	0.51
34:1i:70:ALA:O	34:1i:75:LEU:N	2.33	0.51
38:1m:74:ASN:HB3	38:1m:78:ASN:HD21	1.75	0.51
39:1n:48:ASP:HA	39:1n:51:LYS:HG3	1.92	0.51
5:1E:76:PRO:HD3	44:1s:74:ARG:NH2	2.26	0.51
6:1F:125:GLY:O	6:1F:129:MET:HG3	2.11	0.51
7:1G:449:PRO:O	7:1G:487:TRP:NE1	2.37	0.51
8:1H:113:VAL:O	8:1H:116:ILE:HG22	2.10	0.51
12:1L:327:LEU:O	12:1L:331:MET:HG2	2.10	0.51
12:1L:407:TRP:CD1	12:1L:410:LEU:HD23	2.45	0.51
20:1T:12:LYS:NZ	20:1T:77:VAL:HG21	2.25	0.51
20:1U:60:PHE:H	20:1U:60:PHE:HD2	1.57	0.51
23:1X:9:LEU:O	23:1X:13:LYS:HG3	2.11	0.51
28:1c:32:ILE:O	28:1c:36:LYS:HG2	2.10	0.51
35:1j:8:GLU:O	35:1j:10:ARG:NH1	2.40	0.51
40:1o:45:MET:HE2	40:1o:59:ALA:HB3	1.91	0.51
5:1E:101:GLN:HG3	5:1E:140:ILE:HD11	1.92	0.51
8:1H:24:GLU:OE1	8:1H:271:LEU:HD22	2.10	0.51
8:1H:24:GLU:CD	8:1H:271:LEU:HD22	2.35	0.51
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.22	0.51
12:1L:189:PHE:O	12:1L:194:ASN:N	2.44	0.51
12:1L:313:MET:HB2	12:1L:325:ALA:HB1	1.92	0.51
13:1M:122:PHE:C	13:1M:122:PHE:CD1	2.88	0.51
14:1N:120:GLN:HE21	14:1N:177:LYS:HG2	1.76	0.51
15:1O:288:GLN:NE2	32:1g:29:ASP:OD1	2.41	0.51
20:1T:11:ILE:HG12	20:1T:84:LYS:NZ	2.26	0.51
53:1Y:201:3PE:O31	53:1Y:201:3PE:H351	2.10	0.51
34:1i:89:VAL:O	34:1i:95:THR:HG21	2.10	0.51
38:1m:114:LEU:HB2	38:1m:119:LYS:HB2	1.91	0.51
1:1A:38:GLU:HB2	1:1A:43:PRO:HG3	1.93	0.51
4:1D:76:CYS:H	4:1D:403:ASP:CG	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:140:ILE:HG21	10:1J:65:LEU:HD22	1.92	0.51
8:1H:316:PRO:HG3	25:1Z:57:ARG:HB3	1.92	0.51
13:1M:424:ASN:HA	39:1n:101:TRP:CE2	2.45	0.51
53:1Y:201:3PE:H12	53:1Y:201:3PE:H221	1.93	0.51
34:1i:30:ARG:H	34:1i:30:ARG:HE	1.59	0.51
42:1q:88:ARG:CZ	42:1q:94:THR:HG21	2.41	0.51
2:1B:46:TRP:CH2	50:1H:701:U10:H162	2.46	0.51
3:1C:108:LYS:HB2	3:1C:108:LYS:HZ3	1.74	0.51
4:1D:161:ILE:O	8:1H:279:ARG:HB3	2.11	0.51
5:1E:112:ASN:O	5:1E:115:SER:OG	2.27	0.51
6:1F:224:ASN:HB3	6:1F:227:THR:HG23	1.91	0.51
11:1K:37:MET:CE	11:1K:67:ALA:HA	2.38	0.51
12:1L:145:GLU:OE2	12:1L:176:ARG:NH2	2.43	0.51
12:1L:377:SER:O	12:1L:380:LEU:HD23	2.10	0.51
13:1M:431:THR:HA	13:1M:434:ASN:HB2	1.92	0.51
14:1N:290:LEU:O	14:1N:294:MET:HG2	2.10	0.51
22:1W:42:GLU:HG3	22:1W:94:ILE:HD11	1.92	0.51
24:1Y:137:GLU:HG2	24:1Y:139:LYS:HZ1	1.75	0.51
35:1j:32:MET:HE1	35:1j:33:TRP:CD1	2.46	0.51
4:1D:418:ILE:HA	4:1D:421:GLN:HB2	1.93	0.51
7:1G:373:GLU:CD	7:1G:448:LYS:HZ3	2.19	0.51
8:1H:58:LYS:HZ2	8:1H:217:ALA:N	2.09	0.51
8:1H:135:ALA:HB2	8:1H:201:THR:HG23	1.93	0.51
11:1K:94:ASN:CG	12:1L:583:LEU:HD23	2.36	0.51
12:1L:93:ALA:O	12:1L:97:THR:HG22	2.11	0.51
14:1N:44:LEU:HD13	14:1N:122:ILE:HG21	1.92	0.51
15:1O:63:THR:OG1	15:1O:302:ARG:NH2	2.39	0.51
23:1X:43:MET:HE1	27:1b:52:TYR:CZ	2.46	0.51
23:1X:57:GLU:HA	23:1X:60:LYS:HG2	1.91	0.51
35:1j:32:MET:CE	35:1j:33:TRP:CD1	2.93	0.51
38:1m:80:ARG:HG2	38:1m:82:THR:OG1	2.10	0.51
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.46	0.51
6:1F:242:PHE:O	6:1F:251:SER:OG	2.28	0.51
11:1K:8:ILE:CD1	11:1K:43:MET:HE2	2.41	0.51
12:1L:242:PRO:O	12:1L:246:LEU:HG	2.11	0.51
13:1M:307:TRP:HA	13:1M:310:MET:HE3	1.92	0.51
13:1M:410:MET:O	13:1M:414:THR:OG1	2.16	0.51
14:1N:124:LEU:HB3	14:1N:220:ILE:HD11	1.92	0.51
15:1O:233:LYS:HA	15:1O:236:GLU:HG2	1.93	0.51
20:1T:47:GLN:NE2	20:1T:67:ALA:O	2.43	0.51
34:1i:44:GLN:CD	34:1i:44:GLN:H	2.19	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:92:LEU:HD11	2:1B:100:LEU:HG	1.93	0.51
3:1C:53:HIS:CD2	3:1C:55:ASP:H	2.29	0.51
7:1G:236:SER:HB3	7:1G:259:ASN:HD22	1.77	0.51
7:1G:324:ASP:OD1	7:1G:327:ALA:N	2.34	0.51
10:1J:17:PHE:CD2	11:1K:11:ALA:HB1	2.46	0.51
15:1O:291:ARG:O	15:1O:295:LYS:HG2	2.11	0.51
18:1R:37:GLU:N	18:1R:37:GLU:OE2	2.44	0.51
32:1g:92:GLU:HG2	41:1p:64:HIS:CE1	2.46	0.51
33:1h:12:LYS:HD2	33:1h:12:LYS:C	2.36	0.51
34:1i:1:SAC:C	34:1i:1:SAC:H2A1	2.41	0.51
36:1k:50:TRP:CE2	36:1k:51:ARG:HG2	2.46	0.51
10:1J:153:LEU:O	10:1J:157:THR:OG1	2.20	0.50
12:1L:551:SER:HA	12:1L:555:LEU:HB3	1.92	0.50
13:1M:221:VAL:O	13:1M:340:ARG:NH2	2.44	0.50
14:1N:62:THR:HG21	14:1N:114:TRP:HB3	1.92	0.50
15:1O:281:GLU:N	15:1O:281:GLU:OE1	2.43	0.50
23:1X:31:TYR:CE2	25:1Z:74:LEU:HD11	2.46	0.50
38:1m:5:TYR:OH	38:1m:11:ALA:O	2.29	0.50
12:1L:409:LEU:O	12:1L:412:THR:OG1	2.17	0.50
14:1N:10:ILE:O	14:1N:14:MET:HG2	2.11	0.50
15:1O:199:LEU:HA	15:1O:202:ILE:HD12	1.92	0.50
31:1f:43:LEU:HD21	41:1p:67:PHE:HD1	1.76	0.50
34:1i:40:TRP:O	34:1i:44:GLN:NE2	2.45	0.50
34:1i:119:MET:HE3	34:1i:122:PHE:CE1	2.46	0.50
3:1C:175:ARG:HD3	16:1P:13:ARG:HD2	1.93	0.50
4:1D:14:PHE:HB3	4:1D:19:MET:HE2	1.94	0.50
4:1D:232:ASN:O	4:1D:236:ARG:HG3	2.11	0.50
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.93	0.50
11:1K:93:LEU:HD23	11:1K:93:LEU:H	1.76	0.50
14:1N:73:ALA:CB	14:1N:98:MET:HE2	2.41	0.50
14:1N:255:PRO:HG3	14:1N:260:PHE:CD1	2.47	0.50
15:1O:88:SER:OG	15:1O:90:ASP:OD2	2.28	0.50
15:1O:163:TYR:HE1	15:1O:263:VAL:HG12	1.75	0.50
17:1Q:58:GLU:OE2	17:1Q:58:GLU:C	2.54	0.50
19:1S:62:PRO:HG2	19:1S:79:ASN:HA	1.93	0.50
20:1T:86:VAL:HG12	20:1T:86:VAL:O	2.10	0.50
21:1V:94:LEU:C	21:1V:95:ARG:NH2	2.70	0.50
22:1W:62:LYS:HE2	22:1W:66:MET:HE1	1.93	0.50
25:1Z:65:PHE:O	25:1Z:69:ILE:HD12	2.11	0.50
32:1g:33:GLU:OE2	32:1g:33:GLU:HA	2.11	0.50
1:1A:63:LEU:HD11	11:1K:68:ALA:HB1	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:131:LEU:HD21	43:1r:48:LEU:HD11	1.94	0.50
8:1H:272:TRP:O	8:1H:276:SER:OG	2.29	0.50
12:1L:258:PHE:HD1	12:1L:326:PHE:HE2	1.59	0.50
14:1N:298:TYR:O	14:1N:303:THR:OG1	2.29	0.50
20:1U:54:MET:HE1	20:1U:76:ILE:HG21	1.94	0.50
21:1V:57:MET:HE1	21:1V:70:GLN:HG2	1.92	0.50
24:1Y:117:MET:HA	24:1Y:120:THR:HB	1.92	0.50
28:1c:2:PHE:HD2	28:1c:2:PHE:C	2.19	0.50
41:1p:28:PRO:HA	41:1p:31:TYR:CE2	2.46	0.50
12:1L:97:THR:HA	12:1L:100:ILE:HG12	1.93	0.50
14:1N:316:GLN:HG2	15:1O:302:ARG:HH21	1.77	0.50
1:1A:13:LEU:HD11	50:1H:701:U10:H362	1.94	0.50
1:1A:41:PHE:HB3	22:1W:99:GLN:HE21	1.77	0.50
6:1F:132:ARG:HH22	44:1s:66:PRO:HD3	1.77	0.50
8:1H:233:MET:HG2	8:1H:234:MET:N	2.22	0.50
10:1J:60:TYR:O	10:1J:64:MET:CE	2.59	0.50
12:1L:316:THR:HG21	12:1L:395:ILE:HG12	1.94	0.50
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.94	0.50
13:1M:271:MET:HE3	13:1M:271:MET:C	2.37	0.50
14:1N:112:HIS:CE1	14:1N:164:ILE:HG21	2.47	0.50
14:1N:161:SER:OG	14:1N:184:ILE:O	2.30	0.50
14:1N:215:MET:HA	14:1N:215:MET:HE2	1.93	0.50
16:1P:50:ARG:NH1	56:1P:501:NDP:O2X	2.45	0.50
20:1T:20:LYS:HE3	20:1T:30:LEU:HD23	1.92	0.50
20:1U:72:CYS:O	20:1U:76:ILE:HG13	2.11	0.50
24:1Y:124:VAL:HA	53:1Y:201:3PE:H252	1.94	0.50
29:1d:90:MET:HE1	33:1h:107:GLU:HB2	1.92	0.50
38:1m:44:ARG:O	38:1m:48:LEU:HG	2.11	0.50
39:1n:82:PRO:O	39:1n:90:TYR:N	2.44	0.50
1:1A:108:GLN:O	1:1A:109:LYS:HD3	2.11	0.50
4:1D:283:PHE:O	9:1I:1:THR:OG1	2.30	0.50
12:1L:69:MET:HE1	13:1M:451:PRO:HD2	1.94	0.50
12:1L:357:ARG:NH2	39:1n:77:GLN:O	2.43	0.50
13:1M:430:PHE:HB3	32:1g:46:GLY:HA3	1.94	0.50
16:1P:179:LEU:HD22	16:1P:245:ILE:HD11	1.93	0.50
20:1U:21:LEU:HA	36:1k:18:TYR:CZ	2.47	0.50
23:1X:87:CYS:SG	23:1X:99:CYS:HB3	2.52	0.50
31:1f:26:LEU:HA	31:1f:29:ARG:HB2	1.93	0.50
32:1g:88:TRP:HD1	41:1p:65:ARG:HB3	1.77	0.50
34:1i:124:ASP:N	40:1o:61:TYR:OH	2.45	0.50
36:1k:67:LEU:HD12	36:1k:70:PHE:HD2	1.77	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:85:ILE:CD1	37:1l:88:ARG:HB2	2.42	0.50
5:1E:104:THR:HB	6:1F:349:ARG:HH21	1.77	0.50
6:1F:190:THR:HB	6:1F:204:ARG:HG2	1.93	0.50
7:1G:659:ASP:OD1	7:1G:659:ASP:N	2.43	0.50
13:1M:262:LEU:O	13:1M:265:SER:OG	2.29	0.50
13:1M:441:ILE:HG23	13:1M:442:LEU:HD23	1.94	0.50
14:1N:147:GLN:HB2	33:1h:125:TYR:CE1	2.47	0.50
15:1O:214:MET:HG2	15:1O:217:LYS:HE3	1.94	0.50
15:1O:290:ASP:O	15:1O:294:GLN:HG3	2.12	0.50
20:1U:49:GLU:HB3	36:1k:44:TRP:HE1	1.77	0.50
25:1Z:64:ASP:OD2	25:1Z:64:ASP:C	2.55	0.50
28:1c:2:PHE:C	28:1c:2:PHE:CD2	2.90	0.50
42:1q:94:THR:OG1	42:1q:96:ASP:OD1	2.24	0.50
6:1F:300:GLY:HA2	6:1F:333:ALA:H	1.76	0.50
7:1G:21:GLU:OE1	7:1G:22:PRO:HD2	2.12	0.50
7:1G:100:ASN:HB3	7:1G:135:ARG:HG2	1.93	0.50
7:1G:518:PRO:HB3	7:1G:538:PRO:HD3	1.93	0.50
7:1G:556:MET:HG3	7:1G:556:MET:O	2.10	0.50
9:1I:77:CYS:O	9:1I:105:ARG:HD2	2.12	0.50
28:1c:26:PHE:C	28:1c:26:PHE:CD2	2.88	0.50
36:1k:70:PHE:O	36:1k:70:PHE:HD1	1.95	0.50
37:1l:82:ASP:N	37:1l:82:ASP:OD1	2.44	0.50
37:1l:136:ASN:O	37:1l:136:ASN:ND2	2.45	0.50
8:1H:306:SER:O	8:1H:310:MET:HG2	2.12	0.49
12:1L:366:MET:SD	12:1L:443:ILE:HG22	2.52	0.49
12:1L:528:TYR:HB2	37:1l:105:LEU:HD21	1.92	0.49
13:1M:270:ILE:HD11	13:1M:395:LEU:HB3	1.94	0.49
13:1M:325:MET:HG3	13:1M:437:MET:HE1	1.94	0.49
14:1N:255:PRO:HG3	14:1N:260:PHE:CG	2.46	0.49
15:1O:242:LYS:HG2	15:1O:244:ASP:H	1.77	0.49
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.45	0.49
24:1Y:75:ILE:HG13	24:1Y:76:SER:N	2.27	0.49
29:1d:87:ASP:HA	29:1d:90:MET:HB2	1.94	0.49
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.37	0.49
38:1m:36:LEU:O	38:1m:40:SER:OG	2.27	0.49
1:1A:90:MET:SD	10:1J:151:THR:OG1	2.66	0.49
2:1B:53:ALA:HB2	4:1D:83:LEU:HD11	1.94	0.49
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.51	0.49
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.47	0.49
12:1L:463:PHE:N	12:1L:463:PHE:CD1	2.78	0.49
14:1N:85:THR:OG1	30:1e:18:THR:OG1	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:178:ILE:HG12	14:1N:179:MET:N	2.27	0.49
18:1R:18:TYR:CE2	18:1R:24:ARG:HB2	2.47	0.49
3:1C:40:VAL:HG23	43:1r:68:VAL:HG13	1.94	0.49
4:1D:182:GLU:OE2	9:1I:58:SER:N	2.45	0.49
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.93	0.49
12:1L:142:ILE:HG12	13:1M:370:PRO:HB2	1.93	0.49
12:1L:146:GLY:O	12:1L:150:MET:HB2	2.12	0.49
13:1M:5:ILE:O	13:1M:9:THR:HG22	2.12	0.49
13:1M:81:GLN:HE22	32:1g:57:ASN:HD21	1.59	0.49
14:1N:61:LEU:O	14:1N:65:THR:OG1	2.23	0.49
14:1N:187:MET:HA	14:1N:187:MET:CE	2.37	0.49
16:1P:97:ARG:NH2	56:1P:501:NDP:O3X	2.44	0.49
20:1U:24:LYS:HE3	36:1k:41:ARG:CZ	2.42	0.49
22:1W:107:PHE:O	22:1W:109:GLU:HG2	2.12	0.49
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.47	0.49
29:1d:70:PHE:CD1	29:1d:70:PHE:C	2.90	0.49
46:1d:201:PC1:H153	30:1e:2:PHE:CZ	2.47	0.49
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	1.94	0.49
40:1o:104:GLU:HA	40:1o:107:LEU:HB2	1.95	0.49
2:1B:69:MET:HG3	2:1B:74:VAL:HG13	1.95	0.49
4:1D:352:TYR:HD1	9:1I:86:VAL:HG21	1.77	0.49
5:1E:111:ARG:HB2	5:1E:152:PRO:HD3	1.94	0.49
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.47	0.49
46:1L:702:PC1:H3D1	24:1Y:116:TYR:HD2	1.77	0.49
13:1M:177:LEU:HB3	33:1h:94:LEU:HD21	1.94	0.49
13:1M:296:LEU:H	13:1M:296:LEU:HD12	1.78	0.49
14:1N:36:ASN:ND2	14:1N:134:GLN:OE1	2.44	0.49
16:1P:133:SER:O	16:1P:167:LYS:HA	2.12	0.49
16:1P:145:TYR:HD2	16:1P:286:ARG:CZ	2.26	0.49
23:1X:136:LEU:HD22	23:1X:137:PRO:HD2	1.94	0.49
28:1c:31:LEU:HD21	29:1d:26:LEU:HD11	1.93	0.49
36:1k:71:LYS:HD2	36:1k:72:TRP:CZ3	2.47	0.49
37:1l:47:TYR:OH	37:1l:77:ILE:O	2.28	0.49
37:1l:98:TRP:HB3	38:1m:6:LYS:HZ1	1.76	0.49
37:1l:111:PHE:O	37:1l:115:MET:SD	2.70	0.49
39:1n:50:HIS:CD2	39:1n:62:LEU:HD13	2.47	0.49
2:1B:109:GLU:O	2:1B:109:GLU:OE2	2.31	0.49
11:1K:8:ILE:HD12	11:1K:9:ILE:N	2.27	0.49
11:1K:40:LEU:HD21	14:1N:72:MET:HA	1.94	0.49
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	1.95	0.49
33:1h:114:MET:HE3	33:1h:122:TRP:CE2	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:23:LYS:O	34:1i:23:LYS:HD3	2.12	0.49
36:1k:12:LYS:O	36:1k:13:MET:HE3	2.13	0.49
38:1m:50:TYR:O	39:1n:168:HIS:NE2	2.42	0.49
7:1G:410:GLY:O	7:1G:421:HIS:NE2	2.44	0.49
8:1H:202:GLU:HG2	8:1H:211:PHE:CD1	2.47	0.49
10:1J:130:THR:HG21	25:1Z:124:LEU:HD22	1.94	0.49
12:1L:551:SER:O	12:1L:556:ILE:N	2.46	0.49
12:1L:587:TYR:O	12:1L:590:SER:OG	2.22	0.49
20:1T:7:THR:OG1	20:1T:88:GLU:OE2	2.30	0.49
22:1W:98:LYS:HB3	22:1W:102:HIS:HB2	1.95	0.49
24:1Y:133:GLN:HG3	24:1Y:136:ALA:HB2	1.93	0.49
30:1e:64:GLU:O	30:1e:68:ARG:N	2.30	0.49
32:1g:62:PHE:HB3	33:1h:28:TYR:CD2	2.47	0.49
13:1M:209:LEU:HD11	13:1M:264:LEU:HD12	1.94	0.49
14:1N:44:LEU:HB3	14:1N:122:ILE:HG21	1.94	0.49
14:1N:108:LEU:HD21	14:1N:191:THR:HG21	1.94	0.49
14:1N:236:LYS:O	14:1N:237:MET:HE2	2.13	0.49
15:1O:40:ARG:O	15:1O:44:GLU:HG3	2.12	0.49
15:1O:252:ASP:OD2	15:1O:254:ARG:N	2.46	0.49
18:1R:19:ASP:OD1	18:1R:20:ASP:N	2.45	0.49
20:1T:85:ASP:HA	20:1T:87:TYR:HE1	1.78	0.49
21:1V:57:MET:HE3	21:1V:70:GLN:HE21	1.76	0.49
21:1V:97:LYS:CA	21:1V:97:LYS:CE	2.78	0.49
21:1V:97:LYS:HE2	21:1V:99:TRP:CE2	2.48	0.49
34:1i:43:GLU:HA	34:1i:46:TRP:CE3	2.48	0.49
40:1o:68:CYS:O	40:1o:72:SER:N	2.46	0.49
1:1A:93:PHE:C	1:1A:93:PHE:CD2	2.91	0.49
4:1D:68:LEU:HD12	4:1D:68:LEU:O	2.12	0.49
7:1G:420:ASP:OD1	7:1G:420:ASP:N	2.45	0.49
8:1H:104:PHE:O	8:1H:108:MET:HG2	2.13	0.49
9:1I:156:ASN:ND2	18:1R:36:ASN:OD1	2.46	0.49
10:1J:8:ILE:O	10:1J:12:ILE:HD12	2.12	0.49
10:1J:126:VAL:C	25:1Z:120:MET:HE2	2.38	0.49
12:1L:126:ILE:HD12	12:1L:127:THR:H	1.77	0.49
12:1L:386:LEU:HD12	12:1L:462:ILE:HA	1.94	0.49
12:1L:401:MET:HE3	40:1o:94:TYR:CZ	2.48	0.49
13:1M:275:ILE:HG22	13:1M:279:GLN:NE2	2.27	0.49
14:1N:311:MET:HE3	14:1N:314:LYS:HD2	1.95	0.49
20:1U:35:HIS:HB2	20:1U:39:ASP:H	1.77	0.49
25:1Z:133:ILE:O	25:1Z:137:THR:HG23	2.12	0.49
33:1h:87:TYR:O	33:1h:91:MET:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:96:ASP:OD1	42:1q:96:ASP:N	2.45	0.49
7:1G:318:ILE:HG13	7:1G:522:LEU:HD11	1.95	0.49
8:1H:70:MET:HA	8:1H:73:ILE:HG22	1.94	0.49
8:1H:107:ALA:O	8:1H:110:SER:OG	2.25	0.49
13:1M:410:MET:SD	13:1M:411:LEU:HG	2.52	0.49
15:1O:138:MET:SD	15:1O:143:PHE:HB2	2.53	0.49
16:1P:335:LYS:HD3	16:1P:335:LYS:C	2.38	0.49
24:1Y:8:TYR:CE1	24:1Y:24:SER:HB3	2.48	0.49
25:1Z:97:ILE:HG23	25:1Z:98:MET:HG3	1.94	0.49
27:1b:23:ALA:C	27:1b:27:LEU:HD12	2.38	0.49
27:1b:78:GLU:OE2	27:1b:79:TRP:N	2.46	0.49
8:1H:128:ALA:HA	8:1H:213:VAL:HG11	1.95	0.49
9:1I:60:ARG:HG2	9:1I:172:ASP:OD1	2.12	0.49
10:1J:173:ARG:HH11	10:1J:173:ARG:HG3	1.78	0.49
13:1M:430:PHE:O	13:1M:434:ASN:ND2	2.38	0.49
14:1N:25:HIS:NE2	30:1e:17:MET:HG2	2.28	0.49
14:1N:265:MET:HA	14:1N:265:MET:CE	2.39	0.49
16:1P:145:TYR:HH	56:1P:501:NDP:HO2N	1.46	0.49
20:1T:11:ILE:CG1	20:1T:84:LYS:HZ1	2.26	0.49
24:1Y:94:CYS:O	24:1Y:98:LEU:HB3	2.13	0.49
25:1Z:94:GLU:HA	25:1Z:97:ILE:HG22	1.94	0.49
29:1d:29:PRO:HA	29:1d:32:VAL:HG22	1.94	0.49
32:1g:45:HIS:CG	32:1g:58:MET:HG3	2.48	0.49
37:1l:29:MET:HB3	37:1l:33:ASP:HB2	1.95	0.49
37:1l:41:GLY:H	38:1m:80:ARG:NH2	2.06	0.49
37:1l:108:PHE:HD1	37:1l:108:PHE:O	1.96	0.49
4:1D:269:LEU:HD21	4:1D:373:GLU:HG3	1.94	0.48
5:1E:172:ILE:HG23	5:1E:182:PRO:HG3	1.95	0.48
7:1G:228:ILE:HG21	7:1G:581:GLN:HG3	1.95	0.48
8:1H:54:LYS:HD2	8:1H:54:LYS:C	2.38	0.48
8:1H:310:MET:HE3	27:1b:32:PRO:HD3	1.95	0.48
9:1I:80:CYS:SG	9:1I:82:LEU:HG	2.53	0.48
12:1L:383:MET:SD	12:1L:383:MET:N	2.83	0.48
13:1M:309:PHE:HB3	13:1M:458:LEU:HD13	1.95	0.48
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	1.95	0.48
15:1O:112:LEU:HD13	15:1O:263:VAL:HG11	1.94	0.48
16:1P:22:THR:HG21	16:1P:85:VAL:HG12	1.95	0.48
22:1W:61:ASP:O	22:1W:65:GLU:N	2.43	0.48
32:1g:113:PHE:O	41:1p:158:GLN:NE2	2.46	0.48
34:1i:17:LEU:HD23	34:1i:20:ARG:HH21	1.77	0.48
34:1i:124:ASP:O	34:1i:126:HIS:ND1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:30:ARG:NE	37:1l:33:ASP:OD1	2.38	0.48
4:1D:372:GLY:HA3	4:1D:394:PRO:HB3	1.94	0.48
5:1E:150:ASN:ND2	5:1E:162:GLU:OE2	2.46	0.48
8:1H:39:VAL:HA	42:1q:31:ASN:ND2	2.28	0.48
51:1H:702:CDL:HB4	51:1H:702:CDL:H512	1.53	0.48
12:1L:103:PHE:CE2	12:1L:106:TRP:HZ3	2.31	0.48
12:1L:186:MET:SD	12:1L:196:TRP:NE1	2.86	0.48
12:1L:441:VAL:HG23	35:1j:12:ARG:H	1.78	0.48
14:1N:313:MET:SD	14:1N:313:MET:N	2.87	0.48
20:1T:8:LEU:HD12	20:1T:86:VAL:HG11	1.95	0.48
21:1V:5:LYS:NZ	21:1V:68:GLU:OE2	2.45	0.48
23:1X:58:GLU:OE1	23:1X:58:GLU:N	2.32	0.48
36:1k:61:SER:OG	36:1k:62:PHE:N	2.46	0.48
37:1l:13:TYR:CZ	37:1l:39:ASP:HB2	2.48	0.48
37:1l:117:TRP:O	37:1l:121:ILE:HG12	2.13	0.48
38:1m:53:PRO:HB2	39:1n:129:ARG:HH22	1.77	0.48
41:1p:112:CYS:O	41:1p:116:GLU:HG2	2.13	0.48
1:1A:84:LEU:HD12	1:1A:87:MET:HE2	1.94	0.48
1:1A:105:GLU:O	1:1A:110:GLY:HA3	2.13	0.48
2:1B:70:ASP:OD1	8:1H:34:ARG:NH2	2.47	0.48
4:1D:398:HIS:HB3	4:1D:421:GLN:HE21	1.74	0.48
8:1H:287:HIS:CD2	8:1H:291:LYS:HD2	2.48	0.48
12:1L:53:MET:HB2	12:1L:59:GLN:HE22	1.77	0.48
12:1L:337:ALA:C	12:1L:341:MET:HE1	2.38	0.48
12:1L:462:ILE:HG22	12:1L:463:PHE:HD1	1.78	0.48
13:1M:203:PHE:HB3	13:1M:243:MET:HE2	1.94	0.48
14:1N:34:GLU:OE2	14:1N:34:GLU:HA	2.11	0.48
14:1N:213:LEU:O	14:1N:217:MET:HG2	2.14	0.48
16:1P:301:GLU:OE2	16:1P:301:GLU:C	2.56	0.48
4:1D:224:GLU:HG2	9:1I:36:MET:HE1	1.95	0.48
6:1F:361:GLN:HG3	7:1G:51:ASN:HD21	1.78	0.48
8:1H:195:ARG:HD3	8:1H:274:ARG:HG3	1.96	0.48
11:1K:4:VAL:O	11:1K:8:ILE:HG13	2.12	0.48
12:1L:257:VAL:HG11	12:1L:313:MET:HG2	1.95	0.48
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.48	0.48
12:1L:337:ALA:O	12:1L:341:MET:CE	2.51	0.48
12:1L:338:MET:HA	12:1L:457:LEU:HD23	1.96	0.48
12:1L:483:PRO:O	12:1L:486:MET:HE1	2.13	0.48
13:1M:28:THR:O	13:1M:32:LEU:HG	2.13	0.48
15:1O:73:LEU:HD21	15:1O:295:LYS:HB2	1.95	0.48
19:1S:19:ARG:HG2	19:1S:21:HIS:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:87:CYS:SG	23:1X:99:CYS:CB	3.02	0.48
34:1i:43:GLU:HG2	34:1i:44:GLN:OE1	2.14	0.48
35:1j:39:ARG:NH2	35:1j:43:ASP:OD1	2.35	0.48
4:1D:128:ILE:HD12	4:1D:330:VAL:HG21	1.96	0.48
5:1E:111:ARG:NH1	6:1F:260:GLY:O	2.47	0.48
5:1E:132:THR:OG1	5:1E:134:ASP:OD1	2.22	0.48
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.32	0.48
7:1G:415:LEU:O	7:1G:417:TYR:N	2.46	0.48
10:1J:51:PHE:N	10:1J:139:GLU:OE2	2.46	0.48
10:1J:136:PHE:HE2	27:1b:50:TYR:HB3	1.79	0.48
12:1L:331:MET:HB3	12:1L:387:THR:HB	1.95	0.48
15:1O:64:GLY:HA3	28:1c:2:PHE:CE2	2.48	0.48
15:1O:285:GLY:HA2	32:1g:26:LEU:CD1	2.42	0.48
17:1Q:89:LYS:O	17:1Q:93:VAL:HG12	2.14	0.48
24:1Y:130:GLU:OE2	24:1Y:131:GLY:N	2.46	0.48
31:1f:49:ARG:NH1	33:1h:60:VAL:H	2.10	0.48
33:1h:142:ASP:OD1	33:1h:142:ASP:N	2.42	0.48
34:1i:61:TYR:HA	34:1i:64:TYR:HB3	1.95	0.48
38:1m:18:ASP:N	38:1m:18:ASP:OD1	2.46	0.48
38:1m:48:LEU:O	38:1m:52:ASP:HB2	2.13	0.48
4:1D:244:VAL:HG22	4:1D:292:ASP:HB3	1.96	0.48
10:1J:20:PHE:H	10:1J:20:PHE:HD2	1.62	0.48
12:1L:247:LEU:CA	12:1L:251:THR:OG1	2.61	0.48
12:1L:533:MET:HE3	12:1L:534:HIS:N	2.29	0.48
12:1L:556:ILE:O	12:1L:560:THR:OG1	2.28	0.48
14:1N:91:ASN:OD1	14:1N:94:ALA:N	2.45	0.48
14:1N:288:LEU:HD12	14:1N:288:LEU:H	1.78	0.48
15:1O:157:LYS:HG3	15:1O:158:VAL:HG13	1.95	0.48
16:1P:335:LYS:NZ	16:1P:336:PRO:CD	2.77	0.48
21:1V:113:TRP:CG	21:1V:113:TRP:O	2.64	0.48
22:1W:114:ARG:C	22:1W:114:ARG:CD	2.86	0.48
39:1n:133:GLU:C	39:1n:137:LYS:HZ3	2.21	0.48
40:1o:7:ARG:HB2	40:1o:15:GLU:HB2	1.96	0.48
4:1D:261:ARG:NH1	4:1D:303:GLU:OE2	2.47	0.48
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.48	0.48
12:1L:405:ASN:ND2	12:1L:407:TRP:H	2.12	0.48
13:1M:78:MET:HA	13:1M:81:GLN:OE1	2.13	0.48
14:1N:98:MET:HA	14:1N:101:ALA:HB3	1.94	0.48
33:1h:85:LYS:O	33:1h:89:LYS:HB2	2.14	0.48
34:1i:44:GLN:HA	34:1i:47:ASN:CG	2.39	0.48
38:1m:53:PRO:HB2	39:1n:129:ARG:HH12	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:102:TYR:O	38:1m:106:THR:OG1	2.19	0.48
1:1A:70:ALA:HB2	10:1J:59:ILE:HD11	1.94	0.48
2:1B:50:PHE:CE1	4:1D:54:GLN:OE1	2.66	0.48
3:1C:65:ARG:NH1	4:1D:252:ASN:HD21	2.11	0.48
4:1D:71:GLU:CB	4:1D:72:MET:HE2	2.32	0.48
5:1E:31:ILE:HG13	5:1E:53:LEU:HD23	1.96	0.48
5:1E:191:PHE:H	5:1E:194:GLU:CD	2.22	0.48
6:1F:183:ALA:HA	7:1G:177:ARG:HH22	1.79	0.48
6:1F:248:GLU:O	6:1F:249:ARG:NH1	2.47	0.48
8:1H:206:GLU:HG2	8:1H:207:LEU:HG	1.95	0.48
10:1J:129:ASP:OD1	10:1J:129:ASP:C	2.56	0.48
12:1L:294:THR:O	12:1L:295:GLN:NE2	2.47	0.48
13:1M:207:MET:HG2	13:1M:298:ILE:HG12	1.94	0.48
14:1N:200:MET:HE3	14:1N:200:MET:CA	2.37	0.48
14:1N:326:LEU:O	14:1N:330:ILE:HG12	2.14	0.48
18:1R:11:VAL:HG22	18:1R:17:ALA:HB2	1.95	0.48
27:1b:56:LEU:HD23	27:1b:56:LEU:H	1.79	0.48
37:1l:157:GLU:HB2	40:1o:34:LYS:HE3	1.95	0.48
3:1C:53:HIS:HD2	3:1C:55:ASP:H	1.62	0.48
5:1E:214:GLN:HG3	5:1E:217:LEU:HD22	1.95	0.48
6:1F:153:ILE:HG22	44:1s:58:LEU:HD11	1.96	0.48
7:1G:382:THR:HG23	7:1G:384:PRO:HD3	1.96	0.48
8:1H:24:GLU:HG2	8:1H:228:TYR:OH	2.14	0.48
12:1L:337:ALA:HA	12:1L:340:PHE:HD2	1.78	0.48
12:1L:426:ILE:HD12	12:1L:427:ILE:N	2.29	0.48
13:1M:98:MET:HE2	13:1M:98:MET:N	2.28	0.48
13:1M:354:LEU:HD23	33:1h:18:ASP:HB3	1.95	0.48
13:1M:457:PRO:HA	32:1g:84:ARG:HH12	1.78	0.48
15:1O:23:LYS:HD3	15:1O:167:HIS:CG	2.49	0.48
15:1O:200:GLN:NE2	15:1O:201:ASP:OD1	2.47	0.48
15:1O:232:GLU:O	15:1O:236:GLU:OE2	2.31	0.48
15:1O:294:GLN:O	15:1O:297:THR:OG1	2.23	0.48
16:1P:107:GLU:OE1	16:1P:111:VAL:HB	2.14	0.48
21:1V:65:LYS:HZ1	21:1V:66:LYS:HG3	1.77	0.48
38:1m:4:LYS:HZ1	39:1n:68:GLU:HB3	1.77	0.48
38:1m:74:ASN:HA	38:1m:77:PRO:HG2	1.96	0.48
3:1C:87:GLN:H	3:1C:87:GLN:CD	2.17	0.48
4:1D:62:LEU:HG	4:1D:425:PHE:CE2	2.49	0.48
4:1D:220:PHE:HE1	25:1Z:24:ASN:HD22	1.61	0.48
7:1G:272:ASP:OD2	7:1G:683:THR:N	2.42	0.48
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:628:PRO:O	7:1G:632:ARG:NH2	2.46	0.48
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.49	0.48
10:1J:13:PHE:CE2	11:1K:8:ILE:HG22	2.49	0.48
10:1J:100:GLU:HA	10:1J:103:MET:HG2	1.96	0.48
14:1N:281:LEU:O	14:1N:285:THR:HG22	2.14	0.48
15:1O:291:ARG:HD3	32:1g:29:ASP:OD2	2.14	0.48
16:1P:102:LYS:H	16:1P:102:LYS:CD	2.26	0.48
20:1U:14:ARG:HE	35:1j:11:TYR:HE1	1.61	0.48
37:1I:156:TYR:CD1	40:1o:26:PRO:HB2	2.49	0.48
38:1m:80:ARG:CG	38:1m:82:THR:OG1	2.62	0.48
1:1A:113:TRP:HE1	8:1H:286:MET:HG2	1.79	0.47
5:1E:55:GLN:NE2	5:1E:59:GLY:O	2.35	0.47
7:1G:129:ARG:HB2	43:1r:48:LEU:HD13	1.96	0.47
7:1G:667:THR:OG1	7:1G:668:ILE:N	2.47	0.47
12:1L:107:TYR:CE2	12:1L:348:HIS:HB2	2.48	0.47
12:1L:540:HIS:O	12:1L:544:MET:HG3	2.13	0.47
14:1N:5:ILE:HD12	14:1N:5:ILE:N	2.28	0.47
14:1N:234:TRP:CD2	14:1N:304:MET:HB3	2.49	0.47
15:1O:57:HIS:ND1	15:1O:60:ASP:OD1	2.46	0.47
20:1U:58:PHE:HB3	20:1U:60:PHE:CE2	2.49	0.47
32:1g:62:PHE:HA	32:1g:66:PHE:CE2	2.48	0.47
34:1i:43:GLU:HA	34:1i:46:TRP:CZ3	2.49	0.47
39:1n:67:GLU:HA	39:1n:70:PHE:HD1	1.79	0.47
41:1p:70:VAL:H	41:1p:90:GLN:HE22	1.62	0.47
1:1A:109:LYS:HD3	1:1A:110:GLY:H	1.79	0.47
8:1H:308:PRO:HB2	8:1H:314:ILE:HD13	1.96	0.47
9:1I:54:LYS:NZ	42:1q:79:GLY:O	2.40	0.47
10:1J:50:SER:N	10:1J:139:GLU:OE1	2.46	0.47
12:1L:203:MET:CE	41:1p:109:LEU:HG	2.39	0.47
12:1L:341:MET:O	12:1L:345:SER:N	2.36	0.47
13:1M:278:ARG:NH2	37:1I:82:ASP:OD2	2.41	0.47
14:1N:92:PRO:O	14:1N:96:THR:OG1	2.28	0.47
14:1N:203:LEU:HD22	14:1N:343:LEU:HB3	1.96	0.47
16:1P:240:ASP:HB3	16:1P:337:ALA:HB1	1.96	0.47
20:1U:64:ASP:O	39:1n:17:ARG:NH1	2.46	0.47
27:1b:24:ILE:HD12	27:1b:24:ILE:H	1.79	0.47
37:1I:157:GLU:HG2	40:1o:36:ARG:HB2	1.96	0.47
41:1p:85:PHE:CE1	41:1p:89:MET:HE2	2.49	0.47
2:1B:92:LEU:HG	2:1B:96:MET:SD	2.55	0.47
4:1D:200:HIS:NE2	9:1I:124:GLU:OE2	2.47	0.47
6:1F:117:LYS:HE3	6:1F:117:LYS:HB3	1.73	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:322:LEU:HB3	6:1F:327:THR:HG23	1.95	0.47
9:1I:95:GLU:HB2	9:1I:108:ARG:HB3	1.96	0.47
10:1J:60:TYR:HB3	10:1J:64:MET:CE	2.39	0.47
46:1L:702:PC1:H272	24:1Y:112:ALA:HA	1.95	0.47
13:1M:345:ALA:HB1	13:1M:348:LEU:HD11	1.96	0.47
15:1O:254:ARG:HH12	15:1O:255:THR:CG2	2.28	0.47
20:1T:29:LYS:HZ3	20:1T:40:LEU:HA	1.76	0.47
22:1W:61:ASP:OD2	22:1W:61:ASP:N	2.41	0.47
25:1Z:86:MET:HE3	25:1Z:86:MET:HB2	1.74	0.47
30:1e:90:LYS:O	30:1e:90:LYS:NZ	2.42	0.47
32:1g:58:MET:HE3	32:1g:58:MET:C	2.39	0.47
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.13	0.47
37:1l:147:THR:OG1	37:1l:148:LYS:N	2.45	0.47
1:1A:106:TRP:CZ2	8:1H:291:LYS:HG2	2.49	0.47
2:1B:53:ALA:HA	4:1D:108:TYR:CZ	2.50	0.47
3:1C:137:MET:HE1	3:1C:153:THR:HG23	1.95	0.47
7:1G:366:THR:OG1	7:1G:491:ASN:ND2	2.48	0.47
12:1L:376:GLY:HA2	12:1L:379:ALA:HB3	1.95	0.47
13:1M:395:LEU:HD11	38:1m:100:TRP:CD1	2.49	0.47
13:1M:400:MET:HA	13:1M:403:THR:HB	1.95	0.47
20:1T:56:ASP:OD1	20:1T:57:GLU:N	2.47	0.47
23:1X:87:CYS:HG	23:1X:99:CYS:HG	1.22	0.47
24:1Y:15:THR:OG1	24:1Y:16:GLU:OE2	2.33	0.47
29:1d:94:VAL:HA	29:1d:101:PHE:CE2	2.49	0.47
37:1l:8:MET:HE2	38:1m:66:ARG:NH1	2.29	0.47
38:1m:62:PRO:HA	38:1m:65:ILE:HD13	1.95	0.47
42:1q:47:LYS:HD2	42:1q:49:TYR:OH	2.13	0.47
1:1A:17:LEU:HB3	8:1H:222:MET:HE1	1.97	0.47
6:1F:82:MET:HE3	6:1F:221:THR:OG1	2.14	0.47
6:1F:106:LYS:O	6:1F:110:ILE:HG22	2.14	0.47
6:1F:309:LYS:HA	6:1F:312:CYS:HB2	1.97	0.47
7:1G:16:GLN:NE2	7:1G:17:SER:O	2.48	0.47
7:1G:54:MET:CE	7:1G:94:MET:HE3	2.42	0.47
7:1G:337:ARG:HH11	7:1G:337:ARG:HB2	1.79	0.47
10:1J:95:SER:O	10:1J:98:MET:SD	2.72	0.47
12:1L:234:PRO:HB3	12:1L:304:PHE:HE1	1.79	0.47
12:1L:382:GLY:HA2	12:1L:386:LEU:HD23	1.95	0.47
12:1L:496:MET:O	12:1L:500:LEU:N	2.25	0.47
13:1M:237:LYS:HB3	13:1M:316:MET:SD	2.54	0.47
14:1N:4:ILE:HG12	15:1O:9:VAL:HG22	1.97	0.47
41:1p:145:LEU:HD11	41:1p:154:CYS:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:21:ALA:O	8:1H:60:PRO:HG3	2.14	0.47
4:1D:106:LEU:HD11	4:1D:391:ILE:HD13	1.95	0.47
13:1M:257:MET:HE3	13:1M:257:MET:HB3	1.76	0.47
14:1N:323:MET:HA	51:1O:403:CDL:H721	1.95	0.47
16:1P:162:GLU:CD	16:1P:162:GLU:H	2.22	0.47
21:1V:80:ILE:HD12	21:1V:80:ILE:H	1.80	0.47
23:1X:40:LYS:NZ	27:1b:52:TYR:OH	2.43	0.47
27:1b:44:ILE:HG12	27:1b:80:LEU:HD11	1.96	0.47
29:1d:70:PHE:C	29:1d:70:PHE:HD1	2.22	0.47
35:1j:26:GLU:CD	35:1j:26:GLU:H	2.22	0.47
44:1s:32:PRO:CD	44:1s:32:PRO:O	2.54	0.47
1:1A:1:FME:N	1:1A:4:MET:SD	2.87	0.47
4:1D:72:MET:HE2	4:1D:72:MET:N	2.30	0.47
4:1D:117:ALA:HB2	4:1D:367:ILE:HG12	1.95	0.47
6:1F:13:GLY:HA3	6:1F:274:VAL:HG23	1.95	0.47
7:1G:373:GLU:OE2	7:1G:448:LYS:NZ	2.46	0.47
8:1H:43:TYR:CZ	51:1a:101:CDL:H141	2.49	0.47
9:1I:13:ASP:C	9:1I:13:ASP:OD2	2.58	0.47
10:1J:119:PHE:CG	11:1K:6:MET:HG3	2.49	0.47
11:1K:84:THR:HG23	11:1K:85:TYR:HD1	1.80	0.47
12:1L:126:ILE:HD12	12:1L:127:THR:N	2.29	0.47
12:1L:203:MET:HB3	41:1p:113:GLN:HG3	1.96	0.47
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.96	0.47
12:1L:543:SER:O	12:1L:547:LYS:HD3	2.15	0.47
13:1M:18:SER:OG	13:1M:19:LYS:N	2.48	0.47
13:1M:116:ILE:HD13	13:1M:116:ILE:HA	1.76	0.47
13:1M:451:PRO:O	13:1M:454:ILE:HG13	2.14	0.47
14:1N:109:SER:CB	14:1N:157:MET:HE2	2.44	0.47
15:1O:233:LYS:HE3	15:1O:233:LYS:HB3	1.69	0.47
16:1P:157:ARG:HH21	16:1P:165:ILE:HD12	1.80	0.47
19:1S:17:GLU:OE2	19:1S:19:ARG:NH1	2.47	0.47
19:1S:84:ASP:N	19:1S:84:ASP:OD1	2.46	0.47
24:1Y:116:TYR:O	24:1Y:120:THR:OG1	2.20	0.47
26:1a:57:VAL:HG23	26:1a:59:ARG:HB2	1.95	0.47
51:1a:101:CDL:H332	42:1q:7:LEU:HD21	1.96	0.47
32:1g:71:VAL:O	32:1g:75:THR:HG23	2.14	0.47
37:1l:55:GLN:NE2	37:1l:70:ARG:O	2.45	0.47
40:1o:45:MET:O	40:1o:55:ARG:NH2	2.47	0.47
42:1q:54:GLN:HE21	43:1r:1:ALA:HB1	1.79	0.47
1:1A:66:ASP:O	1:1A:69:ILE:HG13	2.14	0.47
4:1D:37:ASP:OD1	14:1N:51:ARG:HD3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:151:ILE:HG12	4:1D:170:MET:CE	2.45	0.47
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.97	0.47
6:1F:357:GLU:HA	7:1G:177:ARG:HH11	1.79	0.47
13:1M:206:LYS:HA	13:1M:215:TRP:HZ2	1.79	0.47
14:1N:260:PHE:CE2	14:1N:264:TRP:HB2	2.50	0.47
17:1Q:55:TRP:HE1	17:1Q:108:ARG:HH21	1.63	0.47
21:1V:97:LYS:HE2	21:1V:99:TRP:CZ2	2.50	0.47
26:1a:1:MET:HE3	26:1a:1:MET:HB3	1.77	0.47
28:1c:26:PHE:HD2	28:1c:26:PHE:C	2.22	0.47
29:1d:40:CYS:O	29:1d:44:ILE:HG12	2.15	0.47
29:1d:65:VAL:O	29:1d:69:VAL:HG12	2.15	0.47
31:1f:14:ILE:C	31:1f:17:PRO:HD2	2.40	0.47
4:1D:3:GLN:HB2	13:1M:138:ASN:HA	1.97	0.47
4:1D:68:LEU:HD12	4:1D:70:GLY:H	1.80	0.47
5:1E:116:ILE:HG13	5:1E:152:PRO:HB2	1.97	0.47
6:1F:215:VAL:HG12	6:1F:220:THR:HB	1.97	0.47
6:1F:274:VAL:HG12	6:1F:317:MET:HB2	1.97	0.47
8:1H:30:TYR:CE1	9:1I:45:PRO:HG3	2.50	0.47
8:1H:134:ARG:NH1	8:1H:282:TYR:HD2	2.12	0.47
10:1J:98:MET:SD	10:1J:99:MET:N	2.88	0.47
13:1M:316:MET:HE2	13:1M:316:MET:HB2	1.74	0.47
14:1N:321:LYS:HA	14:1N:321:LYS:HD2	1.55	0.47
17:1Q:68:PRO:O	18:1R:27:ARG:NH2	2.47	0.47
21:1V:94:LEU:HB2	21:1V:95:ARG:HH12	1.79	0.47
27:1b:79:TRP:CH2	27:1b:80:LEU:HD13	2.49	0.47
29:1d:78:ARG:HH22	46:1d:201:PC1:H221	1.79	0.47
37:1l:156:TYR:HB2	40:1o:33:ARG:NE	2.26	0.47
39:1n:43:MET:CE	58:1n:201:EHZ:C2	2.93	0.47
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.28	0.47
10:1J:121:GLY:HA2	11:1K:3:LEU:HD23	1.97	0.47
12:1L:489:THR:HA	12:1L:492:ILE:HG12	1.97	0.47
13:1M:346:ARG:HA	13:1M:414:THR:HA	1.96	0.47
14:1N:231:SER:O	14:1N:234:TRP:HD1	1.98	0.47
14:1N:282:MET:HA	14:1N:285:THR:HG22	1.96	0.47
17:1Q:11:ILE:CD1	17:1Q:13:VAL:HG22	2.45	0.47
20:1T:11:ILE:HG12	20:1T:84:LYS:HZ1	1.80	0.47
20:1U:32:VAL:HG22	20:1U:74:GLN:HB3	1.96	0.47
23:1X:88:ILE:HD12	23:1X:99:CYS:SG	2.55	0.47
34:1i:28:SER:HB2	34:1i:31:GLU:HG3	1.97	0.47
34:1i:79:TRP:CD1	41:1p:40:VAL:HG13	2.50	0.47
38:1m:61:ASP:OD2	38:1m:61:ASP:C	2.58	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.47	0.47
10:1J:7:PHE:HD1	10:1J:7:PHE:O	1.98	0.46
12:1L:496:MET:H	12:1L:496:MET:HE3	1.80	0.46
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.50	0.46
13:1M:50:LEU:N	13:1M:58:SER:O	2.49	0.46
13:1M:76:MET:HA	13:1M:229:MET:HE1	1.97	0.46
13:1M:277:LEU:HD21	37:1l:88:ARG:HH22	1.80	0.46
14:1N:132:THR:HB	14:1N:209:ILE:HD12	1.97	0.46
33:1h:7:ARG:NH2	34:1i:27:LEU:O	2.47	0.46
35:1j:60:THR:HG22	35:1j:61:ASP:H	1.81	0.46
35:1j:64:LEU:HD12	40:1o:99:LYS:NZ	2.30	0.46
37:1l:97:SER:HA	38:1m:5:TYR:CD1	2.50	0.46
37:1l:97:SER:HA	38:1m:5:TYR:HD1	1.79	0.46
38:1m:25:SER:HG	38:1m:27:GLU:CD	2.23	0.46
38:1m:123:THR:HB	41:1p:136:LYS:HD3	1.97	0.46
41:1p:38:LEU:HD12	41:1p:42:ARG:HB2	1.96	0.46
43:1r:67:ILE:O	43:1r:67:ILE:HD12	2.16	0.46
44:1s:60:LYS:H	44:1s:60:LYS:HG3	1.52	0.46
2:1B:25:ARG:HH21	2:1B:27:GLU:HB3	1.80	0.46
7:1G:448:LYS:HB3	7:1G:487:TRP:CE2	2.50	0.46
8:1H:203:GLY:O	8:1H:207:LEU:N	2.32	0.46
9:1I:53:GLU:OE1	42:1q:58:ARG:HD2	2.15	0.46
10:1J:1:FME:C	10:1J:3:MET:H	2.28	0.46
12:1L:434:LYS:HE2	39:1n:33:ARG:HG2	1.98	0.46
14:1N:54:GLU:OE2	14:1N:54:GLU:N	2.46	0.46
14:1N:317:PHE:HE2	15:1O:106:LEU:HD21	1.78	0.46
19:1S:23:CYS:HG	19:1S:59:ASP:H	1.64	0.46
22:1W:96:VAL:O	22:1W:96:VAL:CG1	2.54	0.46
23:1X:81:PHE:CD2	26:1a:66:LEU:HD21	2.49	0.46
37:1l:58:ARG:HB3	37:1l:64:TRP:CZ2	2.49	0.46
40:1o:61:TYR:HB2	40:1o:86:TRP:HD1	1.80	0.46
40:1o:82:GLU:OE1	40:1o:82:GLU:N	2.40	0.46
42:1q:12:GLN:OE1	42:1q:12:GLN:C	2.59	0.46
4:1D:8:VAL:O	4:1D:12:GLU:HG2	2.14	0.46
6:1F:132:ARG:NH2	44:1s:66:PRO:HD3	2.30	0.46
6:1F:298:ILE:HB	6:1F:335:ILE:HB	1.97	0.46
7:1G:215:PHE:HB3	9:1I:104:ARG:CD	2.43	0.46
7:1G:532:ILE:O	7:1G:556:MET:HE1	2.15	0.46
8:1H:20:LEU:HD23	8:1H:228:TYR:CD1	2.45	0.46
8:1H:165:LEU:O	8:1H:169:GLN:HG2	2.16	0.46
11:1K:66:PHE:CE2	14:1N:31:ILE:HG12	2.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:106:TRP:O	12:1L:109:HIS:ND1	2.48	0.46
12:1L:279:CYS:O	12:1L:283:ILE:HG13	2.14	0.46
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.26	0.46
13:1M:24:TRP:O	13:1M:28:THR:OG1	2.24	0.46
28:1c:20:THR:HG23	29:1d:63:LEU:HD22	1.98	0.46
29:1d:86:ARG:NH1	33:1h:107:GLU:OE1	2.49	0.46
34:1i:44:GLN:HA	34:1i:47:ASN:ND2	2.31	0.46
37:1l:79:TRP:C	37:1l:79:TRP:CD1	2.94	0.46
40:1o:87:ASP:O	40:1o:91:HIS:N	2.41	0.46
41:1p:88:GLU:O	41:1p:92:ARG:HG3	2.16	0.46
5:1E:178:ALA:O	5:1E:180:LYS:NZ	2.46	0.46
6:1F:57:LEU:O	6:1F:61:LYS:HG2	2.16	0.46
7:1G:556:MET:O	7:1G:556:MET:CG	2.63	0.46
8:1H:20:LEU:HA	8:1H:23:VAL:HG12	1.97	0.46
8:1H:213:VAL:HG23	8:1H:214:GLU:N	2.30	0.46
12:1L:51:LEU:HD21	12:1L:91:PRO:HG3	1.97	0.46
12:1L:292:ALA:HB2	12:1L:304:PHE:HB2	1.97	0.46
12:1L:314:MET:C	12:1L:314:MET:HE2	2.41	0.46
12:1L:485:TYR:HB2	52:1L:701:MYR:H121	1.97	0.46
12:1L:502:LEU:HD23	12:1L:502:LEU:HA	1.78	0.46
12:1L:538:THR:O	12:1L:542:LEU:HG	2.16	0.46
13:1M:361:MET:H	13:1M:361:MET:CE	2.27	0.46
13:1M:425:ASN:HB2	38:1m:57:GLY:HA2	1.97	0.46
14:1N:223:SER:OG	15:1O:271:ASN:ND2	2.48	0.46
14:1N:235:ASN:O	15:1O:293:PHE:CD1	2.68	0.46
14:1N:260:PHE:CZ	14:1N:264:TRP:HB2	2.50	0.46
16:1P:132:ILE:HD11	16:1P:168:PRO:HG2	1.98	0.46
17:1Q:89:LYS:HD3	17:1Q:105:VAL:HG21	1.98	0.46
23:1X:15:GLN:NE2	23:1X:67:LEU:HD21	2.30	0.46
27:1b:30:ILE:HD12	27:1b:31:LEU:N	2.30	0.46
32:1g:73:GLY:O	32:1g:77:VAL:HG12	2.16	0.46
39:1n:88:THR:O	39:1n:92:ARG:NH2	2.48	0.46
39:1n:176:ARG:NH1	39:1n:176:ARG:HA	2.31	0.46
41:1p:47:ALA:O	41:1p:51:ILE:HD13	2.15	0.46
42:1q:1:MET:HE2	42:1q:1:MET:HB2	1.81	0.46
43:1r:101:LYS:O	43:1r:101:LYS:HD3	2.14	0.46
5:1E:145:LEU:HB2	5:1E:153:MET:HE1	1.96	0.46
6:1F:49:LEU:HD13	6:1F:127:ARG:HG2	1.98	0.46
50:1H:701:U10:H172	50:1H:701:U10:H151	1.53	0.46
9:1I:44:GLU:OE2	43:1r:1:ALA:N	2.43	0.46
10:1J:55:MET:HG2	11:1K:61:ILE:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:78:MET:HE1	10:1J:79:TYR:CE1	2.49	0.46
10:1J:79:TYR:HD2	16:1P:325:ARG:HD2	1.80	0.46
12:1L:2:ASN:HB2	12:1L:3:PRO:HD3	1.96	0.46
12:1L:176:ARG:NE	12:1L:176:ARG:HA	2.31	0.46
15:1O:41:GLU:HG3	15:1O:231:ALA:HB1	1.96	0.46
15:1O:188:ASN:HB3	15:1O:191:GLU:HG3	1.96	0.46
15:1O:227:GLU:HB3	15:1O:233:LYS:NZ	2.30	0.46
16:1P:83:LYS:HE3	16:1P:83:LYS:HB3	1.77	0.46
16:1P:168:PRO:HA	16:1P:230:PHE:HB2	1.98	0.46
38:1m:1:SER:H1	39:1n:68:GLU:C	2.21	0.46
41:1p:22:GLN:OE1	41:1p:22:GLN:N	2.46	0.46
2:1B:142:VAL:HG12	2:1B:143:ASP:O	2.16	0.46
7:1G:214:ALA:O	9:1I:104:ARG:NH1	2.49	0.46
8:1H:20:LEU:CD2	8:1H:228:TYR:CD1	2.99	0.46
8:1H:310:MET:CE	27:1b:32:PRO:HD3	2.46	0.46
9:1I:95:GLU:HG3	9:1I:108:ARG:HD2	1.96	0.46
10:1J:100:GLU:O	10:1J:104:VAL:HG12	2.16	0.46
12:1L:176:ARG:HH21	12:1L:179:ASP:CB	2.29	0.46
13:1M:304:GLN:OE1	41:1p:147:ALA:N	2.39	0.46
15:1O:151:HIS:CD2	15:1O:279:LEU:HD11	2.50	0.46
18:1R:26:VAL:O	18:1R:29:SER:OG	2.34	0.46
27:1b:27:LEU:HB3	27:1b:31:LEU:CD2	2.45	0.46
36:1k:19:LYS:HE2	36:1k:19:LYS:H	1.72	0.46
36:1k:21:TRP:C	36:1k:22:LYS:HZ2	2.23	0.46
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.26	0.46
39:1n:30:CYS:HB3	39:1n:35:LYS:HG2	1.97	0.46
39:1n:71:TRP:O	39:1n:74:GLN:HG3	2.15	0.46
42:1q:54:GLN:HG3	43:1r:1:ALA:HA	1.98	0.46
2:1B:48:MET:HE3	2:1B:48:MET:HB3	1.87	0.46
2:1B:154:GLU:HG2	9:1I:137:PHE:HE2	1.81	0.46
4:1D:342:MET:HA	4:1D:342:MET:HE2	1.96	0.46
6:1F:61:LYS:HD3	6:1F:76:GLY:HA3	1.97	0.46
11:1K:8:ILE:HD13	11:1K:43:MET:CE	2.46	0.46
13:1M:263:MET:HE3	38:1m:101:TYR:HA	1.98	0.46
13:1M:367:LEU:HD11	13:1M:408:LEU:CD2	2.46	0.46
14:1N:112:HIS:NE2	14:1N:164:ILE:HG21	2.30	0.46
15:1O:239:GLU:O	15:1O:239:GLU:CD	2.59	0.46
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.16	0.46
25:1Z:57:ARG:HA	25:1Z:60:LEU:HD12	1.98	0.46
35:1j:51:PHE:HD2	40:1o:88:TYR:HD1	1.62	0.46
37:1l:82:ASP:OD2	38:1m:71:ARG:NH2	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:101:TYR:OH	38:1m:105:LYS:NZ	2.49	0.46
3:1C:76:ALA:O	4:1D:392:LYS:HE2	2.16	0.46
3:1C:108:LYS:HB2	3:1C:108:LYS:NZ	2.31	0.46
4:1D:66:MET:N	4:1D:66:MET:HE3	2.31	0.46
5:1E:89:MET:HE1	6:1F:141:GLU:N	2.31	0.46
7:1G:515:ARG:HE	7:1G:532:ILE:HD11	1.80	0.46
13:1M:283:LYS:HE2	13:1M:283:LYS:HB3	1.71	0.46
20:1T:37:MET:N	20:1T:37:MET:SD	2.89	0.46
23:1X:70:PHE:O	23:1X:73:ILE:HG22	2.15	0.46
32:1g:23:THR:C	32:1g:24:ILE:HG13	2.41	0.46
32:1g:80:LEU:HD22	32:1g:81:PRO:HD2	1.98	0.46
33:1h:70:PRO:HA	33:1h:73:ARG:HD3	1.98	0.46
39:1n:25:HIS:CG	39:1n:74:GLN:HA	2.51	0.46
42:1q:14:VAL:HG12	42:1q:23:TYR:CD2	2.51	0.46
2:1B:93:THR:HG22	2:1B:95:LYS:H	1.80	0.46
4:1D:4:TRP:CZ2	13:1M:140:THR:HG23	2.51	0.46
7:1G:10:GLU:HB2	7:1G:19:MET:HE1	1.98	0.46
7:1G:130:PHE:CZ	7:1G:132:GLU:HB2	2.51	0.46
8:1H:197:PRO:HG2	8:1H:198:PHE:CE2	2.51	0.46
9:1I:53:GLU:HG3	42:1q:61:TRP:HB3	1.96	0.46
12:1L:358:LYS:C	12:1L:359:MET:HE2	2.41	0.46
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	1.98	0.46
14:1N:217:MET:HE2	14:1N:326:LEU:HA	1.96	0.46
23:1X:38:PRO:HB3	23:1X:61:LEU:HG	1.98	0.46
29:1d:13:PHE:HE1	29:1d:78:ARG:HD3	1.80	0.46
32:1g:42:PRO:O	33:1h:17:TYR:OH	2.34	0.46
33:1h:45:VAL:HG23	33:1h:46:PHE:HD1	1.79	0.46
37:1l:17:PRO:HA	37:1l:20:ARG:HG3	1.97	0.46
39:1n:94:GLU:HA	39:1n:97:LYS:HZ2	1.80	0.46
12:1L:103:PHE:CE2	12:1L:341:MET:HB2	2.51	0.46
12:1L:573:MET:O	12:1L:576:MET:HG3	2.16	0.46
13:1M:1:FME:HG2	13:1M:111:THR:HG21	1.97	0.46
13:1M:294:MET:HE2	13:1M:294:MET:HA	1.98	0.46
14:1N:29:ILE:HG13	14:1N:86:ILE:HD11	1.98	0.46
15:1O:138:MET:SD	15:1O:138:MET:C	2.99	0.46
16:1P:106:PHE:HD2	16:1P:144:ARG:HB2	1.81	0.46
25:1Z:24:ASN:O	25:1Z:24:ASN:OD1	2.34	0.46
29:1d:36:PHE:C	29:1d:36:PHE:CD2	2.93	0.46
36:1k:70:PHE:CD1	36:1k:74:PHE:HB2	2.51	0.46
42:1q:72:ASP:C	42:1q:72:ASP:OD2	2.59	0.46
7:1G:444:LYS:NZ	7:1G:476:ASN:O	2.40	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:47:THR:O	42:1q:58:ARG:HD3	2.16	0.45
12:1L:378:LEU:C	12:1L:383:MET:HE1	2.41	0.45
12:1L:435:PRO:HG3	36:1k:56:PHE:CD2	2.52	0.45
12:1L:546:GLN:HB2	13:1M:278:ARG:NH1	2.31	0.45
13:1M:206:LYS:HA	13:1M:215:TRP:CZ2	2.50	0.45
13:1M:265:SER:O	13:1M:268:GLY:N	2.49	0.45
13:1M:325:MET:HE1	13:1M:437:MET:O	2.16	0.45
14:1N:100:MET:HE2	14:1N:100:MET:HB2	1.88	0.45
14:1N:176:ARG:NH1	14:1N:225:THR:OG1	2.49	0.45
20:1T:14:ARG:NH1	20:1T:57:GLU:OE2	2.49	0.45
21:1V:84:GLU:OE2	21:1V:85:ASN:N	2.49	0.45
23:1X:146:ARG:HA	23:1X:146:ARG:HD3	1.72	0.45
27:1b:9:LYS:HE2	27:1b:9:LYS:HB3	1.77	0.45
32:1g:58:MET:SD	32:1g:62:PHE:CD2	3.08	0.45
40:1o:25:PRO:HB2	40:1o:28:TYR:HB3	1.98	0.45
5:1E:194:GLU:OE2	6:1F:28:ARG:NH2	2.49	0.45
9:1I:112:ASP:OD2	9:1I:115:LYS:HE3	2.17	0.45
12:1L:373:LEU:HD12	12:1L:431:PHE:CE2	2.52	0.45
13:1M:277:LEU:HA	13:1M:406:TYR:HB3	1.99	0.45
16:1P:233:PRO:HD3	16:1P:307:ALA:HB1	1.98	0.45
32:1g:108:MET:HG3	41:1p:98:ASP:OD1	2.16	0.45
34:1i:41:PRO:O	34:1i:44:GLN:HG2	2.16	0.45
38:1m:4:LYS:HD3	38:1m:4:LYS:HA	1.61	0.45
38:1m:61:ASP:O	38:1m:65:ILE:HG23	2.16	0.45
1:1A:33:LYS:O	2:1B:81:ARG:NH1	2.48	0.45
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.41	0.45
4:1D:74:ARG:HA	4:1D:74:ARG:NH1	2.31	0.45
4:1D:258:VAL:O	4:1D:262:GLY:N	2.34	0.45
7:1G:94:MET:SD	7:1G:120:SER:HA	2.57	0.45
7:1G:185:THR:O	7:1G:185:THR:OG1	2.29	0.45
8:1H:105:MET:HE2	8:1H:237:PHE:CE2	2.50	0.45
8:1H:116:ILE:HD11	8:1H:211:PHE:HA	1.97	0.45
12:1L:439:PRO:HB3	35:1j:12:ARG:HE	1.81	0.45
13:1M:69:THR:HG22	13:1M:234:VAL:HG11	1.98	0.45
13:1M:210:TYR:CD1	13:1M:213:HIS:HE1	2.33	0.45
13:1M:303:ILE:HD11	13:1M:388:TRP:CG	2.51	0.45
15:1O:140:ARG:NH2	15:1O:204:ASN:OD1	2.48	0.45
15:1O:258:ARG:HE	15:1O:258:ARG:HB3	1.61	0.45
16:1P:209:ASP:OD2	16:1P:308:THR:N	2.47	0.45
17:1Q:39:VAL:HG11	17:1Q:108:ARG:HD3	1.97	0.45
24:1Y:21:ALA:HA	24:1Y:70:GLY:HA3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:119:LEU:O	24:1Y:123:LEU:N	2.41	0.45
36:1k:72:TRP:H	36:1k:72:TRP:HE3	1.61	0.45
37:1l:136:ASN:ND2	37:1l:139:TYR:HB2	2.31	0.45
38:1m:25:SER:OG	38:1m:27:GLU:OE2	2.34	0.45
40:1o:83:GLN:HB3	40:1o:87:ASP:OD2	2.17	0.45
2:1B:50:PHE:HZ	2:1B:103:VAL:HG11	1.81	0.45
3:1C:151:ILE:HD11	4:1D:80:ILE:HG12	1.99	0.45
4:1D:92:GLU:OE1	4:1D:92:GLU:O	2.34	0.45
4:1D:94:LYS:NZ	9:1I:88:PRO:O	2.46	0.45
6:1F:232:PRO:O	6:1F:236:ARG:HG3	2.16	0.45
7:1G:455:SER:HB2	7:1G:494:HIS:HA	1.98	0.45
8:1H:52:ALA:O	8:1H:56:VAL:HG22	2.17	0.45
8:1H:79:LEU:HD22	8:1H:79:LEU:HA	1.79	0.45
9:1I:158:GLY:O	9:1I:162:GLU:HB2	2.16	0.45
10:1J:128:TYR:HB2	25:1Z:121:MET:HE2	1.98	0.45
12:1L:337:ALA:O	12:1L:340:PHE:HB2	2.17	0.45
13:1M:73:LEU:HA	13:1M:76:MET:SD	2.56	0.45
13:1M:201:MET:N	13:1M:201:MET:SD	2.89	0.45
13:1M:418:LYS:HE3	37:1l:68:ASP:HB3	1.98	0.45
13:1M:429:SER:CB	13:1M:434:ASN:HD21	2.28	0.45
14:1N:139:LEU:HD23	14:1N:139:LEU:HA	1.86	0.45
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.51	0.45
14:1N:321:LYS:HB3	14:1N:323:MET:CE	2.47	0.45
15:1O:6:LEU:H	15:1O:6:LEU:HD22	1.80	0.45
21:1V:97:LYS:CE	21:1V:99:TRP:CE3	2.93	0.45
24:1Y:16:GLU:HB3	24:1Y:19:ARG:HB2	1.99	0.45
24:1Y:119:LEU:HD23	24:1Y:119:LEU:H	1.82	0.45
26:1a:70:ASP:N	26:1a:70:ASP:OD1	2.49	0.45
39:1n:103:LEU:HD13	39:1n:117:TYR:HE2	1.81	0.45
3:1C:138:PHE:O	3:1C:163:ARG:NE	2.49	0.45
4:1D:174:ARG:HA	4:1D:177:MET:HE3	1.97	0.45
6:1F:12:PHE:CE2	6:1F:247:ARG:HG3	2.52	0.45
7:1G:271:TYR:HA	7:1G:274:LEU:HD12	1.99	0.45
12:1L:533:MET:O	12:1L:537:PRO:HD2	2.16	0.45
13:1M:261:PHE:HB2	13:1M:302:MET:HE1	1.98	0.45
13:1M:261:PHE:HB2	13:1M:302:MET:CE	2.47	0.45
14:1N:179:MET:HE3	14:1N:179:MET:HA	1.99	0.45
15:1O:139:TYR:CZ	15:1O:146:LYS:HB3	2.52	0.45
15:1O:239:GLU:CD	15:1O:239:GLU:C	2.84	0.45
23:1X:90:TYR:O	26:1a:35:GLU:HG3	2.16	0.45
27:1b:77:LEU:H	27:1b:77:LEU:HD23	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:51:ARG:O	29:1d:53:VAL:N	2.43	0.45
38:1m:59:ILE:O	38:1m:59:ILE:HD12	2.16	0.45
42:1q:78:ASP:OD1	42:1q:79:GLY:N	2.49	0.45
1:1A:54:LYS:HE2	4:1D:71:GLU:CB	2.47	0.45
2:1B:72:PHE:HB2	2:1B:74:VAL:HG12	1.98	0.45
3:1C:33:LEU:HA	21:1V:98:PRO:HB2	1.98	0.45
3:1C:117:ILE:HB	3:1C:142:PHE:CD2	2.52	0.45
4:1D:398:HIS:HB3	4:1D:421:GLN:HE22	1.80	0.45
5:1E:89:MET:HG3	6:1F:181:ALA:O	2.17	0.45
6:1F:22:PHE:CE1	6:1F:255:LEU:HD11	2.51	0.45
7:1G:243:ARG:N	7:1G:248:MET:HE1	2.32	0.45
8:1H:20:LEU:HD22	8:1H:232:ILE:HD11	1.98	0.45
8:1H:200:LEU:HD13	8:1H:200:LEU:O	2.17	0.45
10:1J:103:MET:O	10:1J:107:ALA:N	2.50	0.45
10:1J:132:ASP:OD2	10:1J:134:GLY:N	2.33	0.45
12:1L:181:GLY:CA	12:1L:218:LEU:HD12	2.45	0.45
12:1L:457:LEU:O	12:1L:461:SER:OG	2.27	0.45
12:1L:481:THR:HB	40:1o:94:TYR:CD1	2.52	0.45
13:1M:19:LYS:HE3	31:1f:9:ASP:HA	1.97	0.45
13:1M:76:MET:HB2	13:1M:226:ALA:HB1	1.97	0.45
13:1M:434:ASN:C	33:1h:21:PHE:HE2	2.25	0.45
14:1N:95:MET:HE3	14:1N:95:MET:C	2.41	0.45
15:1O:176:VAL:HG12	15:1O:177:PRO:HD3	1.97	0.45
20:1U:73:PRO:HA	20:1U:76:ILE:HB	1.99	0.45
21:1V:94:LEU:C	21:1V:95:ARG:CZ	2.90	0.45
23:1X:138:GLU:OE1	23:1X:138:GLU:N	2.46	0.45
31:1f:38:ARG:HE	31:1f:54:VAL:HG23	1.81	0.45
34:1i:60:ILE:HG13	34:1i:61:TYR:N	2.31	0.45
35:1j:36:ILE:HD12	35:1j:37:LEU:N	2.32	0.45
37:1l:140:LEU:HD21	37:1l:146:PRO:HA	1.99	0.45
5:1E:104:THR:HG22	6:1F:349:ARG:HE	1.80	0.45
5:1E:190:ARG:HD3	5:1E:194:GLU:O	2.16	0.45
6:1F:134:ALA:HB3	6:1F:175:VAL:HG12	1.98	0.45
8:1H:235:ASN:OD1	8:1H:235:ASN:N	2.47	0.45
8:1H:296:LEU:HD12	8:1H:296:LEU:HA	1.83	0.45
11:1K:64:LEU:HD23	11:1K:64:LEU:HA	1.84	0.45
12:1L:71:LEU:O	12:1L:72:GLN:HG2	2.16	0.45
12:1L:119:LYS:HG3	12:1L:123:LEU:HD11	1.98	0.45
12:1L:174:TYR:CD2	12:1L:229:LEU:HA	2.50	0.45
12:1L:419:THR:O	12:1L:423:SER:OG	2.26	0.45
13:1M:264:LEU:O	13:1M:264:LEU:HD22	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:310:ASN:O	14:1N:313:MET:SD	2.75	0.45
18:1R:34:GLU:HG3	42:1q:124:TYR:HD1	1.82	0.45
23:1X:9:LEU:HG	25:1Z:88:ARG:HG2	1.98	0.45
25:1Z:80:ASP:OD1	25:1Z:81:ARG:N	2.50	0.45
25:1Z:94:GLU:OE2	30:1e:74:ARG:NH2	2.50	0.45
26:1a:59:ARG:HG3	26:1a:61:HIS:CE1	2.51	0.45
29:1d:15:PRO:HG2	29:1d:81:TYR:CZ	2.52	0.45
33:1h:61:PRO:HG3	41:1p:63:TYR:HD2	1.81	0.45
42:1q:2:GLU:HA	42:1q:2:GLU:OE2	2.17	0.45
6:1F:42:TRP:N	6:1F:236:ARG:HH22	2.12	0.45
7:1G:194:GLU:H	7:1G:194:GLU:CD	2.24	0.45
9:1I:78:ILE:HG21	18:1R:86:TYR:HA	1.99	0.45
11:1K:95:LEU:O	14:1N:51:ARG:NH1	2.49	0.45
12:1L:26:ILE:HD11	33:1h:26:ARG:HH22	1.81	0.45
13:1M:66:LEU:HD12	13:1M:66:LEU:HA	1.85	0.45
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	1.98	0.45
16:1P:154:LYS:HB3	16:1P:154:LYS:HE3	1.76	0.45
20:1T:43:ASP:OD1	20:1T:46:ASP:N	2.37	0.45
34:1i:56:TRP:O	34:1i:60:ILE:HG12	2.17	0.45
38:1m:41:ARG:O	38:1m:45:GLU:HG2	2.17	0.45
38:1m:41:ARG:HA	38:1m:44:ARG:HB3	1.99	0.45
39:1n:107:HIS:CD2	39:1n:108:PRO:HD2	2.51	0.45
3:1C:40:VAL:HG12	3:1C:50:ILE:HA	1.98	0.45
5:1E:164:LEU:HD13	5:1E:169:ILE:HD12	1.99	0.45
5:1E:177:LYS:HE2	5:1E:177:LYS:HB2	1.79	0.45
7:1G:315:VAL:O	7:1G:340:SER:OG	2.21	0.45
12:1L:68:TRP:N	12:1L:76:LEU:O	2.50	0.45
12:1L:482:MET:HE3	12:1L:482:MET:HB2	1.75	0.45
13:1M:126:LEU:HD21	13:1M:153:THR:HG21	1.99	0.45
13:1M:264:LEU:HD13	13:1M:264:LEU:C	2.42	0.45
14:1N:41:ILE:N	14:1N:42:PRO:HD2	2.32	0.45
20:1T:87:TYR:N	20:1T:87:TYR:CD1	2.84	0.45
23:1X:51:ASP:HB3	23:1X:54:ARG:HG2	1.98	0.45
25:1Z:24:ASN:O	25:1Z:24:ASN:CG	2.60	0.45
32:1g:36:ASN:HD22	32:1g:39:GLU:HG2	1.82	0.45
34:1i:19:ARG:HA	34:1i:19:ARG:HD3	1.63	0.45
38:1m:88:LEU:HA	38:1m:91:LEU:HD11	1.99	0.45
43:1r:18:ASP:OD2	43:1r:18:ASP:C	2.60	0.45
2:1B:165:ARG:O	2:1B:169:ARG:HG3	2.17	0.45
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.32	0.45
4:1D:342:MET:HG3	7:1G:98:LEU:HD22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:205:LEU:HD21	7:1G:53:ARG:HH12	1.81	0.45
10:1J:125:TRP:O	25:1Z:121:MET:HE1	2.17	0.45
12:1L:62:ILE:HD11	12:1L:81:LYS:HE3	1.97	0.45
12:1L:103:PHE:CD2	12:1L:341:MET:HB2	2.51	0.45
12:1L:496:MET:HA	12:1L:499:MET:HB3	1.98	0.45
15:1O:28:ASP:HB3	15:1O:206:TYR:HE1	1.82	0.45
23:1X:46:ARG:CZ	23:1X:52:PRO:HG3	2.47	0.45
29:1d:113:LEU:HD23	32:1g:121:PRO:HG3	1.99	0.45
3:1C:48:LEU:HD23	3:1C:105:ILE:HD11	1.99	0.44
3:1C:135:TRP:NE1	22:1W:88:MET:HE1	2.31	0.44
5:1E:192:SER:HB2	6:1F:112:ARG:HH22	1.81	0.44
8:1H:199:ASP:OD2	8:1H:279:ARG:NH2	2.50	0.44
8:1H:224:PHE:HZ	50:1H:701:U10:H103	1.82	0.44
8:1H:235:ASN:ND2	8:1H:267:THR:HA	2.32	0.44
9:1I:92:ILE:HD13	9:1I:111:ILE:HG12	1.99	0.44
9:1I:160:LYS:HD3	42:1q:110:TRP:CZ3	2.52	0.44
12:1L:243:VAL:O	12:1L:246:LEU:HB2	2.17	0.44
12:1L:353:GLU:OE2	12:1L:355:ASP:N	2.41	0.44
12:1L:495:ILE:O	12:1L:499:MET:N	2.42	0.44
16:1P:26:ALA:HA	16:1P:31:GLY:HA3	1.98	0.44
20:1U:11:ILE:O	20:1U:15:VAL:HG12	2.16	0.44
37:1l:91:THR:HA	38:1m:10:LEU:O	2.17	0.44
37:1l:133:TYR:HB2	37:1l:137:ASP:HA	2.00	0.44
39:1n:94:GLU:OE1	39:1n:94:GLU:N	2.50	0.44
40:1o:75:ASN:ND2	41:1p:23:THR:OG1	2.50	0.44
2:1B:150:PRO:HD3	4:1D:190:HIS:CD2	2.52	0.44
4:1D:107:ASP:OD1	4:1D:424:VAL:HG11	2.18	0.44
4:1D:211:ILE:O	4:1D:215:SER:OG	2.31	0.44
5:1E:156:ILE:HG21	5:1E:176:LEU:HD11	1.98	0.44
6:1F:82:MET:SD	6:1F:129:MET:HB3	2.57	0.44
7:1G:533:THR:HA	7:1G:556:MET:CE	2.45	0.44
7:1G:627:SER:HB3	7:1G:630:LEU:HG	1.98	0.44
8:1H:72:ILE:O	8:1H:75:PRO:HD2	2.16	0.44
12:1L:6:SER:O	12:1L:10:THR:HG23	2.17	0.44
12:1L:10:THR:HG22	34:1i:81:ILE:HD13	1.99	0.44
13:1M:275:ILE:HG22	13:1M:279:GLN:HE22	1.83	0.44
13:1M:283:LYS:HG3	13:1M:340:ARG:HG2	1.97	0.44
15:1O:239:GLU:O	15:1O:239:GLU:OE2	2.35	0.44
19:1S:35:PHE:CE1	19:1S:39:ARG:HB2	2.52	0.44
20:1U:58:PHE:CB	20:1U:60:PHE:CE2	3.00	0.44
31:1f:3:VAL:HA	31:1f:6:ILE:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:39:ASN:HB3	31:1f:55:THR:OG1	2.17	0.44
38:1m:44:ARG:NE	39:1n:148:PRO:HG3	2.32	0.44
44:1s:60:LYS:HE2	44:1s:60:LYS:HB2	1.56	0.44
3:1C:192:GLN:HB2	17:1Q:72:TRP:CD1	2.53	0.44
4:1D:199:VAL:HG23	4:1D:323:ILE:HB	1.99	0.44
4:1D:338:MET:HE1	9:1I:127:PRO:HB3	2.00	0.44
7:1G:36:GLN:HE22	17:1Q:48:GLY:HA2	1.82	0.44
7:1G:237:ASN:HD21	7:1G:255:HIS:CD2	2.35	0.44
7:1G:310:PHE:HE2	7:1G:520:LYS:HD3	1.82	0.44
7:1G:524:LEU:O	7:1G:545:TYR:HA	2.17	0.44
12:1L:297:ASP:O	12:1L:301:ILE:HD13	2.18	0.44
12:1L:384:PRO:HA	12:1L:389:PHE:CD1	2.52	0.44
13:1M:32:LEU:CD2	13:1M:74:PRO:HG2	2.37	0.44
13:1M:197:LEU:HB3	13:1M:201:MET:CE	2.43	0.44
14:1N:341:PRO:HB2	29:1d:79:GLN:HE21	1.82	0.44
15:1O:133:VAL:HG13	15:1O:205:ALA:HB3	2.00	0.44
15:1O:315:LYS:HG3	15:1O:316:TRP:CE3	2.53	0.44
16:1P:164:THR:OG1	16:1P:223:ALA:O	2.28	0.44
20:1T:80:ILE:HG22	20:1T:84:LYS:HE2	1.99	0.44
30:1e:12:ASP:OD2	30:1e:13:LEU:N	2.50	0.44
32:1g:62:PHE:CD1	32:1g:66:PHE:HE2	2.36	0.44
36:1k:83:ALA:O	36:1k:86:TYR:HB3	2.16	0.44
37:1l:68:ASP:O	37:1l:86:ARG:NH2	2.49	0.44
38:1m:47:LEU:HB3	39:1n:165:LEU:HD23	1.98	0.44
39:1n:168:HIS:O	39:1n:172:ARG:HG3	2.17	0.44
40:1o:71:ASP:HB3	41:1p:22:GLN:OE1	2.17	0.44
43:1r:63:MET:N	43:1r:63:MET:HE3	2.32	0.44
1:1A:57:LEU:HD11	10:1J:169:MET:HG2	1.99	0.44
4:1D:167:PHE:CE1	4:1D:171:PHE:CD1	3.06	0.44
7:1G:85:LYS:HE2	7:1G:85:LYS:HB2	1.77	0.44
7:1G:469:ALA:O	7:1G:473:ILE:HG12	2.18	0.44
7:1G:674:THR:O	7:1G:679:ARG:NH1	2.50	0.44
8:1H:24:GLU:OE2	8:1H:271:LEU:HD22	2.18	0.44
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.82	0.44
8:1H:206:GLU:OE2	8:1H:279:ARG:NH1	2.51	0.44
9:1I:117:ILE:HG12	45:1I:201:SF4:S4	2.58	0.44
10:1J:4:TYR:CE2	10:1J:7:PHE:HB2	2.53	0.44
10:1J:13:PHE:O	10:1J:17:PHE:HB2	2.18	0.44
11:1K:11:ALA:O	11:1K:14:ILE:HG12	2.18	0.44
13:1M:13:PRO:O	13:1M:17:MET:HG2	2.17	0.44
14:1N:95:MET:CE	14:1N:99:THR:OG1	2.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:170:LEU:HD11	14:1N:288:LEU:HD23	1.99	0.44
14:1N:325:LEU:HD13	51:1O:403:CDL:H762	2.00	0.44
16:1P:145:TYR:OH	56:1P:501:NDP:O2D	2.20	0.44
20:1T:10:ALA:O	20:1T:14:ARG:HD2	2.18	0.44
20:1T:24:LYS:NZ	20:1T:46:ASP:OD1	2.43	0.44
27:1b:27:LEU:HB3	27:1b:31:LEU:HD21	1.99	0.44
32:1g:84:ARG:O	41:1p:96:LYS:NZ	2.35	0.44
33:1h:48:GLY:O	41:1p:60:TYR:OH	2.35	0.44
35:1j:22:LEU:O	35:1j:26:GLU:OE1	2.35	0.44
38:1m:126:ILE:HG21	41:1p:138:PHE:HB3	1.98	0.44
40:1o:46:ASN:HA	40:1o:55:ARG:HH22	1.82	0.44
44:1s:34:ASP:OD1	44:1s:34:ASP:C	2.61	0.44
6:1F:42:TRP:CD2	6:1F:161:LEU:HD13	2.52	0.44
7:1G:285:ARG:HB3	7:1G:289:GLY:HA2	2.00	0.44
7:1G:609:MET:HE3	7:1G:609:MET:HB3	1.80	0.44
8:1H:235:ASN:HD22	8:1H:266:LEU:C	2.26	0.44
10:1J:67:VAL:O	10:1J:71:THR:HG23	2.18	0.44
11:1K:26:LEU:HB3	11:1K:78:LEU:HD12	1.99	0.44
13:1M:116:ILE:HG12	13:1M:174:LEU:HD13	1.99	0.44
13:1M:361:MET:H	13:1M:361:MET:HE3	1.83	0.44
14:1N:109:SER:C	14:1N:112:HIS:HD1	2.25	0.44
18:1R:49:VAL:HG22	18:1R:90:GLN:HB2	1.99	0.44
19:1S:24:GLN:HB3	19:1S:25:ARG:CZ	2.47	0.44
21:1V:41:ALA:CB	21:1V:99:TRP:CE3	2.97	0.44
31:1f:56:TRP:HB2	33:1h:85:LYS:NZ	2.33	0.44
32:1g:120:LEU:HD12	32:1g:121:PRO:HD2	1.99	0.44
36:1k:12:LYS:HD2	36:1k:14:GLU:N	2.25	0.44
39:1n:167:TRP:O	39:1n:171:THR:OG1	2.31	0.44
40:1o:68:CYS:HB3	40:1o:79:CYS:SG	2.57	0.44
40:1o:72:SER:O	40:1o:75:ASN:N	2.50	0.44
6:1F:109:GLU:OE1	6:1F:112:ARG:NH2	2.51	0.44
6:1F:254:LYS:HG3	6:1F:255:LEU:O	2.17	0.44
8:1H:85:MET:HE3	8:1H:85:MET:HB2	1.49	0.44
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.17	0.44
11:1K:51:THR:HA	30:1e:31:ARG:HG3	1.99	0.44
12:1L:63:ILE:O	12:1L:79:SER:HA	2.18	0.44
12:1L:119:LYS:O	12:1L:123:LEU:CD1	2.60	0.44
12:1L:277:THR:OG1	12:1L:278:LEU:N	2.51	0.44
12:1L:290:LEU:HD23	12:1L:290:LEU:C	2.42	0.44
12:1L:293:ILE:HG13	12:1L:418:LEU:HD12	2.00	0.44
12:1L:323:HIS:CG	12:1L:475:MET:HG3	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:122:PHE:CZ	13:1M:206:LYS:NZ	2.85	0.44
13:1M:266:MET:CA	13:1M:269:MET:HE1	2.40	0.44
13:1M:396:MET:SD	13:1M:396:MET:N	2.89	0.44
14:1N:71:MET:HE3	14:1N:71:MET:HA	1.99	0.44
14:1N:110:PRO:O	14:1N:113:PHE:CE2	2.70	0.44
15:1O:79:LEU:HA	15:1O:96:LEU:HD21	2.00	0.44
20:1T:25:ILE:HD11	20:1T:40:LEU:HD22	1.99	0.44
23:1X:22:SER:HB3	23:1X:88:ILE:HG22	1.99	0.44
29:1d:39:TYR:HE2	29:1d:43:LEU:HD11	1.83	0.44
29:1d:107:LYS:NZ	29:1d:112:ILE:HG13	2.32	0.44
31:1f:7:VAL:O	31:1f:11:TRP:HB3	2.17	0.44
33:1h:12:LYS:HD2	33:1h:12:LYS:O	2.17	0.44
38:1m:21:GLU:O	39:1n:14:LYS:NZ	2.48	0.44
39:1n:130:GLU:H	39:1n:130:GLU:CD	2.25	0.44
1:1A:48:ARG:NH2	8:1H:124:ASN:OD1	2.51	0.44
1:1A:53:MET:SD	1:1A:55:PHE:CD1	3.11	0.44
3:1C:90:PHE:HZ	3:1C:163:ARG:HE	1.66	0.44
4:1D:33:TRP:NE1	15:1O:276:PRO:HD2	2.28	0.44
6:1F:30:ASP:O	6:1F:39:ARG:NH1	2.37	0.44
6:1F:49:LEU:HD21	6:1F:123:LEU:HD12	1.99	0.44
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.98	0.44
6:1F:372:MET:HG2	6:1F:392:LEU:HD11	1.99	0.44
7:1G:47:SER:O	7:1G:161:ARG:NH1	2.50	0.44
8:1H:199:ASP:OD1	8:1H:279:ARG:NE	2.51	0.44
12:1L:274:GLN:NE2	12:1L:320:ASN:OD1	2.51	0.44
12:1L:336:LYS:HD2	12:1L:336:LYS:HA	1.76	0.44
13:1M:378:GLU:C	13:1M:378:GLU:OE1	2.60	0.44
13:1M:399:ASN:HA	13:1M:402:ILE:HG22	1.99	0.44
15:1O:57:HIS:CG	15:1O:68:PRO:HB3	2.52	0.44
15:1O:304:TYR:HA	29:1d:50:ARG:HE	1.83	0.44
20:1U:70:LEU:HD12	20:1U:70:LEU:C	2.43	0.44
29:1d:43:LEU:HD12	29:1d:61:GLN:NE2	2.33	0.44
34:1i:30:ARG:H	34:1i:30:ARG:NE	2.15	0.44
35:1j:59:TRP:CD2	40:1o:99:LYS:HD3	2.53	0.44
37:1l:27:TYR:CE2	37:1l:48:PRO:HD3	2.53	0.44
38:1m:69:TYR:CE1	38:1m:74:ASN:OD1	2.70	0.44
2:1B:46:TRP:CH2	8:1H:54:LYS:NZ	2.86	0.44
3:1C:82:ASP:CG	3:1C:89:ARG:HH21	2.26	0.44
4:1D:24:GLU:O	4:1D:28:TRP:NE1	2.50	0.44
4:1D:49:LEU:HB3	8:1H:126:LYS:HE2	1.99	0.44
5:1E:195:PRO:HG3	6:1F:266:CYS:SG	2.58	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:22:PHE:CE2	6:1F:110:ILE:HD13	2.53	0.44
6:1F:96:ASN:HB2	6:1F:222:VAL:HG13	1.99	0.44
6:1F:249:ARG:HH11	6:1F:249:ARG:HG3	1.82	0.44
6:1F:399:ILE:HG22	7:1G:96:PHE:CZ	2.53	0.44
12:1L:216:LEU:HD13	12:1L:216:LEU:HA	1.88	0.44
12:1L:267:MET:HG3	12:1L:274:GLN:HE21	1.83	0.44
12:1L:386:LEU:H	12:1L:389:PHE:HB3	1.83	0.44
13:1M:209:LEU:O	13:1M:212:LEU:HD12	2.17	0.44
14:1N:120:GLN:NE2	14:1N:176:ARG:HB2	2.33	0.44
14:1N:154:MET:CE	14:1N:191:THR:HB	2.48	0.44
19:1S:50:LEU:HD12	19:1S:52:ILE:HG13	2.00	0.44
19:1S:85:GLN:O	19:1S:88:ARG:HG2	2.18	0.44
20:1U:66:ASP:HA	20:1U:69:LYS:HE3	2.00	0.44
21:1V:93:MET:HE2	21:1V:98:PRO:CD	2.48	0.44
26:1a:69:ILE:HD12	26:1a:69:ILE:O	2.18	0.44
35:1j:22:LEU:O	35:1j:25:ALA:N	2.51	0.44
1:1A:11:VAL:O	1:1A:15:SER:OG	2.28	0.44
6:1F:45:THR:HB	6:1F:167:CYS:SG	2.57	0.44
6:1F:247:ARG:HD3	6:1F:316:LEU:HD23	2.00	0.44
7:1G:504:ASP:HA	19:1S:55:ARG:HE	1.83	0.44
8:1H:97:ASN:OD1	26:1a:40:HIS:NE2	2.35	0.44
8:1H:104:PHE:CZ	8:1H:108:MET:HE2	2.53	0.44
10:1J:60:TYR:C	10:1J:64:MET:HE1	2.43	0.44
10:1J:95:SER:C	10:1J:98:MET:HE3	2.43	0.44
10:1J:133:SER:N	26:1a:42:SER:OG	2.42	0.44
12:1L:69:MET:HB2	12:1L:76:LEU:HB2	2.00	0.44
12:1L:150:MET:HE1	12:1L:153:LEU:HD13	1.99	0.44
12:1L:159:HIS:CE1	39:1n:95:CYS:HB2	2.52	0.44
12:1L:162:THR:O	12:1L:166:THR:HG23	2.18	0.44
12:1L:224:SER:HB2	12:1L:226:GLN:OE1	2.18	0.44
12:1L:294:THR:O	12:1L:294:THR:OG1	2.34	0.44
12:1L:407:TRP:NE1	12:1L:410:LEU:HD23	2.33	0.44
12:1L:516:PRO:HB3	12:1L:521:LYS:HZ3	1.82	0.44
13:1M:197:LEU:CA	13:1M:201:MET:HE1	2.48	0.44
13:1M:346:ARG:H	13:1M:346:ARG:HG3	1.46	0.44
13:1M:363:SER:HB3	13:1M:411:LEU:HD11	2.00	0.44
15:1O:271:ASN:OD1	15:1O:271:ASN:C	2.60	0.44
20:1T:35:HIS:HB3	20:1T:38:LYS:HB2	1.99	0.44
20:1T:46:ASP:O	20:1T:50:ILE:HD12	2.18	0.44
33:1h:81:ASP:OD1	33:1h:82:GLY:N	2.51	0.44
34:1i:73:HIS:O	34:1i:77:PRO:HG2	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:81:VAL:HG22	4:1D:388:ARG:HG2	2.00	0.43
4:1D:88:GLU:OE2	4:1D:430:ARG:NH1	2.49	0.43
5:1E:66:MET:HE2	5:1E:81:TYR:CD1	2.53	0.43
5:1E:103:CYS:SG	5:1E:144:CYS:HA	2.58	0.43
6:1F:302:SER:O	6:1F:414:PRO:HG3	2.18	0.43
7:1G:200:ILE:HG23	7:1G:209:THR:HA	2.00	0.43
7:1G:651:LEU:HD11	19:1S:45:LYS:HG2	2.00	0.43
7:1G:672:TYR:CG	7:1G:684:MET:HE1	2.53	0.43
9:1I:13:ASP:O	9:1I:17:VAL:HG12	2.18	0.43
9:1I:67:LEU:HD12	9:1I:67:LEU:N	2.32	0.43
10:1J:125:TRP:O	25:1Z:121:MET:CE	2.66	0.43
12:1L:234:PRO:O	12:1L:237:MET:HG2	2.16	0.43
12:1L:314:MET:HA	12:1L:317:ILE:HD12	1.99	0.43
12:1L:357:ARG:NH1	39:1n:28:SER:HB2	2.33	0.43
53:1M:502:3PE:H232	14:1N:242:SER:OG	2.18	0.43
16:1P:23:VAL:O	16:1P:48:PRO:HD2	2.18	0.43
16:1P:132:ILE:HG12	56:1P:501:NDP:H6N	1.99	0.43
21:1V:27:TYR:HB3	21:1V:55:LEU:HD12	2.00	0.43
22:1W:20:ILE:O	22:1W:21:PHE:HD1	2.00	0.43
24:1Y:98:LEU:O	24:1Y:102:ALA:N	2.50	0.43
31:1f:28:ARG:HG2	46:1f:101:PC1:H111	2.00	0.43
41:1p:50:PHE:O	41:1p:53:GLN:HG3	2.18	0.43
41:1p:51:ILE:O	41:1p:54:GLN:HG3	2.18	0.43
41:1p:120:TYR:O	41:1p:124:CYS:HB2	2.18	0.43
41:1p:145:LEU:O	41:1p:153:LYS:NZ	2.36	0.43
42:1q:101:LYS:HE2	42:1q:101:LYS:HA	2.00	0.43
1:1A:32:GLU:H	1:1A:32:GLU:CD	2.27	0.43
4:1D:137:ILE:HD13	4:1D:203:LEU:HD13	1.99	0.43
4:1D:173:GLU:H	4:1D:173:GLU:HG2	1.61	0.43
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	2.00	0.43
10:1J:112:GLU:OE2	30:1e:80:ARG:NH1	2.50	0.43
12:1L:287:PHE:HZ	12:1L:527:GLY:HA3	1.83	0.43
12:1L:366:MET:HE2	12:1L:445:GLU:HB3	1.99	0.43
12:1L:373:LEU:HD12	12:1L:431:PHE:HE2	1.82	0.43
14:1N:328:THR:O	14:1N:332:LEU:HD22	2.18	0.43
15:1O:145:ARG:HD3	15:1O:145:ARG:HA	1.68	0.43
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.53	0.43
20:1T:87:TYR:N	20:1T:87:TYR:HD1	2.16	0.43
24:1Y:57:ARG:O	24:1Y:61:THR:HG23	2.17	0.43
25:1Z:58:ARG:HA	25:1Z:58:ARG:HD2	1.82	0.43
31:1f:24:CYS:HB3	46:1f:101:PC1:O14	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:94:LEU:HD13	41:1p:81:ILE:HG13	1.99	0.43
36:1k:33:GLU:O	36:1k:37:ALA:N	2.52	0.43
40:1o:74:PRO:CD	41:1p:28:PRO:HD3	2.47	0.43
4:1D:126:LEU:HD21	4:1D:358:VAL:HG12	2.00	0.43
4:1D:427:GLU:OE1	4:1D:427:GLU:C	2.61	0.43
12:1L:63:ILE:HD13	12:1L:63:ILE:HA	1.84	0.43
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.18	0.43
15:1O:279:LEU:N	15:1O:283:THR:OG1	2.51	0.43
15:1O:315:LYS:HD2	15:1O:315:LYS:HA	1.72	0.43
21:1V:68:GLU:OE2	21:1V:76:ILE:N	2.49	0.43
21:1V:113:TRP:HZ3	21:1V:115:ILE:HD13	1.83	0.43
22:1W:31:ARG:HA	22:1W:34:GLU:OE2	2.18	0.43
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	2.00	0.43
30:1e:9:LEU:HD23	30:1e:9:LEU:HA	1.86	0.43
33:1h:26:ARG:O	33:1h:30:LEU:HB2	2.18	0.43
34:1i:28:SER:HB3	34:1i:30:ARG:NH2	2.33	0.43
34:1i:47:ASN:O	34:1i:51:GLN:NE2	2.51	0.43
34:1i:77:PRO:O	34:1i:80:ILE:HD12	2.18	0.43
35:1j:26:GLU:CD	35:1j:26:GLU:N	2.76	0.43
39:1n:37:ARG:NH2	39:1n:41:CYS:SG	2.92	0.43
43:1r:40:LEU:HD13	43:1r:41:PRO:HD2	2.00	0.43
44:1s:53:ASP:OD2	44:1s:53:ASP:C	2.61	0.43
3:1C:111:THR:HG22	3:1C:112:ASP:O	2.18	0.43
4:1D:393:ALA:HA	4:1D:427:GLU:CD	2.44	0.43
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.53	0.43
11:1K:96:LEU:HB3	14:1N:117:GLU:HB2	2.00	0.43
12:1L:10:THR:HG21	34:1i:78:VAL:HG13	2.00	0.43
12:1L:21:MET:HE3	12:1L:21:MET:HB3	1.78	0.43
12:1L:59:GLN:HB2	34:1i:98:GLU:OE2	2.18	0.43
12:1L:129:MET:HA	12:1L:132:VAL:HG22	1.99	0.43
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	1.99	0.43
12:1L:364:LYS:NZ	36:1k:57:ALA:O	2.52	0.43
12:1L:387:THR:HG22	12:1L:465:GLY:N	2.34	0.43
13:1M:310:MET:HE3	13:1M:310:MET:HB2	1.77	0.43
15:1O:208:LYS:HE3	15:1O:208:LYS:HB3	1.82	0.43
16:1P:35:VAL:O	16:1P:39:GLY:N	2.50	0.43
16:1P:332:GLU:OE2	22:1W:56:VAL:HG12	2.18	0.43
23:1X:79:GLU:HB3	23:1X:80:PRO:HD3	1.99	0.43
31:1f:46:ARG:HH21	31:1f:55:THR:HG23	1.81	0.43
33:1h:95:GLN:HB2	41:1p:82:LEU:HD11	2.00	0.43
33:1h:113:LEU:HB2	33:1h:117:ARG:HH21	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:42:VAL:HB	43:1r:46:HIS:CG	2.54	0.43
1:1A:37:TYR:HA	2:1B:106:GLN:HE22	1.84	0.43
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.33	0.43
2:1B:171:LYS:HD2	2:1B:174:ARG:HH21	1.83	0.43
4:1D:85:ARG:H	4:1D:85:ARG:HG3	1.61	0.43
7:1G:523:PHE:CD1	7:1G:544:ILE:HD13	2.53	0.43
12:1L:246:LEU:HB3	12:1L:247:LEU:H	1.55	0.43
12:1L:313:MET:H	12:1L:313:MET:CE	2.30	0.43
12:1L:439:PRO:HD2	20:1U:57:GLU:O	2.18	0.43
13:1M:220:HIS:O	13:1M:283:LYS:NZ	2.44	0.43
13:1M:361:MET:SD	13:1M:361:MET:N	2.90	0.43
15:1O:41:GLU:CG	15:1O:231:ALA:CB	2.94	0.43
15:1O:56:ILE:O	15:1O:99:TRP:NE1	2.45	0.43
16:1P:32:ARG:HE	16:1P:58:HIS:CE1	2.36	0.43
21:1V:112:LYS:O	21:1V:112:LYS:NZ	2.35	0.43
24:1Y:67:ALA:O	24:1Y:71:LEU:HD22	2.19	0.43
25:1Z:25:LEU:HA	25:1Z:25:LEU:HD23	1.79	0.43
31:1f:3:VAL:O	31:1f:7:VAL:HG12	2.18	0.43
39:1n:54:LYS:HE2	39:1n:54:LYS:HB3	1.87	0.43
1:1A:61:THR:HG22	10:1J:165:VAL:HG23	1.99	0.43
6:1F:120:GLU:O	6:1F:124:VAL:HG22	2.18	0.43
6:1F:150:GLN:HG2	44:1s:54:LEU:HG	2.00	0.43
8:1H:13:ILE:O	8:1H:17:VAL:HG12	2.19	0.43
8:1H:110:SER:O	10:1J:61:LEU:HD21	2.18	0.43
8:1H:237:PHE:HA	8:1H:240:ILE:HG22	2.01	0.43
8:1H:245:ALA:HB3	8:1H:255:TYR:CE1	2.54	0.43
9:1I:44:GLU:HG3	43:1r:0:ACE:H1	2.01	0.43
9:1I:120:GLY:O	9:1I:123:GLN:HG2	2.19	0.43
10:1J:127:ILE:H	10:1J:127:ILE:HG13	1.62	0.43
11:1K:77:LEU:HD12	11:1K:77:LEU:HA	1.86	0.43
12:1L:57:THR:O	34:1i:102:ARG:NH2	2.52	0.43
12:1L:443:ILE:H	12:1L:443:ILE:HG13	1.56	0.43
13:1M:233:ALA:HA	13:1M:320:GLY:HA2	2.01	0.43
15:1O:320:LYS:HG3	28:1c:12:PRO:HG3	2.00	0.43
19:1S:90:LEU:O	19:1S:94:LEU:HG	2.18	0.43
21:1V:75:GLN:N	21:1V:78:GLU:OE1	2.51	0.43
22:1W:22:SER:OG	22:1W:24:ASP:O	2.37	0.43
30:1e:44:HIS:CD2	33:1h:130:LYS:H	2.35	0.43
34:1i:27:LEU:HG	34:1i:31:GLU:HB2	2.01	0.43
36:1k:70:PHE:O	36:1k:70:PHE:CD1	2.72	0.43
41:1p:50:PHE:O	41:1p:50:PHE:HD2	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:93:LEU:HD12	6:1F:129:MET:HE2	2.00	0.43
6:1F:210:PRO:HB3	6:1F:220:THR:HG23	2.00	0.43
7:1G:477:ILE:HD11	7:1G:489:VAL:HG21	2.00	0.43
8:1H:54:LYS:NZ	8:1H:55:LEU:CD2	2.79	0.43
9:1I:150:ASN:ND2	42:1q:124:TYR:OH	2.51	0.43
12:1L:124:PHE:CG	12:1L:247:LEU:HD11	2.53	0.43
12:1L:271:LYS:HA	12:1L:274:GLN:HB2	2.01	0.43
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.18	0.43
16:1P:319:ARG:HA	16:1P:322:ARG:HD3	1.99	0.43
21:1V:39:LYS:HB3	21:1V:39:LYS:HE3	1.73	0.43
22:1W:58:GLN:H	22:1W:58:GLN:CD	2.18	0.43
22:1W:65:GLU:C	22:1W:65:GLU:OE2	2.62	0.43
22:1W:65:GLU:OE2	22:1W:66:MET:N	2.51	0.43
31:1f:28:ARG:CG	46:1f:101:PC1:H111	2.48	0.43
37:1l:98:TRP:CE2	38:1m:10:LEU:HD11	2.54	0.43
41:1p:38:LEU:HD12	41:1p:42:ARG:CB	2.49	0.43
42:1q:6:VAL:HG22	42:1q:9:ARG:HH21	1.84	0.43
1:1A:68:GLU:O	1:1A:72:LEU:HG	2.18	0.43
2:1B:38:ASN:ND2	2:1B:170:GLU:O	2.49	0.43
5:1E:48:LEU:HD21	5:1E:87:TYR:CZ	2.54	0.43
5:1E:60:TRP:CE2	5:1E:94:PRO:HG3	2.53	0.43
8:1H:58:LYS:HZ1	8:1H:217:ALA:HA	1.84	0.43
8:1H:96:ILE:HG23	25:1Z:144:THR:OG1	2.19	0.43
10:1J:23:LYS:N	10:1J:24:PRO:HD2	2.34	0.43
10:1J:141:MET:HE1	30:1e:26:HIS:CE1	2.53	0.43
11:1K:81:VAL:O	11:1K:85:TYR:HB2	2.17	0.43
12:1L:61:MET:HA	41:1p:114:GLN:HE21	1.83	0.43
12:1L:387:THR:HG22	12:1L:465:GLY:H	1.84	0.43
14:1N:234:TRP:CE2	14:1N:304:MET:HB3	2.53	0.43
15:1O:101:TYR:O	15:1O:105:LEU:HD23	2.19	0.43
16:1P:203:GLN:NE2	16:1P:234:ASN:O	2.51	0.43
17:1Q:39:VAL:HG21	17:1Q:108:ARG:HE	1.83	0.43
21:1V:27:TYR:CE2	21:1V:54:LYS:HB3	2.54	0.43
39:1n:174:ARG:NH1	39:1n:176:ARG:O	2.42	0.43
41:1p:89:MET:O	41:1p:93:ARG:HG3	2.19	0.43
1:1A:105:GLU:OE2	1:1A:105:GLU:C	2.62	0.43
5:1E:16:ASN:H	5:1E:19:THR:HG1	1.66	0.43
5:1E:161:TYR:CZ	5:1E:182:PRO:HG2	2.53	0.43
7:1G:338:VAL:O	7:1G:338:VAL:HG12	2.19	0.43
7:1G:453:LEU:HB3	7:1G:492:ILE:HD13	2.00	0.43
8:1H:30:TYR:HB3	9:1I:41:LEU:HD12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:68:ILE:HG12	8:1H:69:SER:N	2.34	0.43
10:1J:87:LYS:HA	10:1J:87:LYS:HD3	1.81	0.43
12:1L:405:ASN:ND2	37:1l:119:GLY:HA3	2.32	0.43
13:1M:194:PHE:HA	13:1M:197:LEU:HD12	2.01	0.43
20:1U:70:LEU:HD11	20:1U:76:ILE:CG1	2.49	0.43
21:1V:41:ALA:O	21:1V:45:LYS:HE3	2.19	0.43
23:1X:73:ILE:HD11	23:1X:106:PHE:HE1	1.84	0.43
32:1g:88:TRP:CZ2	32:1g:92:GLU:HG3	2.53	0.43
34:1i:68:ILE:C	34:1i:68:ILE:HD12	2.44	0.43
34:1i:92:LYS:HB2	34:1i:95:THR:HG22	1.99	0.43
35:1j:63:GLU:HB2	40:1o:99:LYS:HE3	2.01	0.43
3:1C:51:PHE:HD2	21:1V:111:TRP:CD2	2.37	0.43
4:1D:247:ALA:HB1	4:1D:265:ILE:HD11	2.01	0.43
5:1E:18:ASP:N	5:1E:18:ASP:OD1	2.51	0.43
7:1G:320:GLY:N	7:1G:525:LEU:O	2.47	0.43
7:1G:523:PHE:CE1	7:1G:544:ILE:HD13	2.54	0.43
10:1J:82:VAL:HG22	10:1J:83:TRP:N	2.32	0.43
11:1K:70:GLU:OE1	14:1N:34:GLU:OE1	2.36	0.43
12:1L:37:LYS:HG3	12:1L:101:MET:HE1	2.01	0.43
12:1L:82:MET:HG2	12:1L:82:MET:O	2.17	0.43
12:1L:113:PHE:HB3	12:1L:116:ARG:HB3	2.00	0.43
12:1L:452:ASN:HA	12:1L:455:LYS:HE3	2.00	0.43
53:1M:502:3PE:H372	53:1M:502:3PE:H331	2.01	0.43
14:1N:53:THR:HG1	14:1N:54:GLU:H	1.66	0.43
14:1N:89:MET:HE3	14:1N:89:MET:HB3	1.90	0.43
15:1O:108:TYR:HE1	15:1O:163:TYR:HB3	1.84	0.43
15:1O:113:GLU:O	15:1O:117:SER:OG	2.22	0.43
15:1O:312:VAL:HG11	28:1c:2:PHE:HD1	1.84	0.43
16:1P:138:ASP:OD1	16:1P:140:LYS:NZ	2.38	0.43
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.52	0.43
20:1U:22:TYR:CZ	20:1U:24:LYS:HB2	2.54	0.43
20:1U:81:ALA:HA	20:1U:86:VAL:HG22	2.01	0.43
22:1W:42:GLU:O	22:1W:46:THR:N	2.35	0.43
27:1b:31:LEU:N	27:1b:32:PRO:HD2	2.34	0.43
34:1i:100:LYS:NZ	34:1i:101:PRO:HD2	2.29	0.43
36:1k:31:VAL:HG21	39:1n:34:ASP:HB2	2.01	0.43
40:1o:76:PHE:CD1	40:1o:76:PHE:N	2.87	0.43
1:1A:54:LYS:NZ	4:1D:71:GLU:N	2.67	0.42
2:1B:95:LYS:HE3	3:1C:154:GLY:HA2	2.01	0.42
3:1C:52:ILE:HG12	3:1C:109:THR:HG22	2.01	0.42
3:1C:162:PHE:CZ	4:1D:88:GLU:HB2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:417:ILE:O	4:1D:421:GLN:HG2	2.19	0.42
5:1E:142:VAL:HG11	5:1E:145:LEU:HD11	2.00	0.42
6:1F:322:LEU:HD12	6:1F:329:LEU:HA	2.01	0.42
7:1G:88:LYS:HD2	43:1r:52:TYR:HD2	1.84	0.42
12:1L:237:MET:HE3	12:1L:244:SER:CB	2.38	0.42
12:1L:378:LEU:HA	12:1L:381:THR:HG23	2.00	0.42
12:1L:407:TRP:O	12:1L:411:MET:HG2	2.19	0.42
12:1L:525:MET:N	12:1L:525:MET:HE3	2.34	0.42
12:1L:547:LYS:HE2	12:1L:547:LYS:HB2	1.68	0.42
13:1M:153:THR:O	13:1M:157:SER:OG	2.22	0.42
13:1M:175:ASN:ND2	13:1M:178:ILE:H	2.17	0.42
13:1M:207:MET:O	13:1M:294:MET:HG3	2.18	0.42
14:1N:261:MET:HG3	14:1N:340:THR:HG23	2.01	0.42
14:1N:294:MET:HA	14:1N:294:MET:HE3	2.00	0.42
15:1O:108:TYR:CD2	15:1O:108:TYR:O	2.72	0.42
16:1P:140:LYS:HB3	16:1P:140:LYS:HE3	1.38	0.42
18:1R:3:ARG:NH2	18:1R:39:PHE:CE2	2.87	0.42
22:1W:40:TYR:HE1	22:1W:60:ARG:NE	2.17	0.42
22:1W:58:GLN:OE1	22:1W:58:GLN:N	2.39	0.42
24:1Y:61:THR:HG22	24:1Y:103:ARG:HB3	2.01	0.42
29:1d:109:TYR:HA	29:1d:112:ILE:HD12	2.00	0.42
35:1j:65:GLY:HA3	40:1o:30:PHE:CE2	2.54	0.42
3:1C:25:PHE:CE2	43:1r:96:PRO:HG3	2.54	0.42
4:1D:283:PHE:HA	4:1D:309:ARG:NH1	2.33	0.42
6:1F:401:GLY:O	7:1G:64:LYS:NZ	2.51	0.42
7:1G:512:GLU:CD	7:1G:512:GLU:H	2.27	0.42
7:1G:539:LYS:HZ2	7:1G:540:ASP:H	1.66	0.42
12:1L:61:MET:SD	12:1L:82:MET:SD	3.17	0.42
12:1L:581:LYS:HE3	24:1Y:44:PRO:HD3	2.02	0.42
13:1M:212:LEU:HD12	13:1M:212:LEU:C	2.43	0.42
13:1M:269:MET:HG2	13:1M:399:ASN:OD1	2.19	0.42
14:1N:53:THR:O	14:1N:57:THR:OG1	2.22	0.42
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.43	0.42
15:1O:223:TYR:CD2	15:1O:234:VAL:HG12	2.53	0.42
15:1O:295:LYS:HA	15:1O:295:LYS:HD3	1.90	0.42
16:1P:172:PHE:HB2	16:1P:179:LEU:HG	2.01	0.42
21:1V:68:GLU:HG3	21:1V:76:ILE:HD13	2.01	0.42
32:1g:98:LYS:HE3	32:1g:98:LYS:HB3	1.86	0.42
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	2.02	0.42
34:1i:111:GLU:OE1	34:1i:111:GLU:N	2.38	0.42
34:1i:123:PRO:HB2	34:1i:125:GLN:HE21	1.84	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:158:ILE:HD12	40:1o:100:GLU:OE2	2.19	0.42
38:1m:49:GLN:NE2	38:1m:59:ILE:HG12	2.33	0.42
42:1q:13:GLN:HB2	42:1q:23:TYR:HE2	1.84	0.42
43:1r:104:GLU:OE2	43:1r:104:GLU:N	2.52	0.42
1:1A:7:LEU:HD13	8:1H:84:THR:HG21	2.00	0.42
2:1B:126:TYR:CE1	4:1D:85:ARG:HD2	2.54	0.42
3:1C:117:ILE:HD13	3:1C:117:ILE:N	2.34	0.42
6:1F:93:LEU:O	6:1F:134:ALA:HA	2.20	0.42
8:1H:259:PHE:O	8:1H:263:THR:HG23	2.19	0.42
12:1L:435:PRO:HG2	36:1k:51:ARG:HB3	2.02	0.42
12:1L:603:ASN:HD22	24:1Y:2:LYS:HD2	1.85	0.42
15:1O:254:ARG:NH1	15:1O:255:THR:N	2.68	0.42
15:1O:270:LEU:HD23	15:1O:270:LEU:H	1.84	0.42
19:1S:31:GLY:HA3	19:1S:81:PHE:O	2.19	0.42
19:1S:86:VAL:O	19:1S:89:THR:OG1	2.34	0.42
34:1i:101:PRO:HD3	41:1p:14:ARG:NH1	2.34	0.42
36:1k:44:TRP:HB2	39:1n:37:ARG:NE	2.34	0.42
40:1o:88:TYR:HA	40:1o:91:HIS:HB3	2.01	0.42
2:1B:66:ARG:O	9:1I:48:ILE:HG12	2.19	0.42
4:1D:167:PHE:CD1	4:1D:167:PHE:C	2.97	0.42
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.19	0.42
4:1D:220:PHE:O	4:1D:224:GLU:HG3	2.19	0.42
8:1H:218:GLY:O	8:1H:222:MET:HG2	2.19	0.42
10:1J:61:LEU:HD23	10:1J:61:LEU:C	2.45	0.42
11:1K:22:TYR:CE2	11:1K:29:SER:HB2	2.55	0.42
11:1K:59:MET:HG3	14:1N:84:TRP:CH2	2.54	0.42
12:1L:9:LEU:O	12:1L:12:LEU:HD12	2.19	0.42
12:1L:188:TRP:CE3	12:1L:212:PRO:HG3	2.55	0.42
12:1L:297:ASP:OD1	12:1L:298:ILE:N	2.51	0.42
12:1L:571:MET:HE3	12:1L:571:MET:C	2.44	0.42
13:1M:55:THR:O	13:1M:55:THR:OG1	2.33	0.42
13:1M:367:LEU:HD23	13:1M:407:SER:HB2	2.01	0.42
14:1N:109:SER:O	14:1N:111:PHE:N	2.52	0.42
14:1N:235:ASN:ND2	15:1O:293:PHE:HB2	2.33	0.42
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.19	0.42
14:1N:324:LYS:C	14:1N:326:LEU:H	2.27	0.42
14:1N:343:LEU:HD12	14:1N:344:SER:N	2.35	0.42
16:1P:316:GLU:HG3	22:1W:53:ASP:OD2	2.19	0.42
18:1R:32:GLN:OE1	18:1R:32:GLN:C	2.63	0.42
19:1S:41:VAL:O	19:1S:45:LYS:HG3	2.20	0.42
20:1U:63:PRO:HD2	20:1U:79:TYR:OH	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:33:VAL:HG13	21:1V:94:LEU:HD11	2.01	0.42
21:1V:65:LYS:HD2	21:1V:65:LYS:C	2.44	0.42
24:1Y:68:ILE:H	24:1Y:68:ILE:HG13	1.68	0.42
25:1Z:120:MET:O	25:1Z:124:LEU:HD13	2.20	0.42
34:1i:10:ARG:NH2	39:1n:154:PRO:O	2.47	0.42
37:1l:54:SER:H	37:1l:57:GLU:HG3	1.84	0.42
37:1l:98:TRP:HA	37:1l:101:MET:SD	2.60	0.42
38:1m:71:ARG:C	38:1m:75:ILE:HD11	2.45	0.42
43:1r:92:LYS:HD2	43:1r:92:LYS:HA	1.75	0.42
1:1A:35:SER:O	2:1B:106:GLN:NE2	2.49	0.42
4:1D:410:MET:HE3	4:1D:410:MET:HB2	1.89	0.42
7:1G:365:ASN:HB3	7:1G:488:LYS:HD2	2.01	0.42
7:1G:672:TYR:CB	7:1G:684:MET:HE2	2.48	0.42
8:1H:58:LYS:NZ	8:1H:217:ALA:N	2.67	0.42
8:1H:272:TRP:CE2	9:1I:34:LEU:HD22	2.54	0.42
10:1J:18:VAL:HG13	10:1J:96:GLY:HA3	2.00	0.42
11:1K:40:LEU:HD23	14:1N:75:ILE:HG13	2.02	0.42
12:1L:44:PHE:CZ	12:1L:95:PHE:HB2	2.54	0.42
13:1M:276:CYS:SG	13:1M:288:TYR:HB3	2.60	0.42
13:1M:407:SER:CA	13:1M:410:MET:HE1	2.49	0.42
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	2.02	0.42
14:1N:106:LEU:HD21	14:1N:139:LEU:HG	2.01	0.42
15:1O:208:LYS:O	15:1O:212:PRO:HG2	2.20	0.42
20:1T:37:MET:SD	20:1T:71:MET:SD	3.17	0.42
20:1U:7:THR:O	20:1U:11:ILE:HG12	2.19	0.42
20:1U:19:LEU:HD11	20:1U:50:ILE:HG23	2.00	0.42
23:1X:52:PRO:HD2	25:1Z:116:TRP:CE3	2.55	0.42
34:1i:17:LEU:HD23	34:1i:20:ARG:NH2	2.34	0.42
34:1i:82:HIS:O	34:1i:86:LYS:HG2	2.19	0.42
38:1m:93:GLY:O	38:1m:96:PRO:HD2	2.19	0.42
39:1n:129:ARG:O	39:1n:133:GLU:HG2	2.20	0.42
5:1E:51:LEU:HD12	5:1E:69:VAL:HG21	2.01	0.42
5:1E:78:MET:HE2	7:1G:173:GLY:HA3	2.01	0.42
6:1F:95:VAL:HB	6:1F:136:ILE:HG13	2.02	0.42
6:1F:407:LEU:HD23	45:1F:502:SF4:S1	2.60	0.42
7:1G:346:GLU:H	7:1G:346:GLU:HG3	1.68	0.42
7:1G:558:ASP:OD1	7:1G:558:ASP:N	2.52	0.42
12:1L:61:MET:HB2	34:1i:97:VAL:O	2.20	0.42
13:1M:51:ASN:HB3	33:1h:93:ILE:HD12	2.02	0.42
13:1M:156:GLY:C	13:1M:159:PRO:HD2	2.44	0.42
14:1N:109:SER:HB3	14:1N:157:MET:CE	2.47	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:282:MET:HA	14:1N:285:THR:CG2	2.49	0.42
15:1O:56:ILE:HG13	15:1O:99:TRP:NE1	2.35	0.42
15:1O:270:LEU:HB2	15:1O:273:THR:OG1	2.20	0.42
16:1P:246:PHE:CD2	16:1P:251:ARG:HB2	2.54	0.42
17:1Q:127:ARG:NH2	44:1s:70:ARG:HH12	2.18	0.42
20:1T:85:ASP:HA	20:1T:87:TYR:CE1	2.53	0.42
20:1U:48:VAL:O	20:1U:51:ILE:HG13	2.20	0.42
23:1X:67:LEU:HD22	23:1X:71:ARG:HH22	1.84	0.42
24:1Y:91:ILE:H	24:1Y:91:ILE:HG12	1.56	0.42
27:1b:59:ASP:OD1	27:1b:59:ASP:N	2.52	0.42
28:1c:23:THR:O	28:1c:26:PHE:HB3	2.19	0.42
32:1g:58:MET:O	32:1g:62:PHE:HB2	2.19	0.42
36:1k:46:ARG:H	36:1k:46:ARG:HG2	1.57	0.42
37:1l:35:GLU:O	37:1l:49:LYS:N	2.42	0.42
38:1m:110:LYS:O	38:1m:113:LYS:HG2	2.20	0.42
39:1n:107:HIS:O	39:1n:111:LYS:HG3	2.19	0.42
4:1D:25:THR:HA	4:1D:28:TRP:CD1	2.55	0.42
5:1E:192:SER:HB2	6:1F:112:ARG:NH2	2.35	0.42
7:1G:75:LYS:HB3	7:1G:75:LYS:HE3	1.82	0.42
9:1I:113:MET:HG3	9:1I:118:TYR:OH	2.20	0.42
10:1J:22:SER:O	10:1J:22:SER:OG	2.38	0.42
12:1L:15:LEU:O	12:1L:18:PRO:HD2	2.20	0.42
12:1L:405:ASN:HD22	37:1l:119:GLY:CA	2.32	0.42
13:1M:367:LEU:HD21	13:1M:404:ALA:HA	1.99	0.42
20:1T:6:LEU:HG	20:1T:84:LYS:HD2	2.01	0.42
20:1T:17:TYR:CD1	20:1T:17:TYR:C	2.97	0.42
24:1Y:129:LEU:HD13	24:1Y:129:LEU:HA	1.85	0.42
25:1Z:72:MET:HB3	25:1Z:72:MET:HE2	1.80	0.42
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.44	0.42
5:1E:63:ILE:HG13	5:1E:67:ASN:ND2	2.35	0.42
5:1E:97:LYS:HB2	5:1E:136:LEU:HA	2.02	0.42
7:1G:104:ASP:O	7:1G:108:CYS:N	2.52	0.42
7:1G:322:LEU:HD23	7:1G:322:LEU:HA	1.84	0.42
7:1G:350:PRO:HG2	7:1G:467:LEU:HD12	2.02	0.42
8:1H:203:GLY:HA2	8:1H:279:ARG:NH1	2.34	0.42
11:1K:78:LEU:HA	11:1K:81:VAL:HG12	2.02	0.42
12:1L:463:PHE:O	12:1L:467:ILE:HG22	2.20	0.42
13:1M:81:GLN:NE2	32:1g:57:ASN:HD21	2.17	0.42
13:1M:395:LEU:HD21	38:1m:100:TRP:NE1	2.34	0.42
15:1O:87:LYS:HD2	15:1O:87:LYS:HA	1.89	0.42
16:1P:136:ASN:ND2	16:1P:291:ASP:OD1	2.38	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:157:ARG:HH12	16:1P:225:GLY:C	2.28	0.42
17:1Q:23:THR:HG21	17:1Q:99:ASN:OD1	2.20	0.42
20:1U:52:MET:O	20:1U:55:GLU:HB3	2.20	0.42
29:1d:16:ASN:OD1	29:1d:16:ASN:C	2.62	0.42
34:1i:12:GLN:OE1	34:1i:15:ARG:NH2	2.52	0.42
36:1k:18:TYR:CE2	36:1k:22:LYS:HE3	2.55	0.42
38:1m:24:ILE:HD13	38:1m:29:ARG:CZ	2.50	0.42
40:1o:20:ARG:HH22	40:1o:108:LEU:HD11	1.84	0.42
40:1o:65:LEU:HD11	40:1o:86:TRP:HB2	2.01	0.42
41:1p:166:ARG:O	41:1p:170:LYS:HG2	2.19	0.42
1:1A:54:LYS:HE2	4:1D:71:GLU:HB2	2.02	0.42
1:1A:58:VAL:HG11	1:1A:111:LEU:HA	2.01	0.42
1:1A:106:TRP:CH2	8:1H:291:LYS:HG2	2.55	0.42
2:1B:138:ARG:H	2:1B:138:ARG:HG2	1.53	0.42
3:1C:177:ASP:OD2	16:1P:40:ARG:NH2	2.52	0.42
4:1D:7:ASP:OD1	4:1D:8:VAL:N	2.46	0.42
4:1D:34:ASN:HB3	4:1D:36:VAL:HG22	2.01	0.42
6:1F:165:ASN:ND2	6:1F:168:GLY:HA2	2.35	0.42
7:1G:47:SER:OG	7:1G:48:VAL:N	2.53	0.42
12:1L:49:VAL:HA	12:1L:52:LEU:HG	2.02	0.42
12:1L:380:LEU:HD11	12:1L:419:THR:OG1	2.20	0.42
13:1M:196:TRP:CH2	13:1M:200:ILE:HG13	2.55	0.42
15:1O:120:GLN:C	15:1O:120:GLN:OE1	2.63	0.42
16:1P:108:ASP:O	16:1P:113:ILE:HG12	2.20	0.42
16:1P:286:ARG:CZ	16:1P:286:ARG:HB2	2.49	0.42
17:1Q:56:LYS:HA	17:1Q:56:LYS:HD2	1.84	0.42
30:1e:40:ILE:HD13	33:1h:128:ILE:HG21	2.02	0.42
2:1B:48:MET:HG3	2:1B:80:PRO:HG3	2.02	0.42
2:1B:158:TYR:HB2	9:1I:50:TYR:OH	2.20	0.42
4:1D:203:LEU:HG	4:1D:207:LEU:HD22	2.01	0.42
4:1D:283:PHE:HA	4:1D:309:ARG:HH11	1.85	0.42
5:1E:150:ASN:HB3	5:1E:162:GLU:HB3	2.01	0.42
5:1E:162:GLU:O	5:1E:186:PRO:HA	2.19	0.42
6:1F:68:ARG:NH2	6:1F:252:GLY:HA3	2.33	0.42
6:1F:95:VAL:HG11	6:1F:118:LEU:HD21	2.02	0.42
6:1F:176:PHE:HE1	44:1s:62:ARG:HD3	1.85	0.42
6:1F:188:GLU:OE1	6:1F:190:THR:N	2.52	0.42
7:1G:60:GLU:HB3	7:1G:78:ASN:HB3	2.01	0.42
7:1G:337:ARG:HB2	7:1G:337:ARG:NH1	2.35	0.42
7:1G:669:LYS:NZ	7:1G:670:ASP:OD2	2.53	0.42
10:1J:79:TYR:CD2	16:1P:325:ARG:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:95:SER:HB2	10:1J:98:MET:HE3	2.01	0.42
11:1K:96:LEU:HD23	11:1K:96:LEU:HA	1.86	0.42
12:1L:37:LYS:NZ	12:1L:105:MET:HE3	2.35	0.42
12:1L:246:LEU:N	12:1L:249:SER:HB3	2.35	0.42
12:1L:281:GLY:O	12:1L:285:THR:HG23	2.20	0.42
13:1M:102:LEU:O	13:1M:106:LEU:HD23	2.20	0.42
13:1M:222:GLU:OE1	13:1M:222:GLU:N	2.53	0.42
13:1M:445:LEU:HD22	13:1M:445:LEU:H	1.85	0.42
14:1N:312:LYS:HE2	14:1N:312:LYS:HB2	1.87	0.42
17:1Q:69:LEU:O	17:1Q:71:GLY:N	2.53	0.42
20:1T:16:LEU:O	20:1T:20:LYS:HD3	2.20	0.42
20:1U:58:PHE:HB3	20:1U:60:PHE:HE2	1.85	0.42
28:1c:28:TRP:NE1	29:1d:66:THR:HG22	2.34	0.42
34:1i:49:PHE:CD2	34:1i:57:LYS:HG3	2.54	0.42
36:1k:18:TYR:HB3	36:1k:19:LYS:NZ	2.35	0.42
36:1k:83:ALA:O	36:1k:87:LEU:HD12	2.20	0.42
37:1l:85:ILE:HD12	37:1l:88:ARG:H	1.84	0.42
37:1l:99:ASN:HB2	38:1m:6:LYS:HE2	2.01	0.42
41:1p:5:ASP:HB3	41:1p:7:ASP:OD1	2.20	0.42
6:1F:45:THR:O	6:1F:49:LEU:HD23	2.20	0.41
6:1F:68:ARG:HB3	6:1F:254:LYS:HE2	2.02	0.41
6:1F:295:LEU:HD23	6:1F:343:ILE:HD11	2.02	0.41
7:1G:372:GLU:OE2	7:1G:394:ARG:NH1	2.53	0.41
7:1G:606:ILE:HD11	22:1W:119:LEU:HD21	2.02	0.41
8:1H:20:LEU:HG	8:1H:228:TYR:CE1	2.55	0.41
50:1H:701:U10:H471	50:1H:701:U10:H451	1.70	0.41
10:1J:130:THR:HG21	25:1Z:124:LEU:CD2	2.49	0.41
12:1L:98:TRP:O	12:1L:102:GLU:HB2	2.20	0.41
12:1L:285:THR:HB	12:1L:415:ALA:HB2	2.01	0.41
52:1L:701:MYR:H52	52:1L:701:MYR:C1	2.50	0.41
13:1M:159:PRO:HG3	14:1N:284:MET:HE1	2.01	0.41
13:1M:197:LEU:O	13:1M:201:MET:CE	2.68	0.41
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	2.02	0.41
15:1O:108:TYR:HE1	15:1O:163:TYR:CG	2.38	0.41
15:1O:108:TYR:CD2	15:1O:108:TYR:C	2.98	0.41
19:1S:23:CYS:HG	19:1S:26:SER:HG	1.66	0.41
20:1T:35:HIS:CE1	20:1T:71:MET:HG3	2.55	0.41
20:1U:44:SER:O	20:1U:48:VAL:HG23	2.19	0.41
20:1U:51:ILE:HD13	20:1U:67:ALA:HB1	2.02	0.41
33:1h:111:ARG:HG2	33:1h:122:TRP:CZ2	2.52	0.41
34:1i:80:ILE:HD12	34:1i:81:ILE:N	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:41:THR:HG23	40:1o:44:GLU:H	1.84	0.41
40:1o:112:LYS:HD3	40:1o:112:LYS:HA	1.75	0.41
1:1A:53:MET:HE1	1:1A:56:PHE:CA	2.50	0.41
4:1D:23:LYS:HD2	4:1D:23:LYS:HA	1.84	0.41
7:1G:285:ARG:NE	7:1G:557:ALA:O	2.53	0.41
8:1H:27:VAL:HG22	26:1a:5:ILE:HD13	2.02	0.41
10:1J:1:FME:HG3	10:1J:2:THR:HG22	2.01	0.41
12:1L:63:ILE:HG12	12:1L:82:MET:HE1	2.02	0.41
12:1L:487:LYS:HD3	12:1L:488:MET:HE1	2.02	0.41
13:1M:363:SER:CB	13:1M:411:LEU:HD11	2.49	0.41
14:1N:120:GLN:NE2	14:1N:174:GLN:HB3	2.35	0.41
15:1O:29:GLY:HA3	15:1O:35:LYS:HB3	2.03	0.41
15:1O:54:ALA:HB2	15:1O:107:GLN:HB2	2.02	0.41
18:1R:42:ASP:O	18:1R:46:GLU:OE2	2.37	0.41
20:1U:33:ASN:HB3	20:1U:74:GLN:HG2	2.02	0.41
22:1W:40:TYR:CE1	22:1W:60:ARG:CZ	3.03	0.41
23:1X:93:LEU:HD23	23:1X:93:LEU:HA	1.86	0.41
31:1f:45:LYS:HB3	41:1p:68:ARG:HH12	1.85	0.41
37:1l:65:ASP:HB2	37:1l:72:ASN:HA	2.02	0.41
41:1p:145:LEU:HD23	41:1p:145:LEU:HA	1.89	0.41
2:1B:86:MET:HB3	2:1B:86:MET:HE2	1.64	0.41
3:1C:149:ARG:HH21	4:1D:79:HIS:CE1	2.38	0.41
3:1C:161:PRO:HA	3:1C:166:PHE:CD2	2.55	0.41
4:1D:217:ASN:HA	43:1r:22:LYS:HD2	2.01	0.41
7:1G:147:LYS:HE3	7:1G:702:SER:HB2	2.03	0.41
7:1G:284:ILE:HA	7:1G:558:ASP:O	2.19	0.41
7:1G:350:PRO:HD3	7:1G:458:LEU:HB3	2.02	0.41
7:1G:580:ALA:O	7:1G:633:TYR:HA	2.21	0.41
8:1H:155:LEU:HD23	8:1H:155:LEU:HA	1.87	0.41
12:1L:54:PHE:HB3	12:1L:55:MET:HE2	2.01	0.41
12:1L:161:ARG:NE	39:1n:91:GLU:OE2	2.47	0.41
12:1L:287:PHE:CZ	12:1L:527:GLY:HA3	2.55	0.41
46:1L:702:PC1:H2B1	24:1Y:116:TYR:CE1	2.53	0.41
13:1M:142:ARG:NH2	14:1N:303:THR:HG22	2.36	0.41
13:1M:357:THR:C	13:1M:361:MET:HE1	2.45	0.41
14:1N:73:ALA:HB1	14:1N:98:MET:HE2	2.01	0.41
14:1N:98:MET:HE3	14:1N:98:MET:HB2	1.82	0.41
15:1O:39:ALA:O	15:1O:123:VAL:HG11	2.20	0.41
15:1O:171:TYR:OH	15:1O:203:GLU:OE2	2.37	0.41
19:1S:15:LEU:HA	19:1S:15:LEU:HD12	1.75	0.41
20:1U:84:LYS:HG3	20:1U:86:VAL:HG13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:94:LEU:O	21:1V:95:ARG:NH2	2.53	0.41
22:1W:50:PHE:CZ	22:1W:98:LYS:O	2.73	0.41
25:1Z:123:GLU:HB3	30:1e:75:LEU:HD11	2.03	0.41
33:1h:94:LEU:HD23	33:1h:94:LEU:HA	1.87	0.41
36:1k:86:TYR:C	36:1k:86:TYR:CD2	2.98	0.41
37:1l:138:LEU:HB3	37:1l:141:GLU:HB2	2.01	0.41
38:1m:91:LEU:O	38:1m:96:PRO:HD3	2.19	0.41
43:1r:69:MET:SD	43:1r:69:MET:C	3.03	0.41
4:1D:28:TRP:CD1	4:1D:28:TRP:N	2.88	0.41
7:1G:624:GLU:HB2	7:1G:631:VAL:HG21	2.01	0.41
8:1H:22:LEU:HB2	8:1H:48:PRO:CG	2.51	0.41
8:1H:76:ILE:O	8:1H:80:SER:OG	2.25	0.41
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.53	0.41
10:1J:9:LEU:HD22	10:1J:39:VAL:HG23	2.02	0.41
12:1L:137:LEU:HB3	12:1L:182:PHE:HE1	1.85	0.41
12:1L:174:TYR:HA	12:1L:177:ILE:HD12	2.02	0.41
13:1M:220:HIS:NE2	13:1M:231:LEU:HB3	2.36	0.41
13:1M:293:HIS:NE2	13:1M:366:ASN:OD1	2.53	0.41
20:1U:73:PRO:HA	20:1U:76:ILE:HD12	2.03	0.41
23:1X:101:LYS:HE2	23:1X:101:LYS:HB2	1.70	0.41
25:1Z:111:PHE:CD2	25:1Z:117:VAL:HG11	2.55	0.41
31:1f:30:SER:O	31:1f:34:LEU:HG	2.20	0.41
32:1g:36:ASN:HD21	32:1g:38:TYR:HB2	1.85	0.41
32:1g:55:LEU:O	32:1g:59:ARG:HG3	2.20	0.41
37:1l:7:ASP:OD1	37:1l:8:MET:N	2.52	0.41
38:1m:65:ILE:HG12	38:1m:66:ARG:N	2.34	0.41
1:1A:18:VAL:HG23	8:1H:222:MET:HE3	2.00	0.41
1:1A:48:ARG:HD3	1:1A:48:ARG:HA	1.87	0.41
2:1B:122:GLY:N	9:1I:114:THR:OG1	2.53	0.41
2:1B:145:TYR:N	9:1I:141:THR:O	2.31	0.41
6:1F:74:PRO:O	6:1F:77:LEU:N	2.54	0.41
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.52	0.41
6:1F:280:ILE:O	6:1F:286:GLY:N	2.50	0.41
7:1G:363:LEU:HA	7:1G:363:LEU:HD23	1.77	0.41
8:1H:268:ILE:O	8:1H:272:TRP:N	2.53	0.41
10:1J:31:LEU:O	10:1J:35:VAL:HG12	2.21	0.41
10:1J:74:MET:HE2	10:1J:74:MET:HB3	1.74	0.41
11:1K:93:LEU:HD21	12:1L:584:ILE:HD13	2.02	0.41
12:1L:107:TYR:CD2	12:1L:348:HIS:HB2	2.55	0.41
12:1L:246:LEU:O	12:1L:249:SER:N	2.47	0.41
13:1M:14:MET:HE2	13:1M:26:ASN:HB3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:124:LEU:HD23	14:1N:124:LEU:HA	1.93	0.41
14:1N:205:LEU:O	14:1N:209:ILE:HG12	2.20	0.41
16:1P:27:THR:O	16:1P:27:THR:OG1	2.32	0.41
16:1P:243:GLN:OE1	16:1P:243:GLN:HA	2.21	0.41
20:1U:36:PHE:HA	20:1U:40:LEU:HB2	2.02	0.41
33:1h:76:ALA:HA	33:1h:80:TYR:HB2	2.03	0.41
34:1i:55:PRO:O	34:1i:59:VAL:HG23	2.20	0.41
34:1i:77:PRO:HA	34:1i:80:ILE:HD11	2.02	0.41
37:1l:136:ASN:HD22	37:1l:139:TYR:HB2	1.84	0.41
38:1m:6:LYS:HD2	38:1m:7:PRO:O	2.21	0.41
40:1o:21:MET:HB2	40:1o:104:GLU:HG2	2.02	0.41
4:1D:19:MET:HB3	14:1N:173:THR:OG1	2.20	0.41
4:1D:43:LEU:HD13	11:1K:86:GLY:N	2.35	0.41
6:1F:32:ARG:HH11	44:1s:42:GLN:HE21	1.68	0.41
6:1F:361:GLN:N	45:1F:502:SF4:S3	2.93	0.41
6:1F:371:TRP:CE2	7:1G:130:PHE:HD1	2.38	0.41
7:1G:26:VAL:HG23	7:1G:71:MET:O	2.20	0.41
7:1G:135:ARG:HG3	7:1G:135:ARG:HH11	1.85	0.41
7:1G:196:SER:OG	7:1G:265:ASP:OD2	2.27	0.41
8:1H:52:ALA:HB2	50:1H:701:U10:C24	2.49	0.41
11:1K:35:GLY:HA2	11:1K:38:LEU:HD13	2.03	0.41
12:1L:101:MET:HE3	12:1L:102:GLU:N	2.36	0.41
12:1L:260:LEU:HD23	12:1L:260:LEU:HA	1.94	0.41
14:1N:109:SER:HB2	14:1N:110:PRO:HD2	2.02	0.41
14:1N:175:LEU:HD22	14:1N:296:LEU:HD11	2.01	0.41
14:1N:324:LYS:NZ	29:1d:60:ARG:HH12	2.18	0.41
15:1O:3:TYR:HD1	15:1O:7:ALA:HB3	1.85	0.41
16:1P:80:SER:O	16:1P:84:VAL:HG23	2.20	0.41
16:1P:192:PRO:HA	16:1P:256:TYR:HB3	2.03	0.41
17:1Q:133:LYS:HE3	17:1Q:133:LYS:HB3	1.83	0.41
20:1T:60:PHE:HD2	20:1T:60:PHE:H	1.68	0.41
23:1X:6:LEU:O	25:1Z:88:ARG:NH1	2.54	0.41
30:1e:44:HIS:CE1	33:1h:130:LYS:HG2	2.55	0.41
31:1f:39:ASN:N	33:1h:88:GLU:OE2	2.53	0.41
31:1f:49:ARG:HH12	33:1h:60:VAL:H	1.68	0.41
39:1n:176:ARG:HA	39:1n:176:ARG:CZ	2.51	0.41
40:1o:16:PRO:HB3	40:1o:21:MET:HG2	2.03	0.41
1:1A:41:PHE:CE1	2:1B:99:ALA:HB2	2.56	0.41
4:1D:20:TYR:HD2	12:1L:571:MET:SD	2.43	0.41
4:1D:76:CYS:O	4:1D:78:PRO:HD3	2.21	0.41
4:1D:167:PHE:HE1	4:1D:171:PHE:CD1	2.39	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:93:LYS:HE2	5:1E:93:LYS:HB2	1.82	0.41
5:1E:123:LYS:HD2	5:1E:170:GLU:CD	2.46	0.41
5:1E:210:GLY:HA2	6:1F:43:TYR:CE2	2.56	0.41
7:1G:147:LYS:N	7:1G:209:THR:O	2.53	0.41
7:1G:210:SER:OG	7:1G:213:TYR:HB3	2.21	0.41
8:1H:1:FME:HE2	26:1a:29:PHE:CE2	2.53	0.41
9:1I:111:ILE:HG13	9:1I:154:LEU:HD11	2.03	0.41
10:1J:55:MET:SD	10:1J:59:ILE:HG12	2.61	0.41
12:1L:37:LYS:O	12:1L:41:SER:OG	2.30	0.41
12:1L:135:ASN:HA	12:1L:198:LEU:HD12	2.03	0.41
12:1L:435:PRO:HB2	12:1L:437:PHE:HD1	1.86	0.41
13:1M:20:HIS:HB2	13:1M:89:THR:HG21	2.03	0.41
13:1M:277:LEU:HD21	13:1M:405:LEU:HD22	2.01	0.41
14:1N:347:ASN:HD21	29:1d:2:MET:HE2	1.86	0.41
15:1O:44:GLU:HG3	15:1O:44:GLU:H	1.67	0.41
15:1O:232:GLU:C	15:1O:236:GLU:OE2	2.63	0.41
20:1U:47:GLN:OE1	20:1U:71:MET:HE1	2.20	0.41
23:1X:37:LYS:H	23:1X:37:LYS:HG2	1.69	0.41
23:1X:43:MET:HB2	23:1X:43:MET:HE2	1.82	0.41
24:1Y:113:ALA:O	24:1Y:114:CYS:C	2.63	0.41
32:1g:45:HIS:CE1	32:1g:58:MET:HG3	2.56	0.41
1:1A:106:TRP:HH2	27:1b:18:LEU:HD21	1.86	0.41
3:1C:12:ARG:CZ	4:1D:124:LYS:HG3	2.51	0.41
4:1D:223:ASP:OD1	4:1D:305:ARG:NH2	2.31	0.41
4:1D:261:ARG:HD3	4:1D:285:VAL:HB	2.02	0.41
4:1D:413:ASP:OD2	8:1H:281:ARG:NH1	2.54	0.41
6:1F:16:LYS:HE2	6:1F:16:LYS:HB2	1.80	0.41
8:1H:2:PHE:HZ	8:1H:96:ILE:HD11	1.86	0.41
8:1H:129:LEU:HD13	8:1H:129:LEU:HA	1.92	0.41
10:1J:109:LYS:HG3	10:1J:110:GLU:CD	2.46	0.41
10:1J:152:TRP:CD2	30:1e:13:LEU:HD22	2.55	0.41
11:1K:45:THR:HA	11:1K:48:ILE:HD11	2.03	0.41
13:1M:329:LEU:HD22	13:1M:359:TRP:CD2	2.55	0.41
13:1M:368:ALA:HB2	13:1M:374:ASN:ND2	2.36	0.41
14:1N:213:LEU:HD23	14:1N:329:MET:HE3	2.03	0.41
16:1P:335:LYS:NZ	16:1P:336:PRO:CG	2.84	0.41
16:1P:335:LYS:HZ3	16:1P:336:PRO:HD2	1.85	0.41
20:1T:62:ILE:O	20:1T:62:ILE:HG13	2.20	0.41
20:1T:75:GLU:OE1	20:1T:75:GLU:N	2.53	0.41
20:1U:24:LYS:CG	36:1k:41:ARG:NH2	2.80	0.41
21:1V:34:LEU:HD11	21:1V:47:THR:HG22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:12:ARG:HB3	36:1k:50:TRP:CG	2.56	0.41
37:1l:69:LEU:HD12	37:1l:86:ARG:HD3	2.02	0.41
1:1A:6:THR:HG21	8:1H:87:VAL:HG21	2.02	0.41
1:1A:71:LEU:HD12	1:1A:71:LEU:HA	1.85	0.41
3:1C:193:GLU:OE2	7:1G:223:ARG:NH2	2.54	0.41
4:1D:78:PRO:O	4:1D:80:ILE:HG23	2.21	0.41
5:1E:161:TYR:OH	5:1E:182:PRO:HG2	2.21	0.41
5:1E:201:SER:OG	6:1F:20:ARG:NH1	2.54	0.41
6:1F:153:ILE:HD12	6:1F:175:VAL:HG21	2.02	0.41
6:1F:270:GLU:HG2	6:1F:279:LEU:HD12	2.03	0.41
7:1G:126:ASP:OD1	43:1r:56:ARG:NH2	2.43	0.41
7:1G:234:VAL:HG11	7:1G:390:LEU:HB2	2.02	0.41
7:1G:248:MET:N	7:1G:248:MET:SD	2.93	0.41
7:1G:268:ARG:HD2	7:1G:269:PHE:CZ	2.56	0.41
7:1G:272:ASP:OD1	7:1G:272:ASP:N	2.54	0.41
7:1G:651:LEU:O	7:1G:652:VAL:HG22	2.21	0.41
8:1H:70:MET:HE2	8:1H:70:MET:HB2	1.77	0.41
8:1H:102:VAL:HG13	8:1H:150:LEU:HD13	2.03	0.41
10:1J:70:TYR:HD2	11:1K:75:LEU:HB3	1.86	0.41
10:1J:138:GLU:HG2	30:1e:28:ILE:HG21	2.02	0.41
11:1K:70:GLU:OE1	14:1N:34:GLU:CD	2.64	0.41
12:1L:15:LEU:HD13	12:1L:122:VAL:HG13	2.03	0.41
12:1L:124:PHE:CD1	12:1L:247:LEU:HG	2.56	0.41
12:1L:358:LYS:HA	12:1L:358:LYS:HD3	1.69	0.41
12:1L:482:MET:HE3	12:1L:486:MET:SD	2.61	0.41
12:1L:552:LEU:HD21	38:1m:89:GLY:HA2	2.02	0.41
12:1L:553:LEU:HD22	12:1L:553:LEU:HA	1.75	0.41
12:1L:557:TRP:HZ3	38:1m:79:PHE:HZ	1.69	0.41
13:1M:199:CYS:HB2	13:1M:250:LEU:HD21	2.02	0.41
14:1N:25:HIS:O	14:1N:29:ILE:HG12	2.21	0.41
14:1N:71:MET:HE2	14:1N:75:ILE:HG12	2.03	0.41
14:1N:235:ASN:HD21	15:1O:293:PHE:HB2	1.86	0.41
15:1O:140:ARG:HH22	15:1O:204:ASN:HB3	1.86	0.41
15:1O:168:VAL:HG13	15:1O:219:GLU:HB2	2.03	0.41
15:1O:278:TYR:O	32:1g:25:ARG:NH1	2.54	0.41
17:1Q:15:GLU:H	17:1Q:15:GLU:CD	2.22	0.41
18:1R:32:GLN:HE22	18:1R:34:GLU:HG2	1.86	0.41
20:1T:49:GLU:OE1	22:1W:40:TYR:CE2	2.74	0.41
20:1T:52:MET:HE2	22:1W:41:ARG:HH21	1.86	0.41
20:1T:63:PRO:HD2	20:1T:66:ASP:OD2	2.21	0.41
22:1W:98:LYS:HB3	22:1W:98:LYS:HE3	1.80	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:8:THR:HA	25:1Z:88:ARG:NH2	2.36	0.41
23:1X:84:TYR:CZ	23:1X:103:GLN:HB2	2.56	0.41
26:1a:4:GLU:O	26:1a:7:PRO:HD2	2.21	0.41
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	2.02	0.41
32:1g:67:SER:O	32:1g:69:VAL:N	2.54	0.41
33:1h:32:THR:C	33:1h:35:PRO:HD2	2.45	0.41
35:1j:51:PHE:CD2	40:1o:88:TYR:HD1	2.38	0.41
36:1k:44:TRP:HB2	39:1n:37:ARG:CZ	2.51	0.41
37:1l:81:LEU:O	37:1l:85:ILE:HG23	2.21	0.41
39:1n:149:ARG:HD2	39:1n:149:ARG:HA	1.66	0.41
41:1p:77:GLU:HB2	41:1p:80:ASP:CB	2.50	0.41
42:1q:83:PRO:HA	42:1q:113:HIS:CD2	2.56	0.41
43:1r:105:LEU:HD12	43:1r:105:LEU:HA	1.85	0.41
3:1C:83:VAL:HB	3:1C:86:ARG:HD2	2.03	0.41
4:1D:4:TRP:CG	13:1M:140:THR:HG1	2.39	0.41
4:1D:43:LEU:HD22	11:1K:86:GLY:HA3	2.03	0.41
4:1D:230:THR:O	4:1D:294:TYR:OH	2.35	0.41
4:1D:399:LEU:HD13	4:1D:423:ILE:HD13	2.03	0.41
6:1F:188:GLU:HG3	6:1F:405:CYS:HB2	2.02	0.41
6:1F:278:GLU:O	6:1F:282:LYS:HG2	2.21	0.41
7:1G:405:LYS:HB3	7:1G:405:LYS:HE2	1.70	0.41
8:1H:161:THR:HG21	26:1a:40:HIS:CE1	2.55	0.41
11:1K:12:PHE:HE1	11:1K:36:MET:HB3	1.85	0.41
11:1K:26:LEU:N	11:1K:88:ASP:OD2	2.53	0.41
11:1K:61:ILE:O	11:1K:65:VAL:HG23	2.21	0.41
12:1L:341:MET:N	12:1L:341:MET:SD	2.94	0.41
12:1L:501:ALA:HA	12:1L:504:LEU:HB2	2.03	0.41
13:1M:209:LEU:HG	13:1M:264:LEU:CD1	2.51	0.41
13:1M:265:SER:O	13:1M:269:MET:CE	2.69	0.41
14:1N:164:ILE:HD12	14:1N:164:ILE:N	2.36	0.41
15:1O:64:GLY:HA3	28:1c:2:PHE:HE2	1.85	0.41
16:1P:26:ALA:HB3	16:1P:47:VAL:HG13	2.02	0.41
16:1P:36:ASN:HB2	16:1P:62:MET:HE2	2.03	0.41
17:1Q:69:LEU:HG	17:1Q:70:MET:CE	2.37	0.41
18:1R:10:LYS:HE2	18:1R:10:LYS:HB3	1.83	0.41
22:1W:69:LYS:HG3	22:1W:70:ASN:OD1	2.21	0.41
53:1Y:201:3PE:H221	53:1Y:201:3PE:H2	1.87	0.41
33:1h:61:PRO:HG2	33:1h:66:TYR:CZ	2.56	0.41
33:1h:69:HIS:O	33:1h:73:ARG:HG3	2.21	0.41
34:1i:121:GLU:H	34:1i:121:GLU:HG3	1.72	0.41
36:1k:31:VAL:HG13	39:1n:38:TYR:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:99:PRO:HB2	39:1n:101:TRP:CD1	2.56	0.41
42:1q:137:TRP:CZ2	42:1q:140:PRO:HD3	2.56	0.41
1:1A:26:GLN:HG3	46:1B:202:PC1:H32	2.03	0.40
1:1A:41:PHE:HB3	22:1W:99:GLN:NE2	2.36	0.40
2:1B:33:LEU:CD1	46:1B:202:PC1:H3A1	2.51	0.40
2:1B:157:LEU:HD23	2:1B:157:LEU:HA	1.83	0.40
3:1C:116:PRO:HD3	22:1W:20:ILE:CD1	2.51	0.40
4:1D:224:GLU:CB	9:1I:36:MET:HE1	2.50	0.40
4:1D:287:ILE:HD13	9:1I:2:TYR:HB2	2.02	0.40
6:1F:53:PRO:HD3	6:1F:127:ARG:NH1	2.36	0.40
8:1H:224:PHE:CZ	50:1H:701:U10:H103	2.55	0.40
9:1I:69:ARG:NH1	9:1I:73:GLY:O	2.54	0.40
10:1J:99:MET:O	10:1J:103:MET:SD	2.79	0.40
10:1J:143:ILE:H	10:1J:143:ILE:HG13	1.74	0.40
11:1K:12:PHE:CE2	14:1N:72:MET:HG2	2.56	0.40
12:1L:44:PHE:CE1	12:1L:95:PHE:HB2	2.56	0.40
12:1L:377:SER:O	12:1L:380:LEU:HG	2.21	0.40
12:1L:599:MET:SD	12:1L:599:MET:N	2.93	0.40
13:1M:101:LEU:HD12	13:1M:101:LEU:HA	1.81	0.40
13:1M:116:ILE:O	13:1M:120:ILE:HG12	2.21	0.40
13:1M:219:ALA:O	13:1M:223:ALA:N	2.54	0.40
14:1N:44:LEU:HD11	14:1N:59:TYR:CD1	2.56	0.40
19:1S:84:ASP:HB2	19:1S:88:ARG:HH21	1.86	0.40
24:1Y:139:LYS:HD2	24:1Y:139:LYS:H	1.86	0.40
27:1b:80:LEU:HD12	27:1b:80:LEU:HA	1.81	0.40
29:1d:45:ASP:OD2	29:1d:49:ARG:NE	2.54	0.40
34:1i:89:VAL:HG12	34:1i:95:THR:OG1	2.21	0.40
35:1j:18:THR:O	35:1j:21:GLN:HG2	2.21	0.40
35:1j:19:ARG:HE	35:1j:19:ARG:HB3	1.46	0.40
35:1j:62:GLU:C	35:1j:62:GLU:CD	2.88	0.40
42:1q:120:THR:O	42:1q:122:GLN:N	2.46	0.40
1:1A:7:LEU:O	1:1A:11:VAL:HG22	2.22	0.40
2:1B:59:MET:O	2:1B:62:MET:HB3	2.21	0.40
3:1C:175:ARG:HE	3:1C:186:GLU:CD	2.30	0.40
6:1F:34:LYS:HB2	6:1F:34:LYS:HE2	1.83	0.40
6:1F:52:GLY:O	6:1F:56:ILE:HG12	2.22	0.40
7:1G:377:ILE:HG13	7:1G:450:MET:HB3	2.02	0.40
8:1H:169:GLN:HG2	8:1H:169:GLN:H	1.68	0.40
12:1L:111:ASP:OD2	39:1n:96:TYR:OH	2.39	0.40
12:1L:144:TRP:CZ2	12:1L:223:LYS:HB2	2.56	0.40
12:1L:217:LEU:HD13	12:1L:276:MET:HG3	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:231:PRO:O	12:1L:235:SER:OG	2.29	0.40
12:1L:482:MET:HA	12:1L:483:PRO:HD3	1.89	0.40
13:1M:154:LEU:HA	13:1M:154:LEU:HD12	1.79	0.40
13:1M:159:PRO:HD3	14:1N:284:MET:HE1	2.03	0.40
13:1M:267:TRP:CE2	13:1M:271:MET:HG2	2.56	0.40
14:1N:261:MET:CG	14:1N:340:THR:HG23	2.52	0.40
14:1N:313:MET:HA	14:1N:316:GLN:CD	2.47	0.40
17:1Q:17:LEU:HD23	17:1Q:98:LYS:CD	2.51	0.40
22:1W:28:ALA:O	22:1W:32:VAL:HG23	2.21	0.40
23:1X:37:LYS:O	23:1X:41:GLU:HG3	2.21	0.40
23:1X:121:LEU:HD12	23:1X:121:LEU:HA	1.93	0.40
33:1h:115:ARG:HB2	33:1h:123:TYR:CE2	2.56	0.40
35:1j:71:GLU:N	35:1j:71:GLU:CD	2.72	0.40
4:1D:73:VAL:O	4:1D:74:ARG:NH1	2.55	0.40
4:1D:228:MET:HG2	9:1I:33:GLY:HA2	2.02	0.40
4:1D:377:TYR:HB3	4:1D:390:LYS:HB3	2.03	0.40
5:1E:78:MET:HG2	7:1G:171:ASP:C	2.46	0.40
10:1J:126:VAL:O	25:1Z:120:MET:HE2	2.22	0.40
12:1L:382:GLY:HA2	12:1L:386:LEU:CD2	2.52	0.40
12:1L:439:PRO:HA	36:1k:50:TRP:CZ2	2.56	0.40
12:1L:492:ILE:C	12:1L:496:MET:HE1	2.43	0.40
12:1L:552:LEU:HA	12:1L:556:ILE:HB	2.02	0.40
13:1M:139:GLN:OE1	13:1M:139:GLN:N	2.54	0.40
13:1M:285:LEU:O	13:1M:289:SER:N	2.47	0.40
14:1N:304:MET:H	14:1N:304:MET:HG3	1.57	0.40
14:1N:325:LEU:HA	14:1N:328:THR:HB	2.02	0.40
15:1O:182:ARG:HA	15:1O:185:LYS:HE2	2.04	0.40
15:1O:237:ASP:OD1	15:1O:238:ILE:N	2.54	0.40
16:1P:226:LYS:HE3	16:1P:226:LYS:HB2	1.87	0.40
17:1Q:97:GLU:C	17:1Q:100:GLY:H	2.29	0.40
20:1U:22:TYR:OH	20:1U:46:ASP:OD1	2.39	0.40
20:1U:52:MET:HA	20:1U:55:GLU:HB2	2.03	0.40
20:1U:65:ILE:C	20:1U:65:ILE:HD12	2.47	0.40
22:1W:32:VAL:HG21	58:1W:201:EHZ:O3	2.21	0.40
32:1g:96:LEU:HD12	32:1g:100:ARG:HH12	1.86	0.40
35:1j:10:ARG:HH22	35:1j:16:GLN:NE2	2.19	0.40
36:1k:29:GLU:HG2	36:1k:30:THR:N	2.36	0.40
41:1p:31:TYR:O	41:1p:35:ILE:HG23	2.22	0.40
41:1p:41:ASP:N	41:1p:41:ASP:OD1	2.54	0.40
41:1p:51:ILE:HG23	41:1p:55:HIS:CE1	2.56	0.40
42:1q:72:ASP:OD2	42:1q:73:THR:N	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:58:GLU:HG2	2:1B:151:PRO:O	2.22	0.40
3:1C:113:GLU:OE2	17:1Q:98:LYS:NZ	2.40	0.40
3:1C:182:ARG:HG3	22:1W:101:THR:HG22	2.03	0.40
4:1D:349:PHE:CE2	9:1I:82:LEU:HD21	2.57	0.40
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.22	0.40
5:1E:89:MET:HE1	6:1F:140:GLY:C	2.46	0.40
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	2.02	0.40
7:1G:500:VAL:HG21	7:1G:576:THR:HA	2.03	0.40
8:1H:12:PRO:HB3	26:1a:15:CYS:O	2.22	0.40
10:1J:141:MET:HE1	30:1e:26:HIS:ND1	2.36	0.40
12:1L:139:GLN:HA	12:1L:142:ILE:HD12	2.02	0.40
12:1L:142:ILE:HA	13:1M:370:PRO:HB2	2.04	0.40
12:1L:327:LEU:HD23	12:1L:391:SER:HB3	2.02	0.40
12:1L:375:ILE:HG12	35:1j:32:MET:HG2	2.03	0.40
13:1M:92:LYS:O	13:1M:96:ILE:HG12	2.21	0.40
13:1M:243:MET:HB3	13:1M:301:ILE:HG21	2.03	0.40
13:1M:334:TYR:O	13:1M:338:HIS:N	2.54	0.40
14:1N:277:ILE:HD12	24:1Y:134:VAL:HG22	2.03	0.40
14:1N:277:ILE:HD13	53:1Y:201:3PE:H261	2.04	0.40
14:1N:318:GLU:H	14:1N:318:GLU:CD	2.23	0.40
20:1T:14:ARG:HD3	20:1T:58:PHE:CE1	2.56	0.40
21:1V:94:LEU:CA	21:1V:97:LYS:HD2	2.48	0.40
23:1X:47:TRP:CZ3	33:1h:141:PRO:HG3	2.56	0.40
25:1Z:99:LYS:HA	25:1Z:99:LYS:HD3	1.83	0.40
29:1d:90:MET:HE1	33:1h:107:GLU:CB	2.52	0.40
39:1n:83:GLU:H	39:1n:83:GLU:CD	2.29	0.40
41:1p:66:GLU:N	41:1p:66:GLU:OE1	2.54	0.40
4:1D:183:ARG:NH2	4:1D:207:LEU:HA	2.37	0.40
4:1D:375:GLY:O	4:1D:392:LYS:N	2.52	0.40
6:1F:21:ILE:HG21	6:1F:230:VAL:HG12	2.04	0.40
7:1G:141:ASN:ND2	7:1G:695:ILE:HD11	2.37	0.40
7:1G:200:ILE:HG22	17:1Q:45:MET:HE1	2.02	0.40
7:1G:505:LEU:HD23	7:1G:505:LEU:HA	1.90	0.40
7:1G:584:LYS:NZ	17:1Q:106:GLU:OE2	2.55	0.40
7:1G:672:TYR:CB	7:1G:684:MET:CE	2.95	0.40
8:1H:11:ILE:HB	8:1H:12:PRO:HD3	2.04	0.40
8:1H:85:MET:HE2	8:1H:108:MET:HB2	2.03	0.40
10:1J:1:FME:C	10:1J:3:MET:N	2.84	0.40
10:1J:107:ALA:HB1	11:1K:3:LEU:HD11	2.03	0.40
10:1J:143:ILE:HA	11:1K:58:MET:HG2	2.04	0.40
12:1L:104:SER:O	12:1L:108:MET:N	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:131:ILE:HG12	53:1M:502:3PE:H392	2.03	0.40
53:1M:502:3PE:H262	14:1N:243:LEU:HD12	2.04	0.40
14:1N:55:ALA:O	14:1N:118:VAL:HG23	2.21	0.40
15:1O:70:ASP:OD2	15:1O:73:LEU:N	2.53	0.40
15:1O:148:CYS:SG	15:1O:279:LEU:HD13	2.62	0.40
16:1P:105:ASP:OD1	16:1P:107:GLU:HB3	2.21	0.40
16:1P:135:LEU:HB3	16:1P:169:SER:HA	2.04	0.40
21:1V:71:LEU:HD13	21:1V:79:VAL:HG11	2.03	0.40
21:1V:115:ILE:HD12	21:1V:115:ILE:HA	1.79	0.40
30:1e:20:GLN:O	30:1e:24:GLN:NE2	2.55	0.40
32:1g:37:LEU:HD13	32:1g:49:LYS:HZ1	1.87	0.40
33:1h:22:LEU:O	33:1h:26:ARG:HG2	2.22	0.40
37:1l:50:LEU:HB2	37:1l:78:HIS:CD2	2.47	0.40
39:1n:54:LYS:HB3	39:1n:55:ASP:H	1.68	0.40
39:1n:125:LYS:HD3	39:1n:125:LYS:HA	1.88	0.40
41:1p:77:GLU:HB2	41:1p:80:ASP:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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%)	103 (91%)	9 (8%)	1 (1%)	14	47
2	1B	153/258 (59%)	138 (90%)	15 (10%)	0	100	100
3	1C	207/264 (78%)	199 (96%)	8 (4%)	0	100	100
4	1D	427/476 (90%)	402 (94%)	25 (6%)	0	100	100
5	1E	212/249 (85%)	195 (92%)	16 (8%)	1 (0%)	24	57
6	1F	430/464 (93%)	414 (96%)	16 (4%)	0	100	100
7	1G	697/727 (96%)	655 (94%)	41 (6%)	1 (0%)	48	79

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	1H	316/318 (99%)	292 (92%)	21 (7%)	3 (1%)	14	47
9	1I	174/239 (73%)	168 (97%)	6 (3%)	0	100	100
10	1J	173/175 (99%)	160 (92%)	10 (6%)	3 (2%)	7	35
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	552 (91%)	47 (8%)	5 (1%)	16	49
13	1M	457/459 (100%)	438 (96%)	19 (4%)	0	100	100
14	1N	345/347 (99%)	322 (93%)	22 (6%)	1 (0%)	36	67
15	1O	318/357 (89%)	298 (94%)	20 (6%)	0	100	100
16	1P	340/377 (90%)	324 (95%)	16 (5%)	0	100	100
17	1Q	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
18	1R	94/123 (76%)	89 (95%)	5 (5%)	0	100	100
19	1S	85/99 (86%)	79 (93%)	6 (7%)	0	100	100
20	1T	83/156 (53%)	76 (92%)	7 (8%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
22	1W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	21	54
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	43 (92%)	4 (8%)	0	100	100
29	1d	117/123 (95%)	104 (89%)	12 (10%)	1 (1%)	14	47
30	1e	97/106 (92%)	88 (91%)	9 (9%)	0	100	100
31	1f	55/135 (41%)	49 (89%)	6 (11%)	0	100	100
32	1g	98/154 (64%)	83 (85%)	14 (14%)	1 (1%)	12	44
33	1h	136/189 (72%)	126 (93%)	10 (7%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
37	1l	154/186 (83%)	142 (92%)	12 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	1m	126/129 (98%)	114 (90%)	12 (10%)	0	100	100
39	1n	170/179 (95%)	157 (92%)	13 (8%)	0	100	100
40	1o	120/137 (88%)	110 (92%)	10 (8%)	0	100	100
41	1p	171/176 (97%)	162 (95%)	9 (5%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	12 (8%)	0	100	100
43	1r	90/114 (79%)	86 (96%)	4 (4%)	0	100	100
44	1s	43/471 (9%)	38 (88%)	4 (9%)	1 (2%)	5	30
All	All	8194/9744 (84%)	7656 (93%)	519 (6%)	19 (0%)	44	74

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	109	LYS
7	1G	652	VAL
8	1H	68	ILE
8	1H	92	PRO
10	1J	2	THR
10	1J	85	SER
23	1X	28	ALA
29	1d	53	VAL
10	1J	116	ILE
8	1H	208	VAL
12	1L	4	PHE
12	1L	562	LEU
12	1L	549	ALA
5	1E	157	ASN
12	1L	484	LEU
12	1L	600	THR
14	1N	110	PRO
44	1s	32	PRO
32	1g	68	ILE

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	99/99 (100%)	92 (93%)	7 (7%)	13	38
2	1B	131/212 (62%)	127 (97%)	4 (3%)	35	59
3	1C	190/227 (84%)	181 (95%)	9 (5%)	23	49
4	1D	371/405 (92%)	352 (95%)	19 (5%)	21	48
5	1E	183/207 (88%)	178 (97%)	5 (3%)	39	62
6	1F	346/368 (94%)	333 (96%)	13 (4%)	29	55
7	1G	588/610 (96%)	548 (93%)	40 (7%)	14	40
8	1H	274/274 (100%)	261 (95%)	13 (5%)	23	49
9	1I	151/201 (75%)	145 (96%)	6 (4%)	28	54
10	1J	140/140 (100%)	131 (94%)	9 (6%)	16	42
11	1K	84/84 (100%)	78 (93%)	6 (7%)	13	38
12	1L	539/539 (100%)	504 (94%)	35 (6%)	15	42
13	1M	408/408 (100%)	386 (95%)	22 (5%)	20	46
14	1N	310/310 (100%)	293 (94%)	17 (6%)	19	46
15	1O	283/307 (92%)	273 (96%)	10 (4%)	32	57
16	1P	296/323 (92%)	282 (95%)	14 (5%)	23	49
17	1Q	117/152 (77%)	108 (92%)	9 (8%)	12	37
18	1R	79/97 (81%)	73 (92%)	6 (8%)	12	37
19	1S	77/82 (94%)	73 (95%)	4 (5%)	21	47
20	1T	79/133 (59%)	77 (98%)	2 (2%)	42	63
20	1U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	96 (96%)	4 (4%)	28	54
22	1W	107/112 (96%)	103 (96%)	4 (4%)	30	56
23	1X	153/154 (99%)	145 (95%)	8 (5%)	21	47
24	1Y	101/102 (99%)	96 (95%)	5 (5%)	22	48
25	1Z	123/124 (99%)	115 (94%)	8 (6%)	15	42
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	57
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	38
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	107/109 (98%)	102 (95%)	5 (5%)	23	49
30	1e	87/94 (93%)	84 (97%)	3 (3%)	32	57
31	1f	54/113 (48%)	51 (94%)	3 (6%)	19	46

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	1g	92/129 (71%)	86 (94%)	6 (6%)	15	42
33	1h	121/158 (77%)	116 (96%)	5 (4%)	27	53
34	1i	119/120 (99%)	112 (94%)	7 (6%)	18	44
35	1j	62/84 (74%)	56 (90%)	6 (10%)	8	30
36	1k	63/76 (83%)	60 (95%)	3 (5%)	23	49
37	1l	141/161 (88%)	135 (96%)	6 (4%)	26	51
38	1m	113/114 (99%)	111 (98%)	2 (2%)	51	69
39	1n	156/160 (98%)	153 (98%)	3 (2%)	50	68
40	1o	110/120 (92%)	107 (97%)	3 (3%)	39	62
41	1p	154/156 (99%)	149 (97%)	5 (3%)	34	59
42	1q	131/131 (100%)	125 (95%)	6 (5%)	24	50
43	1r	85/98 (87%)	82 (96%)	3 (4%)	32	57
44	1s	44/351 (12%)	41 (93%)	3 (7%)	14	40
All	All	7219/8272 (87%)	6864 (95%)	355 (5%)	24	48

All (355) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	15	SER
1	1A	28	ASN
1	1A	31	SER
1	1A	53	MET
1	1A	71	LEU
1	1A	84	LEU
1	1A	101	SER
2	1B	30	VAL
2	1B	93	THR
2	1B	152	THR
2	1B	160	ILE
3	1C	7	THR
3	1C	33	LEU
3	1C	43	SER
3	1C	97	LEU
3	1C	123	VAL
3	1C	172	VAL
3	1C	188	VAL
3	1C	199	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	1C	201	SER
4	1D	18	VAL
4	1D	47	LEU
4	1D	61	VAL
4	1D	76	CYS
4	1D	128	ILE
4	1D	199	VAL
4	1D	205	LEU
4	1D	215	SER
4	1D	219	SER
4	1D	246	THR
4	1D	256	SER
4	1D	323	ILE
4	1D	324	LYS
4	1D	325	VAL
4	1D	351	LEU
4	1D	384	SER
4	1D	411	LEU
4	1D	414	VAL
4	1D	428	VAL
5	1E	53	LEU
5	1E	61	LEU
5	1E	105	THR
5	1E	114	ASP
5	1E	217	LEU
6	1F	63	SER
6	1F	110	ILE
6	1F	119	VAL
6	1F	177	VAL
6	1F	207	PRO
6	1F	212	ASP
6	1F	218	CYS
6	1F	225	VAL
6	1F	272	MET
6	1F	307	ILE
6	1F	312	CYS
6	1F	336	VAL
6	1F	399	ILE
7	1G	33	VAL
7	1G	53	ARG
7	1G	65	VAL
7	1G	123	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	1G	131	LEU
7	1G	140	LYS
7	1G	148	THR
7	1G	174	THR
7	1G	185	THR
7	1G	215	PHE
7	1G	222	THR
7	1G	227	SER
7	1G	236	SER
7	1G	284	ILE
7	1G	290	LEU
7	1G	291	LEU
7	1G	323	VAL
7	1G	340	SER
7	1G	351	THR
7	1G	366	THR
7	1G	375	ASP
7	1G	377	ILE
7	1G	398	SER
7	1G	404	LEU
7	1G	420	ASP
7	1G	467	LEU
7	1G	477	ILE
7	1G	480	SER
7	1G	531	CYS
7	1G	532	ILE
7	1G	536	ASP
7	1G	558	ASP
7	1G	583	THR
7	1G	632	ARG
7	1G	649	SER
7	1G	652	VAL
7	1G	662	VAL
7	1G	669	LYS
7	1G	698	VAL
7	1G	700	GLU
8	1H	14	LEU
8	1H	17	VAL
8	1H	68	ILE
8	1H	79	LEU
8	1H	111	LEU
8	1H	129	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1H	170	GLU
8	1H	178	SER
8	1H	198	PHE
8	1H	212	ASN
8	1H	233	MET
8	1H	240	ILE
8	1H	276	SER
9	1I	18	THR
9	1I	31	VAL
9	1I	69	ARG
9	1I	97	GLU
9	1I	104	ARG
9	1I	143	THR
10	1J	60	TYR
10	1J	66	VAL
10	1J	70	TYR
10	1J	111	GLU
10	1J	130	THR
10	1J	135	PHE
10	1J	157	THR
10	1J	161	LEU
10	1J	165	VAL
11	1K	31	LEU
11	1K	45	THR
11	1K	54	THR
11	1K	77	LEU
11	1K	83	ASN
11	1K	93	LEU
12	1L	30	ASN
12	1L	31	LEU
12	1L	36	VAL
12	1L	49	VAL
12	1L	71	LEU
12	1L	73	THR
12	1L	86	SER
12	1L	110	SER
12	1L	111	ASP
12	1L	125	LEU
12	1L	126	ILE
12	1L	206	ASN
12	1L	216	LEU
12	1L	244	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	1L	248	HIS
12	1L	253	VAL
12	1L	277	THR
12	1L	294	THR
12	1L	295	GLN
12	1L	298	ILE
12	1L	356	ILE
12	1L	404	THR
12	1L	405	ASN
12	1L	407	TRP
12	1L	443	ILE
12	1L	476	THR
12	1L	481	THR
12	1L	494	THR
12	1L	502	LEU
12	1L	553	LEU
12	1L	556	ILE
12	1L	557	TRP
12	1L	565	THR
12	1L	581	LYS
12	1L	585	LYS
13	1M	41	LEU
13	1M	54	LEU
13	1M	55	THR
13	1M	62	SER
13	1M	80	SER
13	1M	84	LEU
13	1M	88	THR
13	1M	116	ILE
13	1M	143	LEU
13	1M	183	SER
13	1M	195	MET
13	1M	225	ILE
13	1M	291	VAL
13	1M	297	VAL
13	1M	321	LEU
13	1M	322	THR
13	1M	346	ARG
13	1M	350	THR
13	1M	373	ILE
13	1M	394	ILE
13	1M	413	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	1M	421	HIS
14	1N	96	THR
14	1N	115	VAL
14	1N	146	SER
14	1N	162	ILE
14	1N	178	ILE
14	1N	198	THR
14	1N	201	THR
14	1N	217	MET
14	1N	241	THR
14	1N	267	ILE
14	1N	277	ILE
14	1N	282	MET
14	1N	323	MET
14	1N	328	THR
14	1N	335	LEU
14	1N	337	LEU
14	1N	345	SER
15	1O	1	LEU
15	1O	6	LEU
15	1O	24	VAL
15	1O	41	GLU
15	1O	70	ASP
15	1O	122	VAL
15	1O	235	VAL
15	1O	250	ASP
15	1O	283	THR
15	1O	299	LEU
16	1P	14	SER
16	1P	43	SER
16	1P	101	THR
16	1P	109	VAL
16	1P	140	LYS
16	1P	156	VAL
16	1P	171	ILE
16	1P	184	SER
16	1P	193	LEU
16	1P	220	ASP
16	1P	242	VAL
16	1P	280	THR
16	1P	323	THR
16	1P	340	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
17	1Q	13	VAL
17	1Q	47	SER
17	1Q	49	VAL
17	1Q	52	THR
17	1Q	74	SER
17	1Q	84	LEU
17	1Q	85	THR
17	1Q	105	VAL
17	1Q	117	SER
18	1R	14	THR
18	1R	50	SER
18	1R	58	SER
18	1R	71	VAL
18	1R	79	THR
18	1R	81	THR
19	1S	25	ARG
19	1S	29	SER
19	1S	84	ASP
19	1S	87	THR
20	1T	6	LEU
20	1T	19	LEU
21	1V	33	VAL
21	1V	48	GLU
21	1V	97	LYS
21	1V	115	ILE
22	1W	17	VAL
22	1W	51	GLN
22	1W	83	VAL
22	1W	101	THR
23	1X	4	VAL
23	1X	8	THR
23	1X	91	SER
23	1X	127	VAL
23	1X	130	VAL
23	1X	131	LYS
23	1X	164	SER
23	1X	170	THR
24	1Y	3	THR
24	1Y	15	THR
24	1Y	36	SER
24	1Y	68	ILE
24	1Y	91	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
25	1Z	4	SER
25	1Z	10	MET
25	1Z	86	MET
25	1Z	100	ASP
25	1Z	113	THR
25	1Z	117	VAL
25	1Z	121	MET
25	1Z	137	THR
26	1a	38	VAL
26	1a	63	THR
27	1b	18	LEU
27	1b	27	LEU
27	1b	39	ASN
27	1b	76	SER
27	1b	78	GLU
29	1d	3	SER
29	1d	40	CYS
29	1d	53	VAL
29	1d	54	VAL
29	1d	100	ASP
30	1e	18	THR
30	1e	87	LYS
30	1e	96	HIS
31	1f	1	MET
31	1f	26	LEU
31	1f	28	ARG
32	1g	23	THR
32	1g	40	LYS
32	1g	74	SER
32	1g	91	ARG
32	1g	114	ASP
32	1g	116	ASN
33	1h	47	ILE
33	1h	97	GLU
33	1h	114	MET
33	1h	127	THR
33	1h	140	THR
34	1i	33	VAL
34	1i	43	GLU
34	1i	50	LEU
34	1i	78	VAL
34	1i	86	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
34	1i	92	LYS
34	1i	103	ILE
35	1j	7	ILE
35	1j	10	ARG
35	1j	18	THR
35	1j	19	ARG
35	1j	63	GLU
35	1j	64	LEU
36	1k	46	ARG
36	1k	51	ARG
36	1k	85	TYR
37	1l	5	THR
37	1l	16	THR
37	1l	53	ARG
37	1l	83	MET
37	1l	156	TYR
37	1l	157	GLU
38	1m	10	LEU
38	1m	65	ILE
39	1n	10	THR
39	1n	98	VAL
39	1n	109	SER
40	1o	19	LEU
40	1o	27	ASP
40	1o	118	GLU
41	1p	30	THR
41	1p	31	TYR
41	1p	58	ASN
41	1p	89	MET
41	1p	161	ARG
42	1q	95	ASP
42	1q	104	THR
42	1q	120	THR
42	1q	125	VAL
42	1q	129	THR
42	1q	142	THR
43	1r	7	ILE
43	1r	24	GLN
43	1r	106	SER
44	1s	36	SER
44	1s	60	LYS
44	1s	72	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	10	ASN
3	1C	27	GLN
3	1C	46	ASN
3	1C	128	ASN
4	1D	3	GLN
4	1D	129	GLN
4	1D	280	GLN
6	1F	148	ASN
6	1F	416	GLN
7	1G	16	GLN
7	1G	43	HIS
7	1G	237	ASN
7	1G	308	GLN
7	1G	392	ASN
7	1G	459	GLN
7	1G	655	GLN
8	1H	47	GLN
8	1H	287	HIS
9	1I	156	ASN
12	1L	274	GLN
12	1L	603	ASN
13	1M	138	ASN
13	1M	168	GLN
13	1M	192	ASN
13	1M	213	HIS
13	1M	422	HIS
14	1N	120	GLN
14	1N	150	ASN
14	1N	235	ASN
14	1N	322	GLN
15	1O	72	GLN
15	1O	76	ASN
15	1O	107	GLN
15	1O	114	HIS
15	1O	167	HIS
15	1O	184	GLN
15	1O	271	ASN
16	1P	2	HIS
16	1P	260	HIS
17	1Q	121	ASN
19	1S	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	1T	35	HIS
21	1V	52	ASN
21	1V	70	GLN
22	1W	26	ASN
23	1X	15	GLN
23	1X	63	ASN
25	1Z	90	ASN
28	1c	35	HIS
29	1d	61	GLN
30	1e	44	HIS
31	1f	13	HIS
32	1g	36	ASN
32	1g	41	ASN
32	1g	57	ASN
32	1g	116	ASN
34	1i	51	GLN
36	1k	90	GLN
37	1l	78	HIS
38	1m	78	ASN
39	1n	25	HIS
39	1n	65	GLN
39	1n	74	GLN
39	1n	77	GLN
40	1o	64	GLN
41	1p	133	GLN
42	1q	113	HIS
42	1q	135	GLN
43	1r	46	HIS
43	1r	109	GLN
44	1s	40	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
12	FME	1L	1	34,12	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
1	FME	1A	1	1	8,9,10	0.53	0	8,9,11	1.03	1 (12%)
8	FME	1H	1	8	8,9,10	0.54	0	8,9,11	0.97	1 (12%)
10	FME	1J	1	10	8,9,10	0.54	0	8,9,11	1.13	1 (12%)
14	FME	1N	1	14	8,9,10	0.54	0	8,9,11	0.95	1 (12%)
34	SAC	1i	1	-	7,8,9	0.53	0	7,9,11	1.54	1 (14%)
11	FME	1K	1	11	8,9,10	0.55	0	8,9,11	0.97	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	FME	1M	1	13	-	0/7/9/11	-
12	FME	1L	1	34,12	-	0/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
10	FME	1J	1	10	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
34	SAC	1i	1	-	-	5/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.97	117.14	124.77
1	1A	1	FME	O-C-CA	-2.61	118.05	124.77
11	1K	1	FME	O-C-CA	-2.55	118.21	124.77
12	1L	1	FME	O-C-CA	-2.53	118.25	124.77
10	1J	1	FME	O-C-CA	-2.53	118.26	124.77
14	1N	1	FME	O-C-CA	-2.53	118.28	124.77
8	1H	1	FME	O-C-CA	-2.52	118.28	124.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1M	1	FME	O-C-CA	-2.52	118.29	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	CB-CA-N-CN
34	1i	1	SAC	C-CA-CB-OG
34	1i	1	SAC	C2A-C1A-N-CA
34	1i	1	SAC	OAC-C1A-N-CA
34	1i	1	SAC	N-CA-CB-OG
11	1K	1	FME	N-CA-CB-CG
34	1i	1	SAC	C-CA-N-C1A

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1M	1	FME	1	0
1	1A	1	FME	1	0
8	1H	1	FME	2	0
10	1J	1	FME	4	0
34	1i	1	SAC	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 29 ligands modelled in this entry, 3 are monoatomic - leaving 26 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	SF4	1I	201	9	0,12,12	-	-	-		
48	FMN	1F	501	-	33,33,33	0.63	0	48,50,50	0.66	1 (2%)
58	EHZ	1W	201	-	31,36,37	0.20	0	36,44,47	1.05	1 (2%)
46	PC1	1d	201	29,30	38,38,53	0.32	0	44,46,61	0.48	0
45	SF4	1F	502	6	0,12,12	-	-	-		
45	SF4	1B	201	2	0,12,12	-	-	-		
47	FES	1E	301	5	0,4,4	-	-	-		
51	CDL	1O	403	14,15	66,66,99	0.98	3 (4%)	72,78,111	1.40	5 (6%)
51	CDL	1a	101	42,26	60,60,99	0.33	0	66,72,111	0.44	0
52	MYR	1L	701	-	13,14,15	0.28	0	12,13,15	0.29	0
53	3PE	1M	502	13	37,37,50	0.31	0	40,42,55	0.41	0
56	NDP	1P	501	-	51,52,52	0.52	0	71,80,80	0.78	2 (2%)
46	PC1	1L	702	-	45,45,53	0.29	0	51,53,61	0.34	0
46	PC1	1M	501	-	34,34,53	0.32	0	40,42,61	0.38	0
45	SF4	1G	801	7	0,12,12	-	-	-		
58	EHZ	1n	201	-	31,36,37	0.26	0	36,44,47	0.97	1 (2%)
46	PC1	1B	202	2	33,33,53	0.33	0	39,41,61	0.34	0
50	U10	1H	701	-	63,63,63	0.60	2 (3%)	78,79,79	0.76	4 (5%)
47	FES	1G	804	7	0,4,4	-	-	-		
53	3PE	1Y	201	24	34,34,50	0.47	0	37,39,55	0.89	2 (5%)
46	PC1	1f	101	31	24,24,53	0.36	0	30,32,61	0.65	0
45	SF4	1I	202	9	0,12,12	-	-	-		
45	SF4	1G	802	7	0,12,12	-	-	-		
46	PC1	1q	201	42	47,47,53	0.29	0	53,55,61	0.32	0
54	GTP	1O	401	55	33,34,34	0.60	0	50,54,54	0.64	0
51	CDL	1H	702	8	50,50,99	0.36	0	56,62,111	0.60	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	1I	201	9	-	-	0/6/5/5
48	FMN	1F	501	-	-	3/18/18/18	0/3/3/3
58	EHZ	1W	201	-	-	4/42/44/45	-
46	PC1	1d	201	29,30	-	11/42/42/57	-
45	SF4	1F	502	6	-	-	0/6/5/5
45	SF4	1B	201	2	-	-	0/6/5/5
47	FES	1E	301	5	-	-	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	CDL	1O	403	14,15	-	13/76/76/110	-
51	CDL	1a	101	42,26	-	2/71/71/110	-
52	MYR	1L	701	-	-	3/12/12/13	-
56	NDP	1P	501	-	-	4/34/77/77	0/5/5/5
53	3PE	1M	502	13	-	4/41/41/54	-
46	PC1	1L	702	-	-	7/49/49/57	-
46	PC1	1M	501	-	-	3/38/38/57	-
45	SF4	1G	801	7	-	-	0/6/5/5
58	EHZ	1n	201	-	-	10/42/44/45	-
46	PC1	1B	202	2	-	12/37/37/57	-
50	U10	1H	701	-	-	22/63/87/87	0/1/1/1
47	FES	1G	804	7	-	-	0/1/1/1
53	3PE	1Y	201	24	-	11/38/38/54	-
46	PC1	1f	101	31	-	4/27/27/57	-
45	SF4	1I	202	9	-	-	0/6/5/5
45	SF4	1G	802	7	-	-	0/6/5/5
46	PC1	1q	201	42	-	9/51/51/57	-
54	GTP	1O	401	55	-	0/22/38/38	0/3/3/3
51	CDL	1H	702	8	-	8/61/61/110	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	1O	403	CDL	C71-CB7	5.28	1.66	1.50
51	1O	403	CDL	OB9-CB7	4.74	1.36	1.22
50	1H	701	U10	C4-C5	-2.58	1.41	1.48
50	1H	701	U10	C4-C3	2.07	1.43	1.36
51	1O	403	CDL	OB8-CB7	2.05	1.39	1.33

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1O	403	CDL	OB8-CB7-C71	-7.24	89.76	111.83
58	1W	201	EHZ	C10-S1-C9	5.85	119.14	101.84
51	1O	403	CDL	OB8-CB7-OB9	5.58	137.58	123.63
58	1n	201	EHZ	C10-S1-C9	5.38	117.73	101.84
51	1O	403	CDL	OB8-CB6-CB4	5.17	123.31	108.40
56	1P	501	NDP	P2B-O2B-C2B	-4.19	112.23	123.43
53	1Y	201	3PE	O21-C21-C22	3.35	118.73	111.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	1O	403	CDL	CB6-OB8-CB7	3.28	129.11	117.12
56	1P	501	NDP	O4D-C1D-C2D	-2.76	100.70	106.62
50	1H	701	U10	O4-C4-C5	-2.70	107.54	116.64
50	1H	701	U10	O3-C3-C2	2.55	125.25	116.64
51	1H	702	CDL	OB6-CB5-C51	2.55	117.00	111.48
53	1Y	201	3PE	O13-C11-C12	-2.47	100.14	109.17
50	1H	701	U10	C4-C3-C2	-2.30	116.46	120.69
50	1H	701	U10	O4-C4-C3	2.27	132.24	123.64
51	1O	403	CDL	OB9-CB7-C71	2.27	132.66	123.78
48	1F	501	FMN	C4-N3-C2	-2.09	121.93	125.64

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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
46	1L	702	PC1	C11-O13-P-O14
46	1L	702	PC1	C1-O11-P-O14
46	1M	501	PC1	O11-C1-C2-O21
46	1d	201	PC1	C11-O13-P-O12
46	1d	201	PC1	C11-O13-P-O11
46	1d	201	PC1	C12-C11-O13-P
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	C2-C1-O11-P
46	1q	201	PC1	C11-O13-P-O14
51	1H	702	CDL	C1-CA2-OA2-PA1
51	1H	702	CDL	CA3-OA5-PA1-OA2
51	1H	702	CDL	CA3-OA5-PA1-OA3
51	1H	702	CDL	OB7-CB5-OB6-CB4
51	1H	702	CDL	C51-CB5-OB6-CB4
51	1O	403	CDL	CA2-OA2-PA1-OA5
52	1L	701	MYR	O1-C1-C2-C3
53	1Y	201	3PE	O22-C21-O21-C2
53	1Y	201	3PE	C22-C21-O21-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
58	1W	201	EHZ	O2-C9-S1-C10
58	1W	201	EHZ	C8-C9-S1-C10
58	1n	201	EHZ	C12-C13-C14-N2
58	1n	201	EHZ	C18-C17-C20-O6
50	1H	701	U10	C45-C44-C46-C47
50	1H	701	U10	C15-C14-C16-C17
50	1H	701	U10	C25-C24-C26-C27
50	1H	701	U10	C35-C34-C36-C37
50	1H	701	U10	C50-C49-C51-C52
50	1H	701	U10	C13-C14-C16-C17
50	1H	701	U10	C23-C24-C26-C27
50	1H	701	U10	C33-C34-C36-C37
50	1H	701	U10	C48-C49-C51-C52
50	1H	701	U10	C43-C44-C46-C47
50	1H	701	U10	C4-C3-O3-C3M
46	1q	201	PC1	C37-C38-C39-C3A
46	1q	201	PC1	C3A-C3B-C3C-C3D
46	1d	201	PC1	C35-C36-C37-C38
50	1H	701	U10	C14-C16-C17-C18
53	1Y	201	3PE	C31-C32-C33-C34
46	1q	201	PC1	C35-C36-C37-C38
58	1n	201	EHZ	C5-C6-C7-O1
58	1n	201	EHZ	C1-C2-C3-C4
46	1d	201	PC1	C2-C1-O11-P
48	1F	501	FMN	C4'-C5'-O5'-P
51	1O	403	CDL	CA4-CA3-OA5-PA1
51	1O	403	CDL	C56-C57-C58-C59
46	1M	501	PC1	O11-C1-C2-C3
58	1n	201	EHZ	C5-C6-C7-C8
46	1L	702	PC1	C33-C34-C35-C36
46	1q	201	PC1	C31-C32-C33-C34
53	1Y	201	3PE	C32-C33-C34-C35
58	1n	201	EHZ	O3-C12-C13-C14
51	1H	702	CDL	CA4-CA3-OA5-PA1
53	1Y	201	3PE	O21-C2-C3-O31
50	1H	701	U10	C2-C3-O3-C3M
46	1L	702	PC1	C27-C28-C29-C2A
46	1q	201	PC1	C39-C3A-C3B-C3C
53	1M	502	3PE	C34-C35-C36-C37
53	1M	502	3PE	O31-C31-C32-C33
46	1B	202	PC1	C1-C2-C3-O31
46	1B	202	PC1	C12-C11-O13-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	1L	702	PC1	C12-C11-O13-P
46	1q	201	PC1	C12-C11-O13-P
50	1H	701	U10	C5-C6-C7-C8
53	1Y	201	3PE	C12-C11-O13-P
46	1L	702	PC1	O13-C11-C12-N
46	1f	101	PC1	O13-C11-C12-N
51	1O	403	CDL	CB7-C71-C72-C73
51	1a	101	CDL	C12-C13-C14-C15
56	1P	501	NDP	C2D-C1D-N1N-C2N
56	1P	501	NDP	C2D-C1D-N1N-C6N
58	1n	201	EHZ	C19-C17-C20-O6
51	1O	403	CDL	C1-CA2-OA2-PA1
46	1B	202	PC1	O21-C2-C3-O31
46	1B	202	PC1	C1-O11-P-O14
51	1H	702	CDL	CA2-OA2-PA1-OA4
51	1O	403	CDL	CA2-OA2-PA1-OA3
53	1M	502	3PE	C11-O13-P-O14
53	1Y	201	3PE	C1-O11-P-O13
53	1Y	201	3PE	C11-O13-P-O14
46	1B	202	PC1	C31-C32-C33-C34
46	1B	202	PC1	O22-C21-C22-C23
53	1Y	201	3PE	C35-C36-C37-C38
50	1H	701	U10	C30-C29-C31-C32
58	1n	201	EHZ	C7-C8-C9-O2
50	1H	701	U10	C40-C39-C41-C42
46	1B	202	PC1	O21-C21-C22-C23
51	1O	403	CDL	C55-C56-C57-C58
52	1L	701	MYR	C4-C5-C6-C7
58	1W	201	EHZ	N2-C15-C16-C17
56	1P	501	NDP	O4D-C1D-N1N-C6N
58	1n	201	EHZ	N1-C12-C13-C14
50	1H	701	U10	C28-C29-C31-C32
50	1H	701	U10	C38-C39-C41-C42
51	1O	403	CDL	OB6-CB4-CB6-OB8
50	1H	701	U10	C5-C4-O4-C4M
46	1d	201	PC1	C39-C3A-C3B-C3C
53	1Y	201	3PE	C2-C1-O11-P
46	1f	101	PC1	C11-C12-N-C15
51	1H	702	CDL	OB5-CB3-CB4-OB6
46	1f	101	PC1	C11-C12-N-C14
53	1Y	201	3PE	C1-C2-C3-O31
48	1F	501	FMN	C2'-C3'-C4'-O4'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
46	1L	702	PC1	C24-C25-C26-C27
46	1q	201	PC1	C33-C34-C35-C36
50	1H	701	U10	C41-C42-C43-C44
52	1L	701	MYR	C11-C10-C9-C8
58	1W	201	EHZ	O4-C15-C16-C17
51	1O	403	CDL	C53-C54-C55-C56
51	1O	403	CDL	CB3-CB4-CB6-OB8
58	1n	201	EHZ	C4-C5-C6-C7
46	1M	501	PC1	C31-C32-C33-C34
51	1O	403	CDL	C72-C71-CB7-OB8
48	1F	501	FMN	O3'-C3'-C4'-C5'
50	1H	701	U10	C51-C52-C53-C54
51	1O	403	CDL	C12-C11-CA5-OA6
46	1q	201	PC1	C23-C24-C25-C26
56	1P	501	NDP	O4D-C1D-N1N-C2N
53	1M	502	3PE	O21-C2-C3-O31
51	1O	403	CDL	C72-C71-CB7-OB9
50	1H	701	U10	C16-C17-C18-C19
51	1a	101	CDL	C72-C71-CB7-OB8

There are no ring outliers.

21 monomers are involved in 67 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1I	201	SF4	1	0
48	1F	501	FMN	1	0
58	1W	201	EHZ	2	0
46	1d	201	PC1	4	0
45	1F	502	SF4	3	0
51	1O	403	CDL	3	0
51	1a	101	CDL	4	0
52	1L	701	MYR	2	0
53	1M	502	3PE	4	0
56	1P	501	NDP	8	0
46	1L	702	PC1	5	0
46	1M	501	PC1	1	0
58	1n	201	EHZ	4	0
46	1B	202	PC1	2	0
50	1H	701	U10	8	0
47	1G	804	FES	1	0
53	1Y	201	3PE	7	0
46	1f	101	PC1	3	0

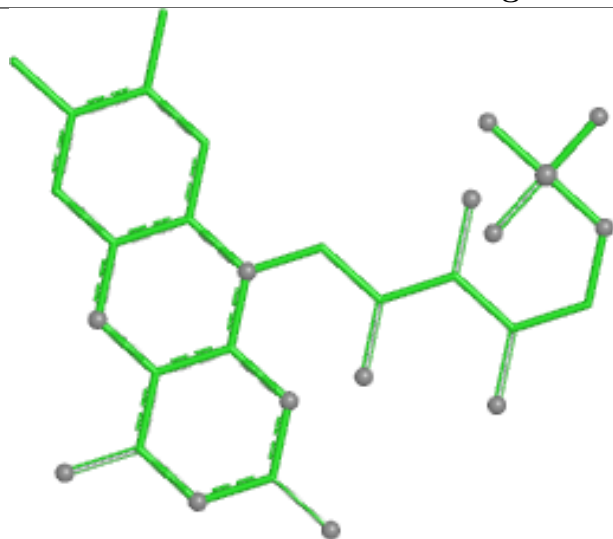
Continued on next page...

Continued from previous page...

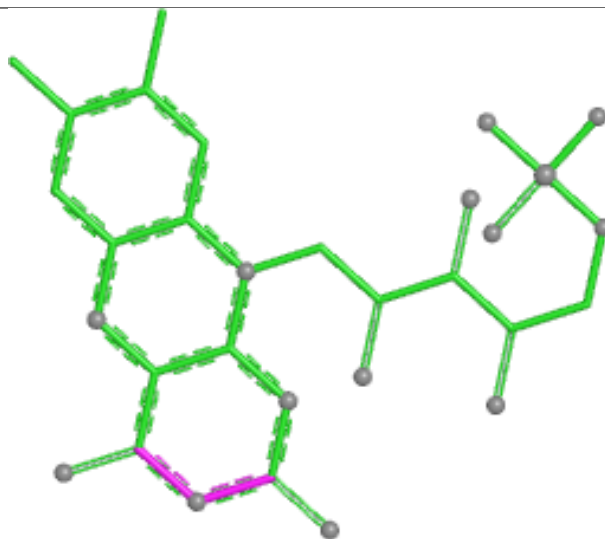
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1q	201	PC1	1	0
54	1O	401	GTP	1	0
51	1H	702	CDL	2	0

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.

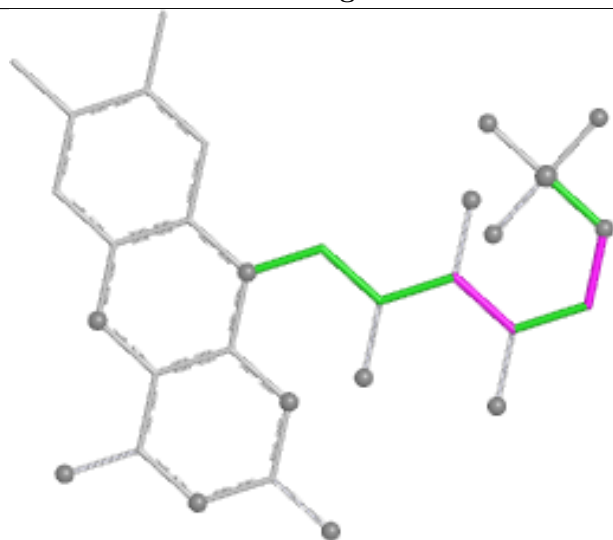
Ligand FMN 1F 501



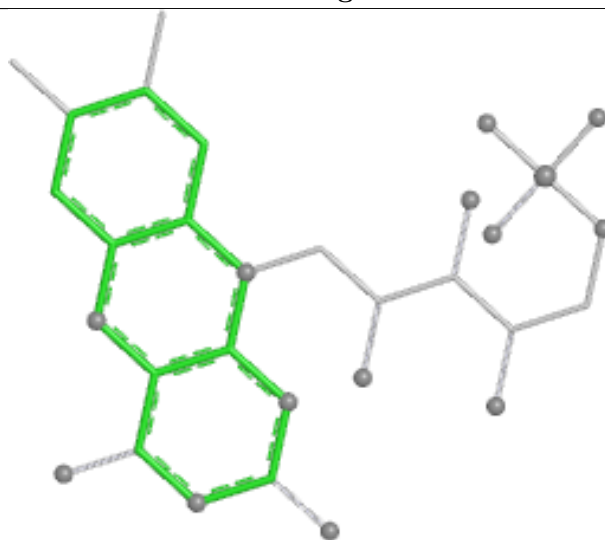
Bond lengths



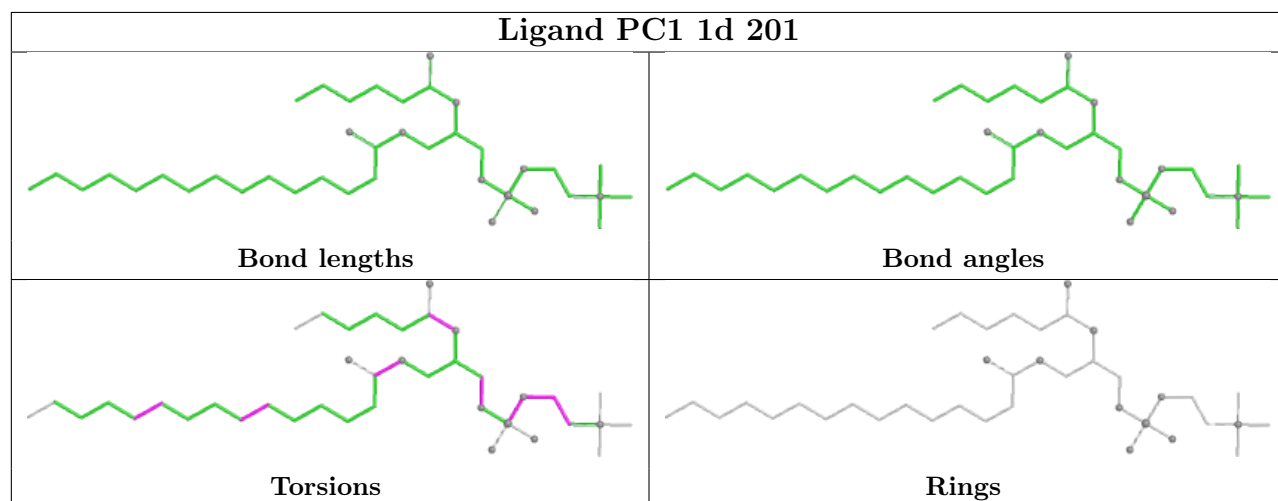
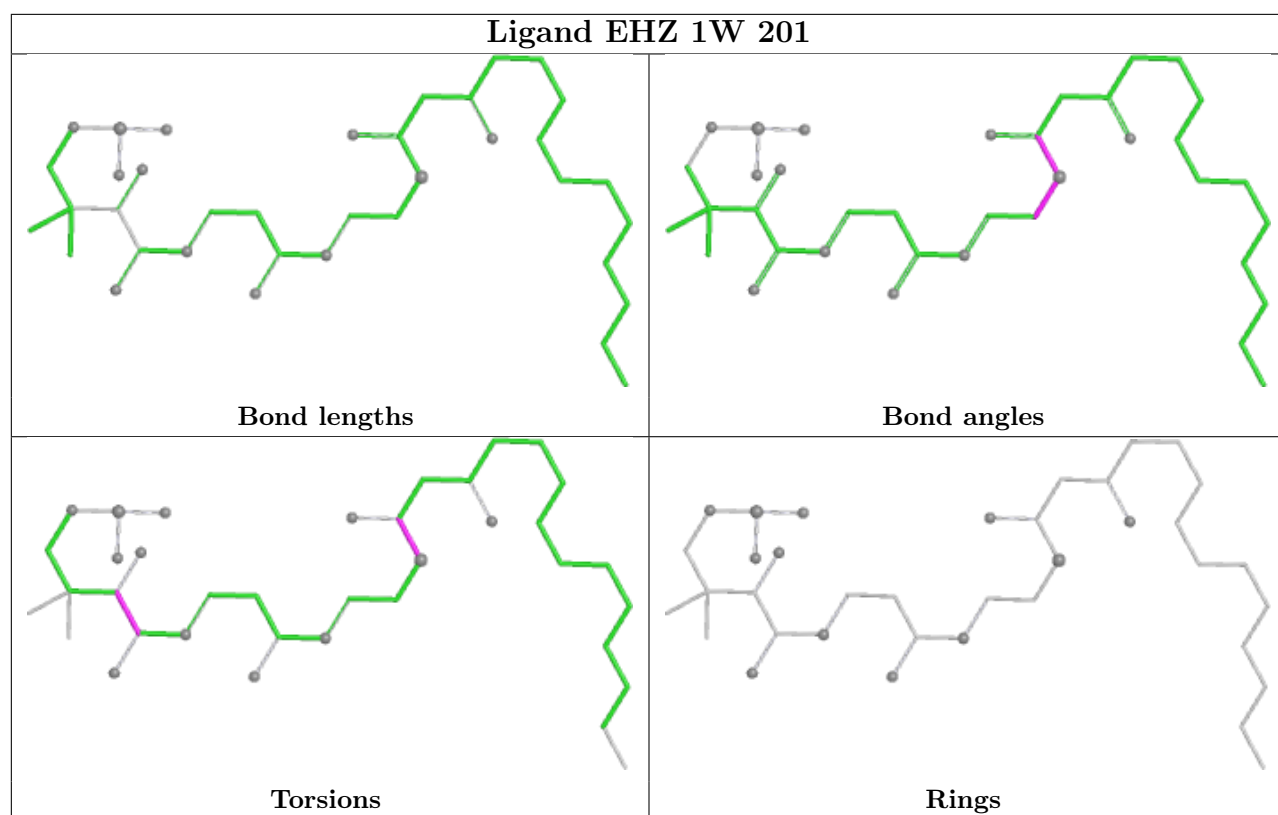
Bond angles

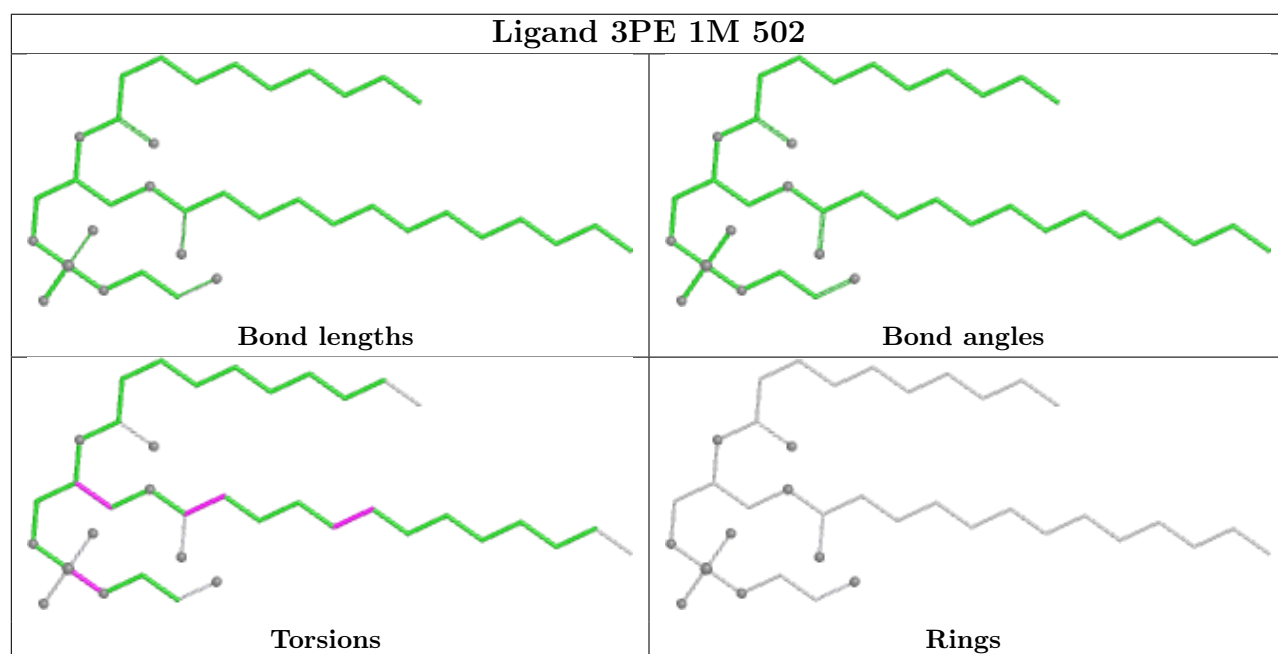
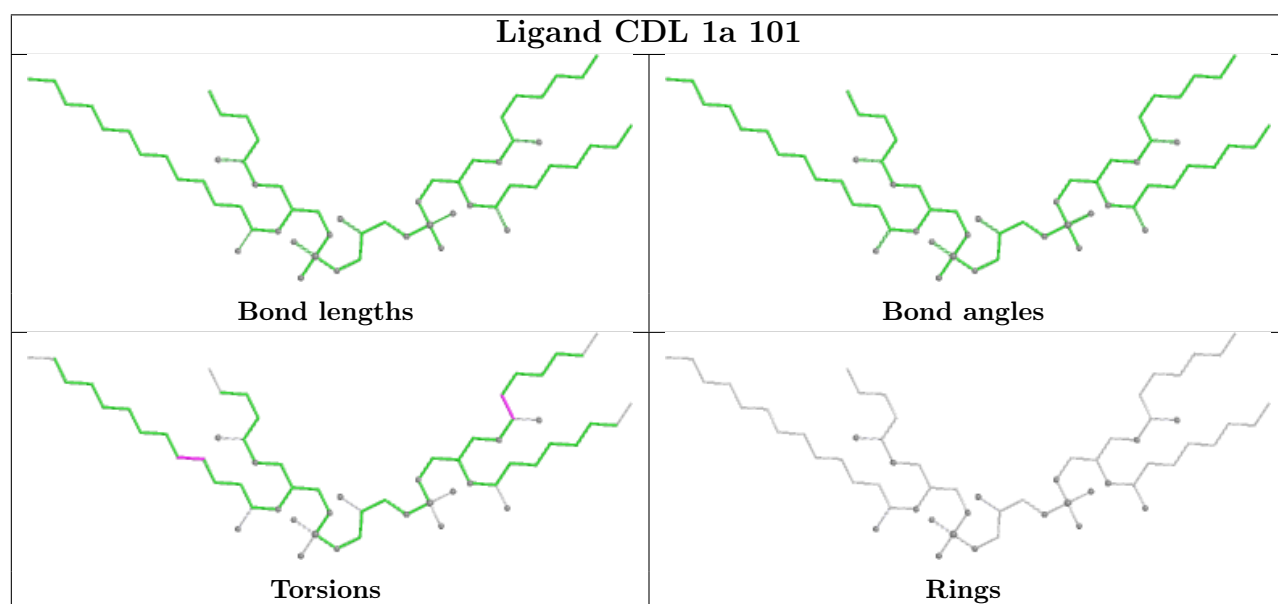
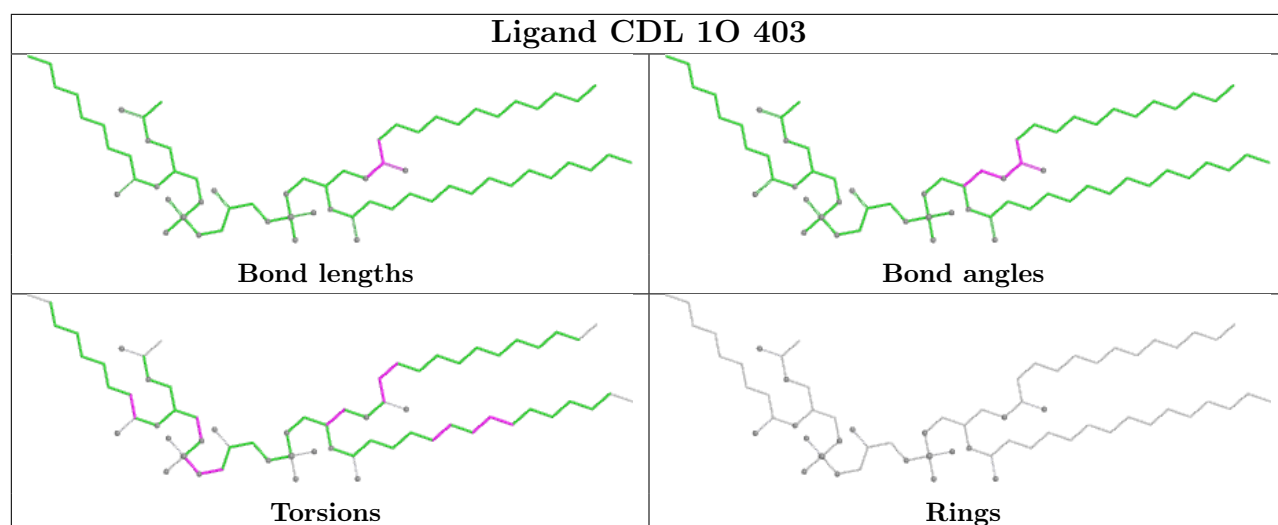


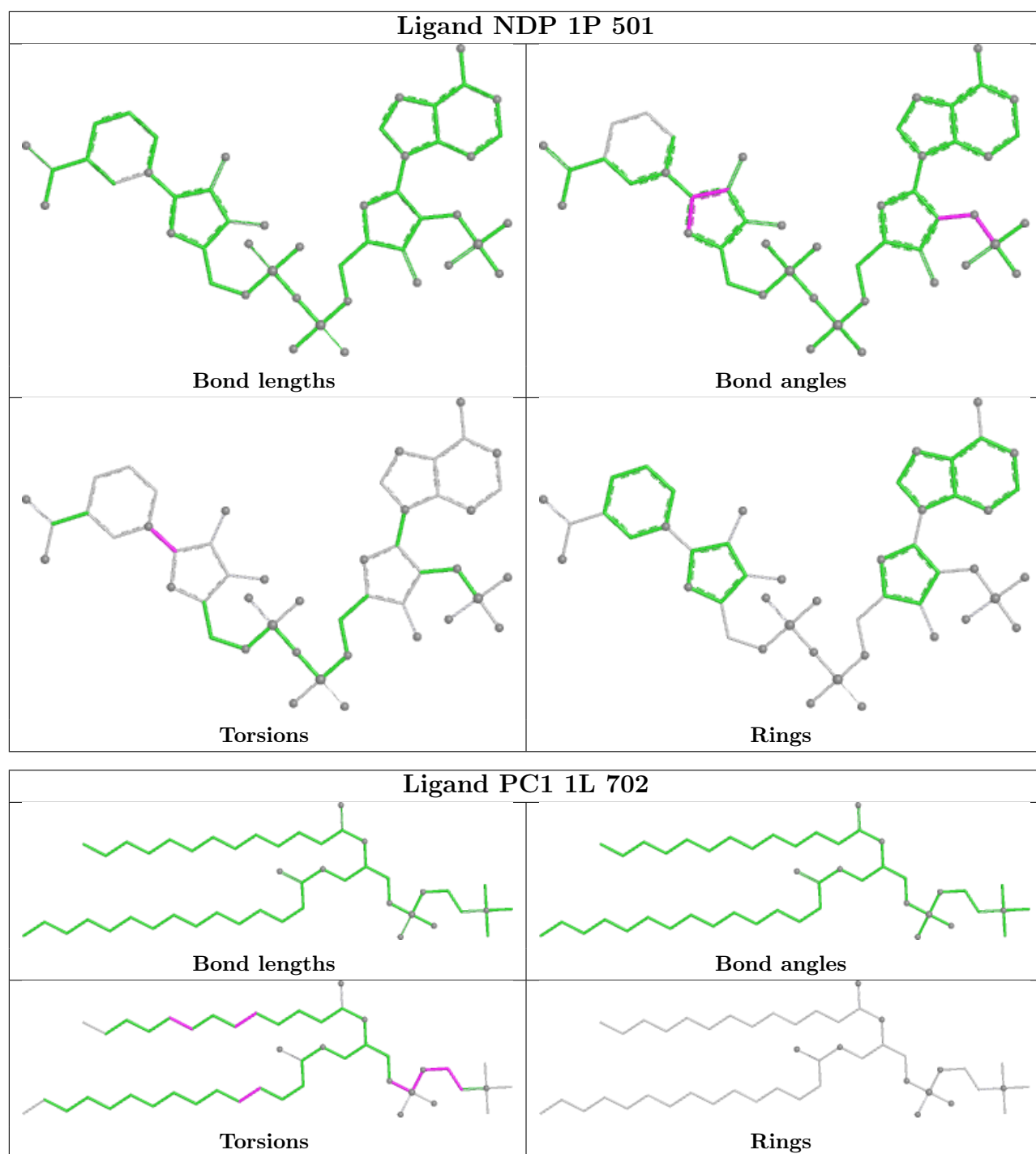
Torsions

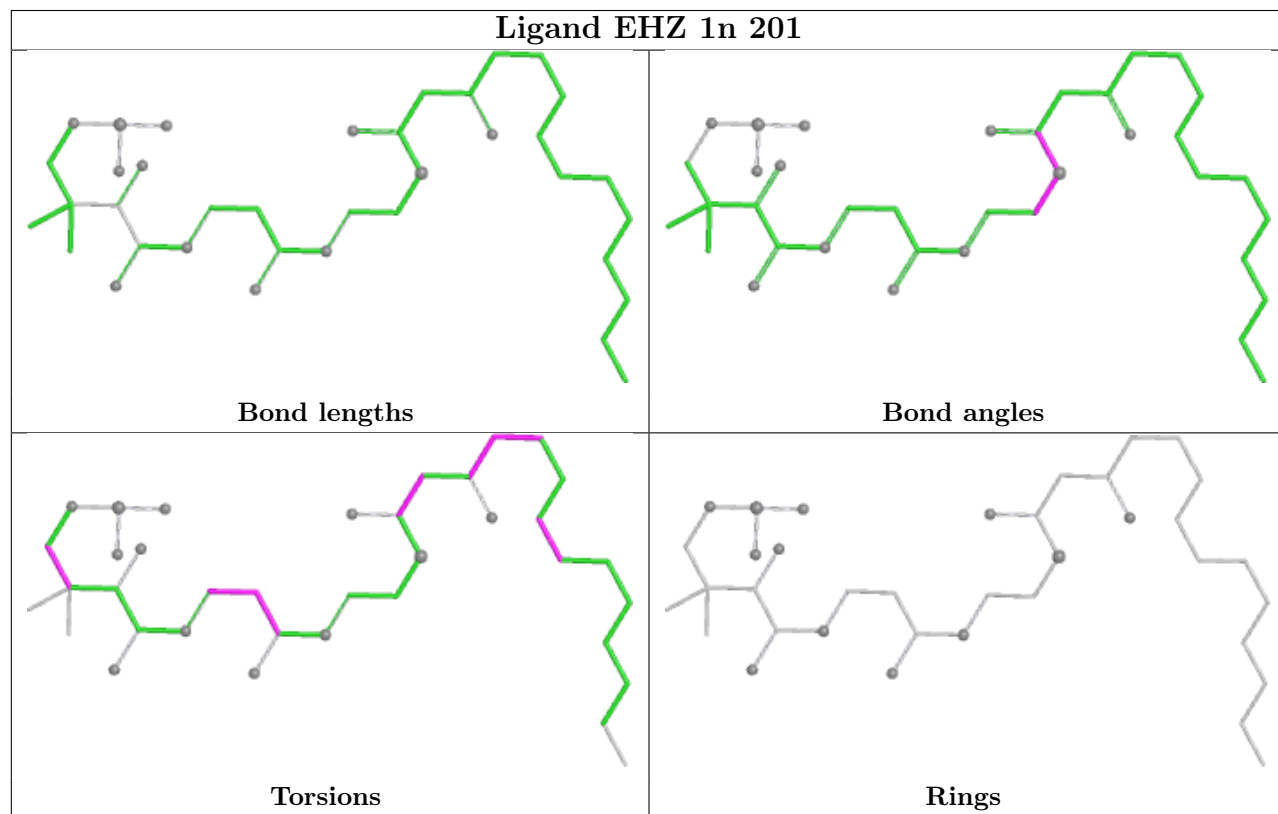
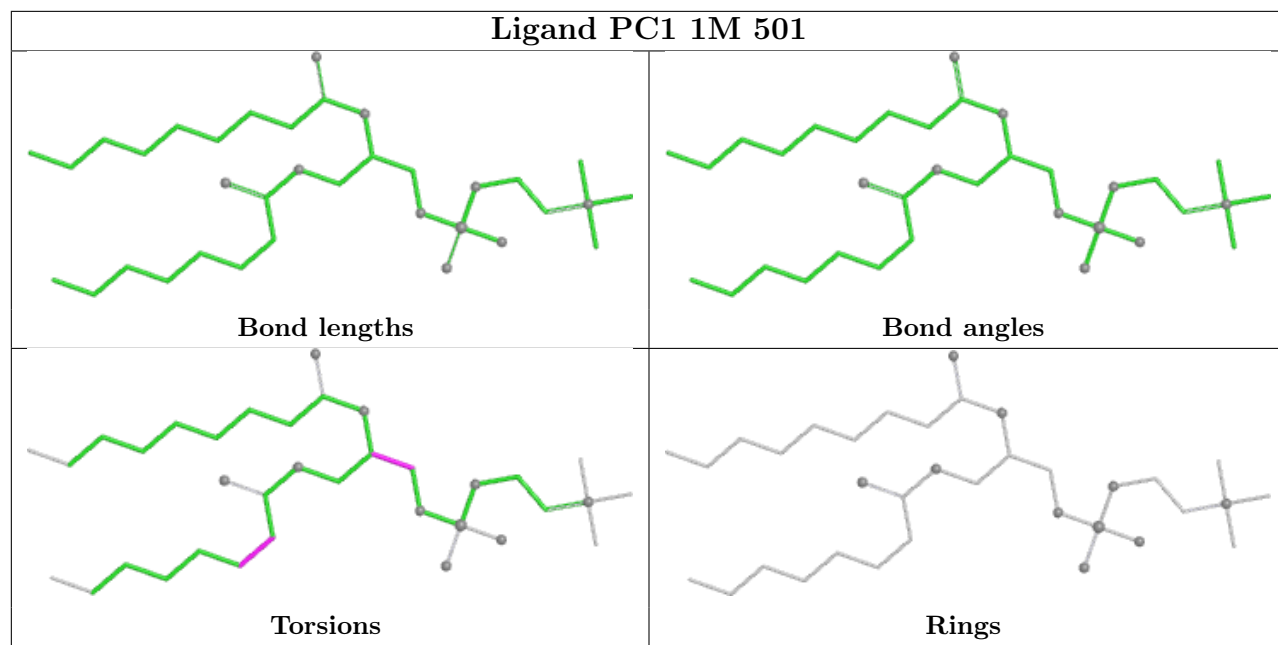


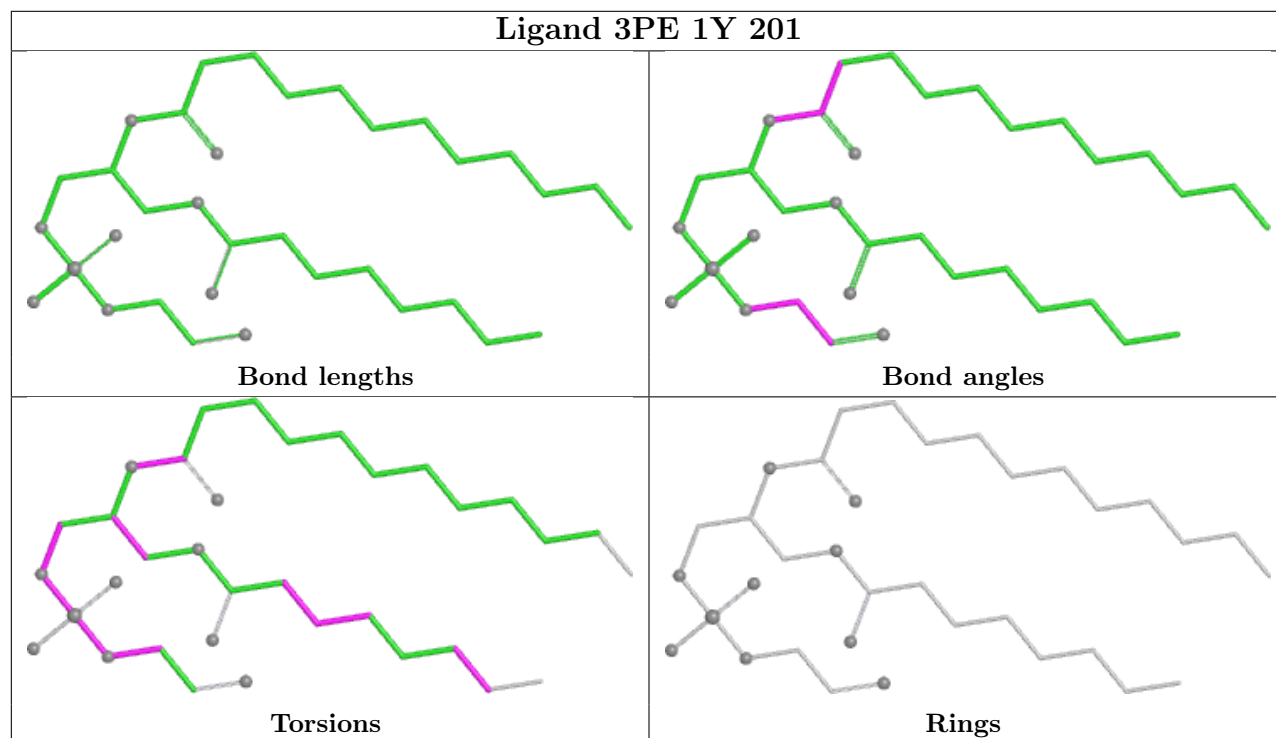
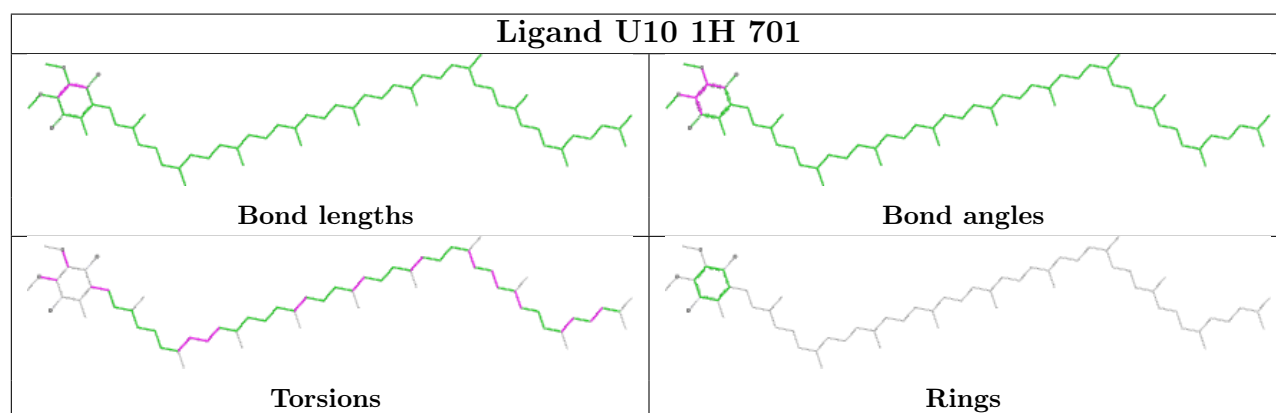
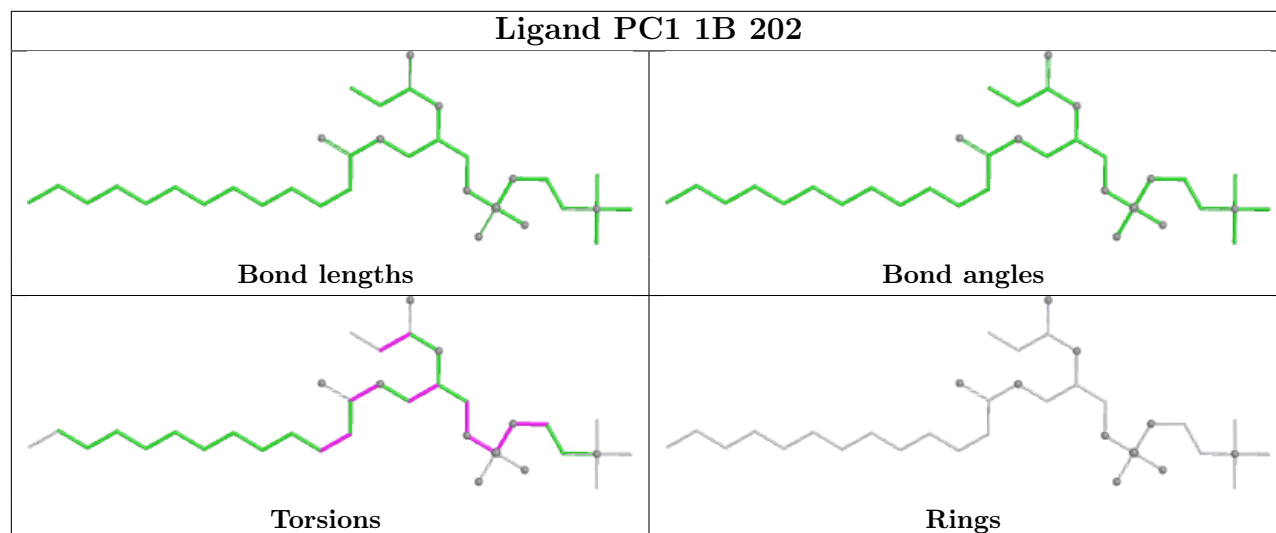
Rings

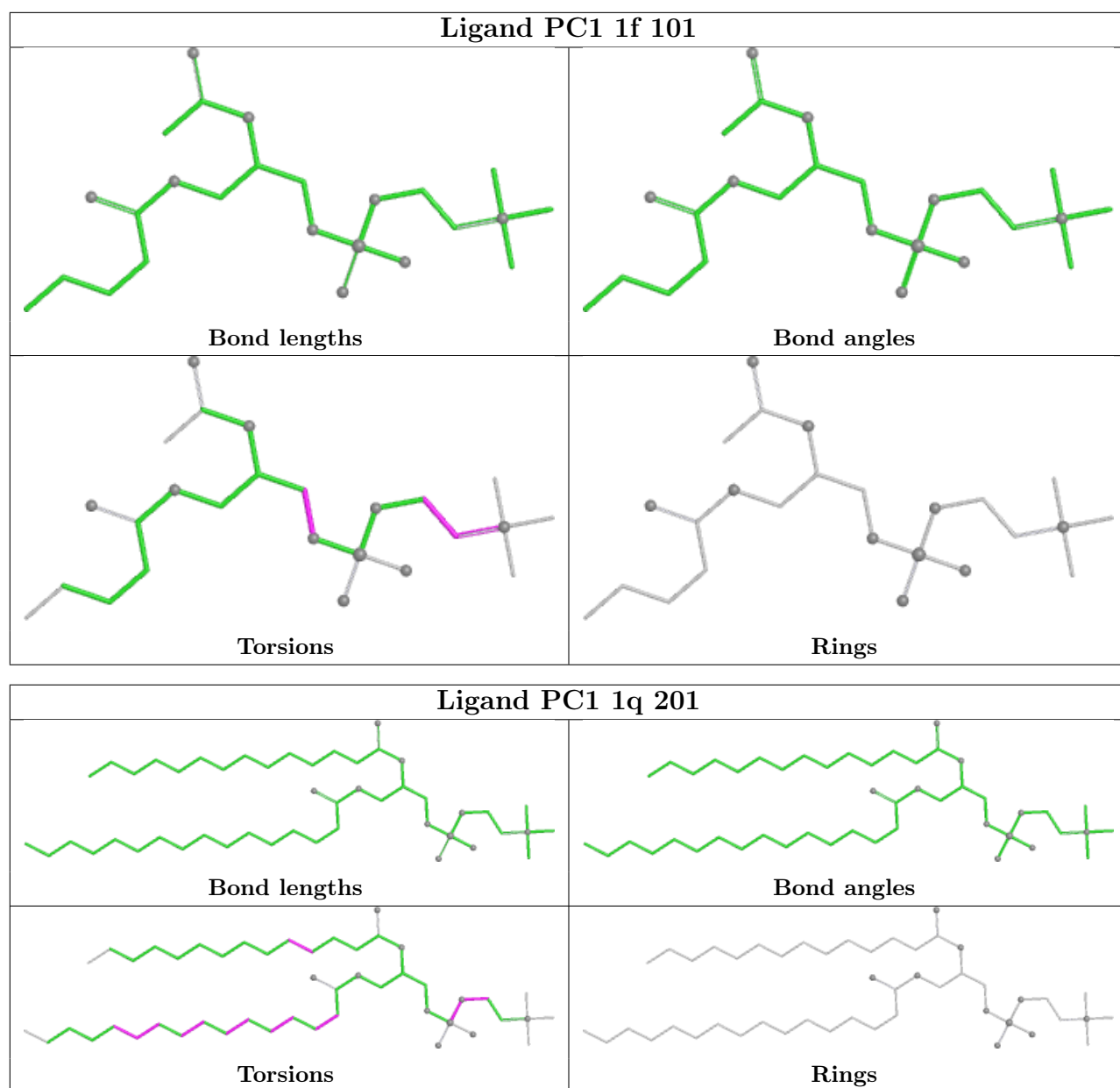


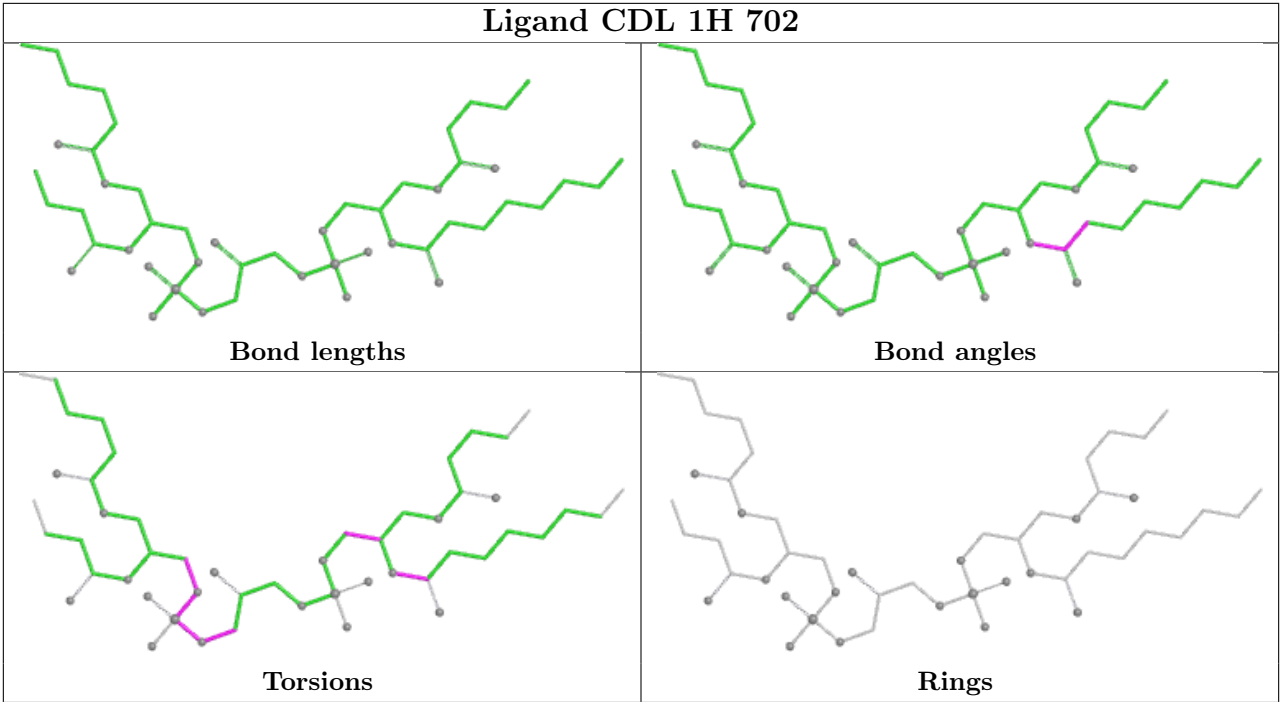












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	6.44
1	1i	1:SAC	C	2:GLY	N	3.63

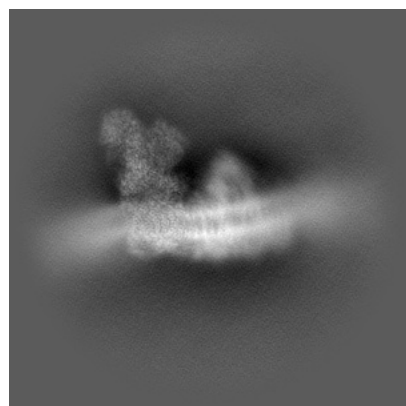
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42176. These allow visual inspection of the internal detail of the map and identification of artifacts.

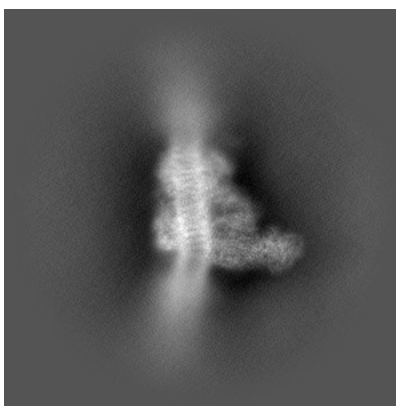
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

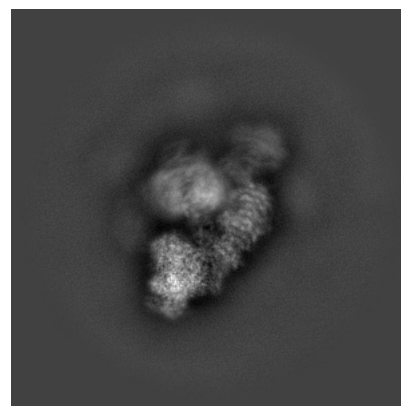
6.1.1 Primary map



X

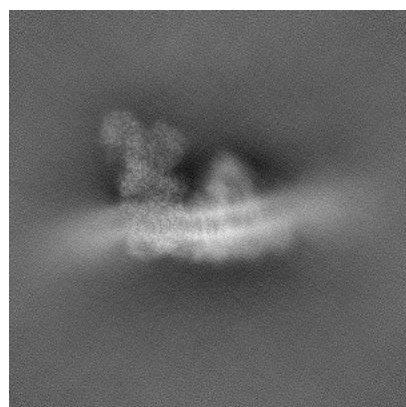


Y

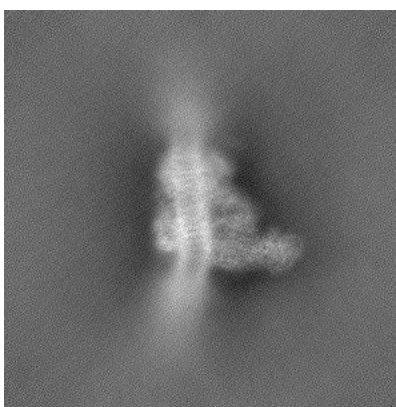


Z

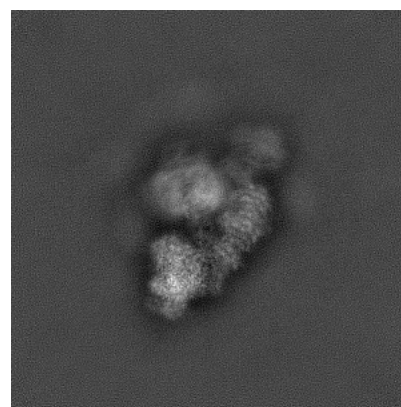
6.1.2 Raw map



X



Y

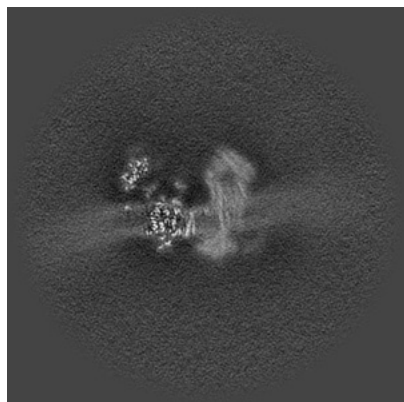


Z

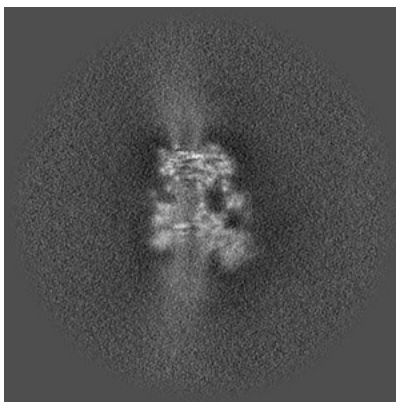
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

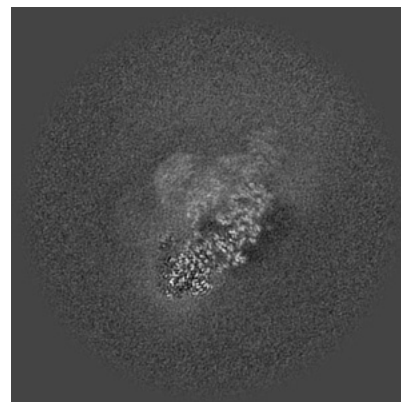
6.2.1 Primary map



X Index: 200

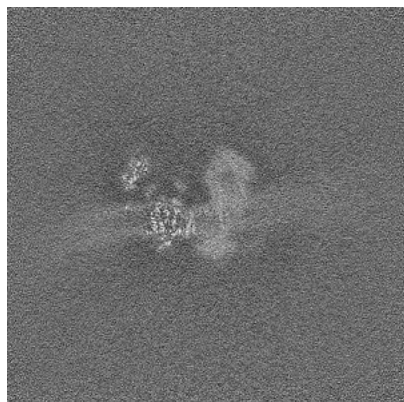


Y Index: 200

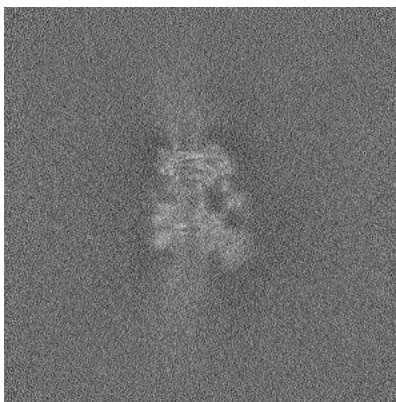


Z Index: 200

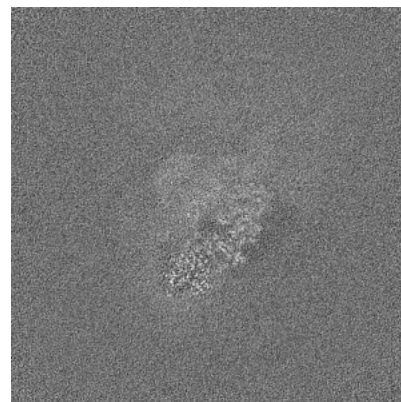
6.2.2 Raw map



X Index: 200



Y Index: 200

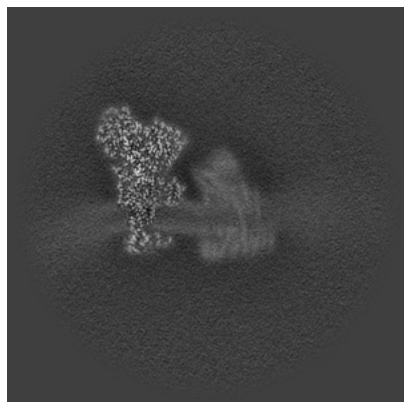


Z Index: 200

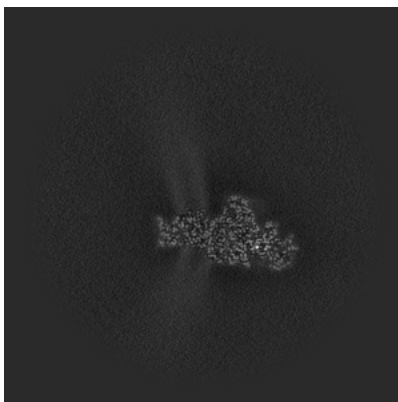
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

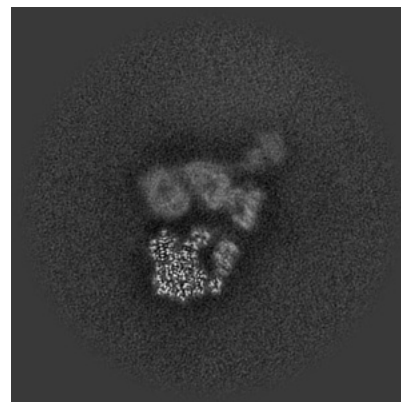
6.3.1 Primary map



X Index: 163

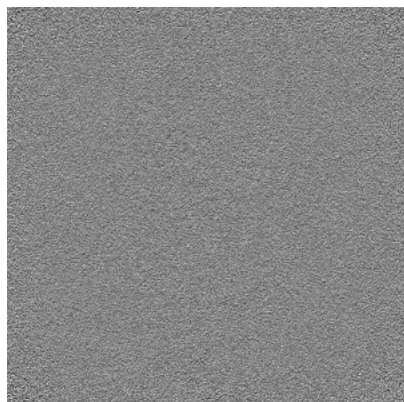


Y Index: 127

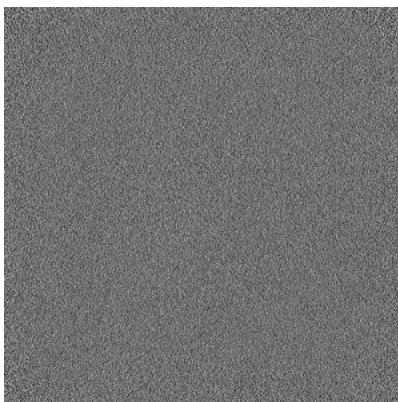


Z Index: 225

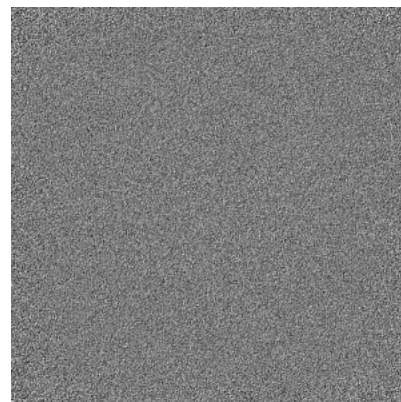
6.3.2 Raw map



X Index: 0



Y Index: 0

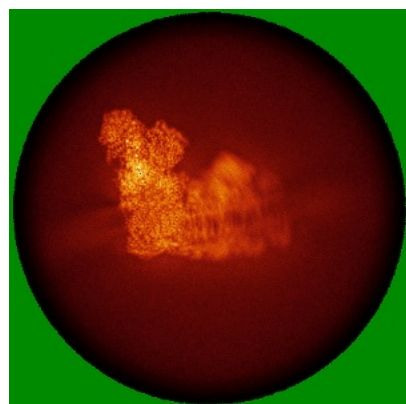


Z Index: 0

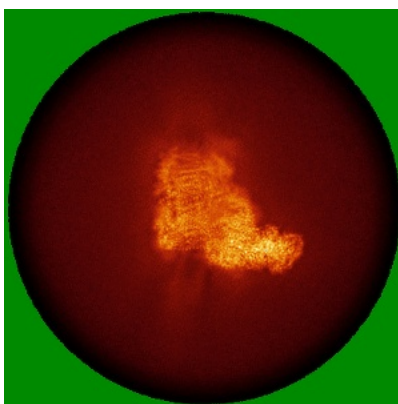
The images above show the largest variance slices of the map in three orthogonal directions.

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

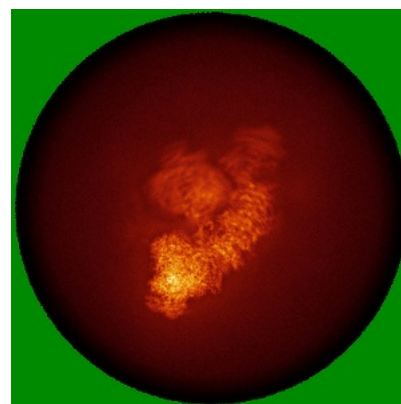
6.4.1 Primary map



X

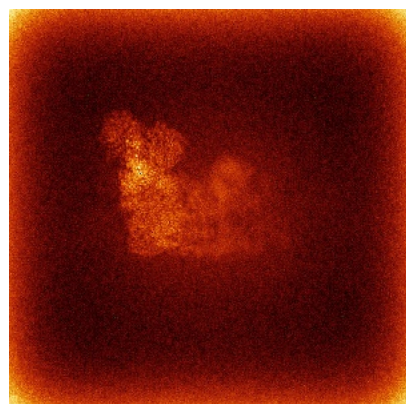


Y

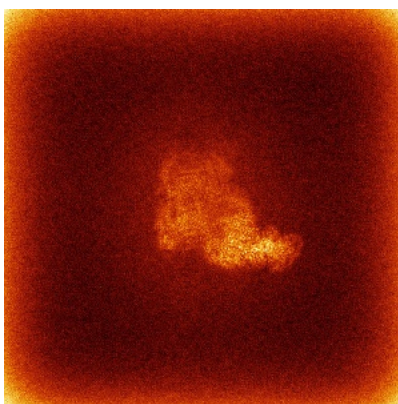


Z

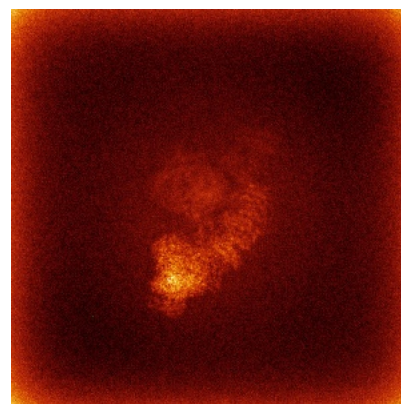
6.4.2 Raw map



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.

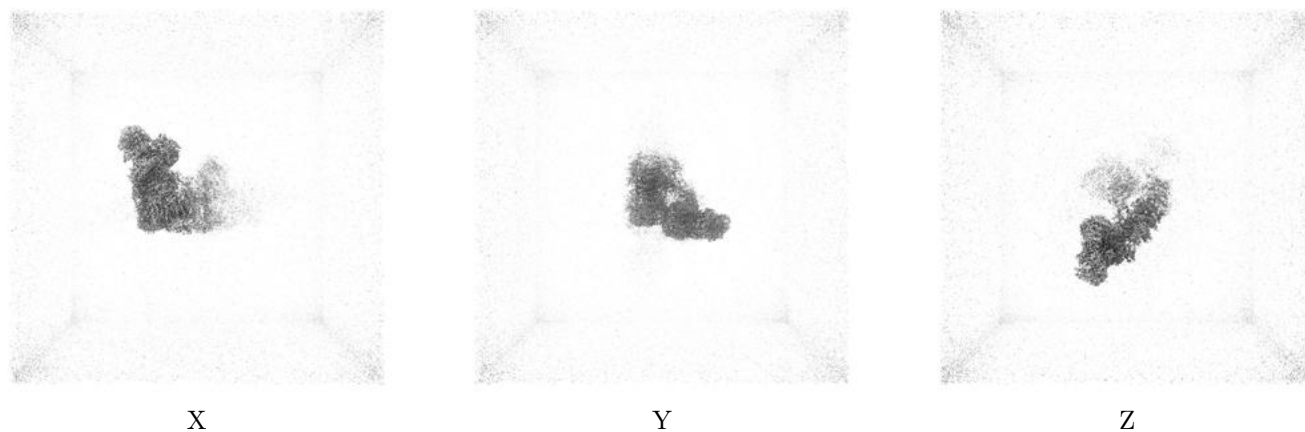
6.5 Orthogonal surface views [i](#)

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.

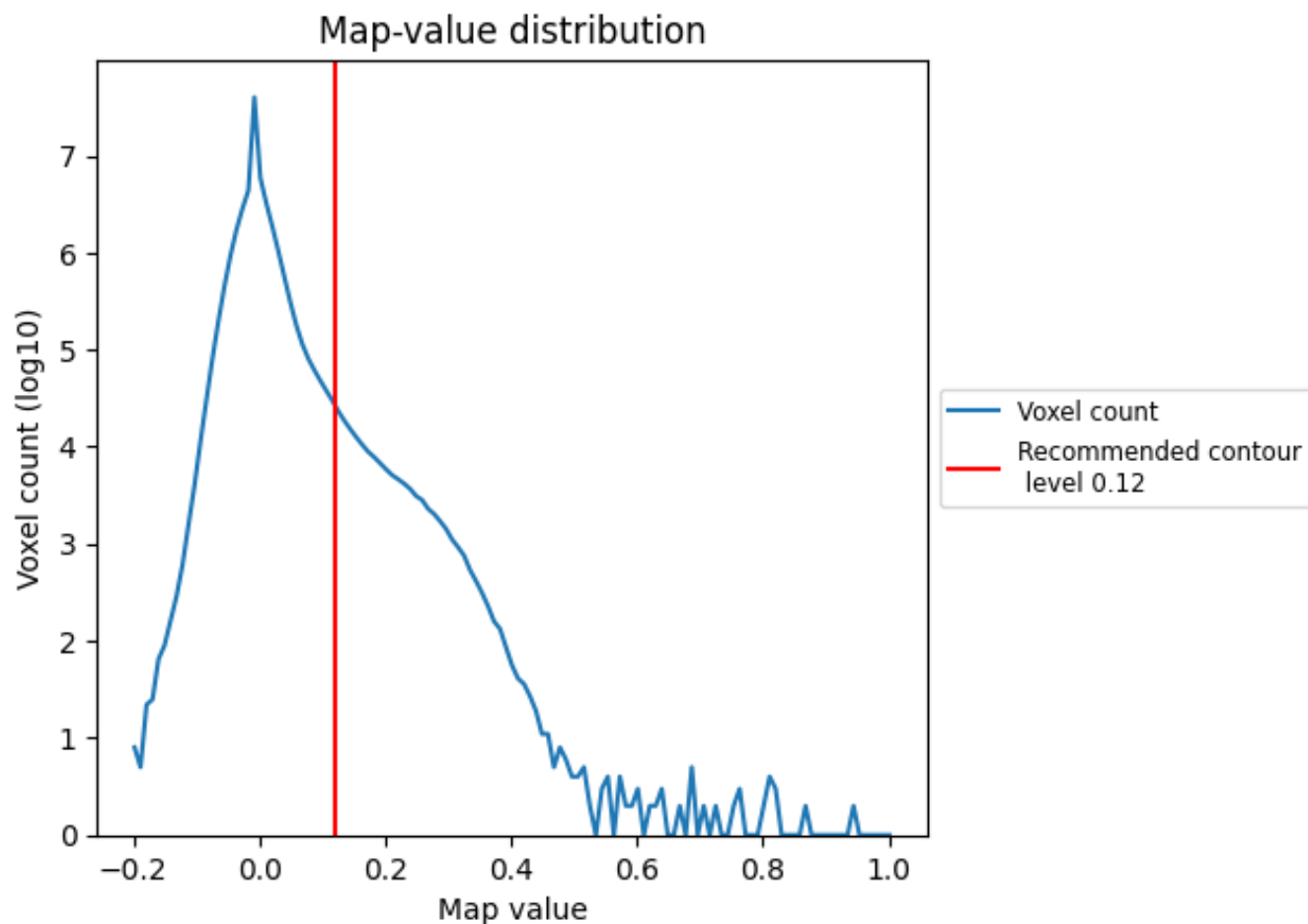
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

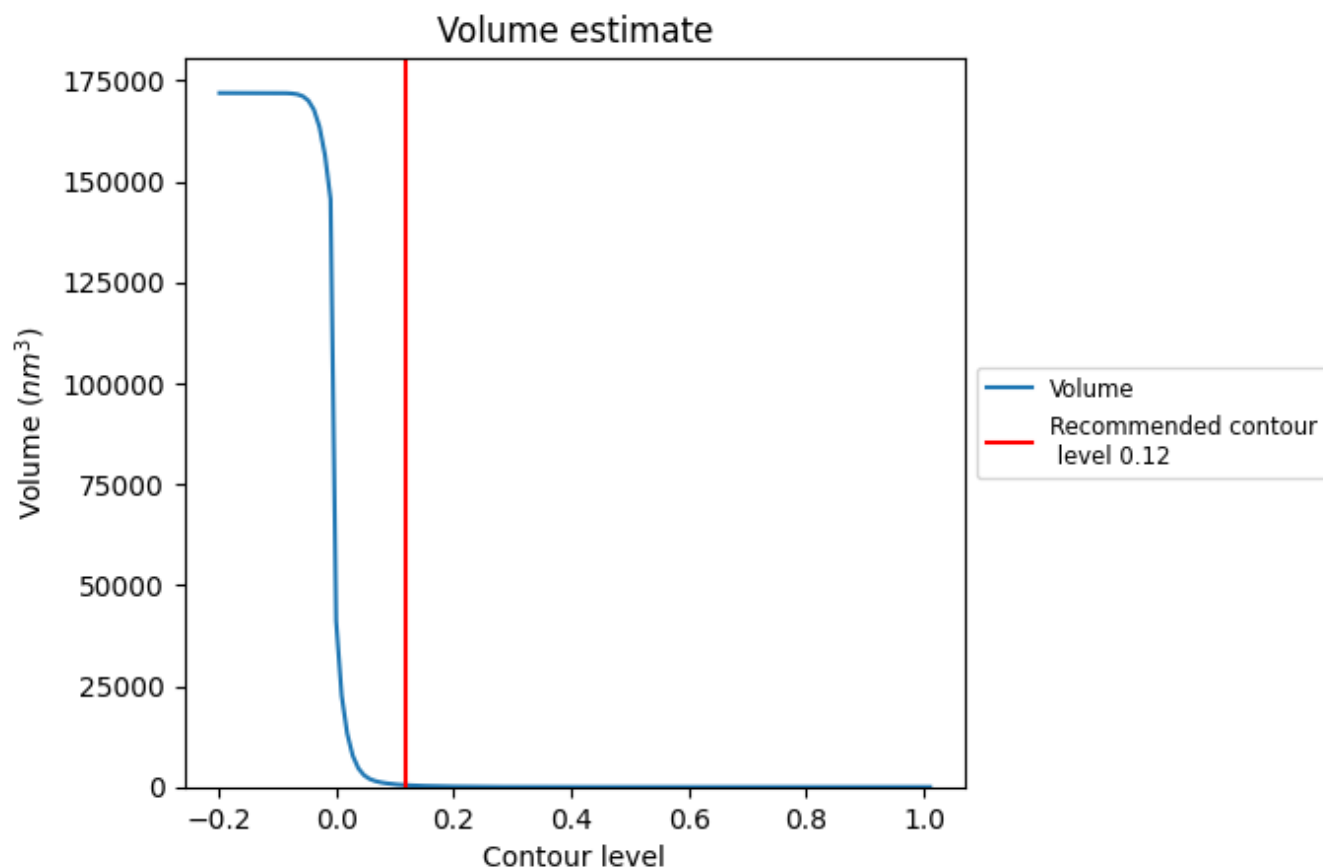
This section contains the results of statistical analysis of the map.

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.

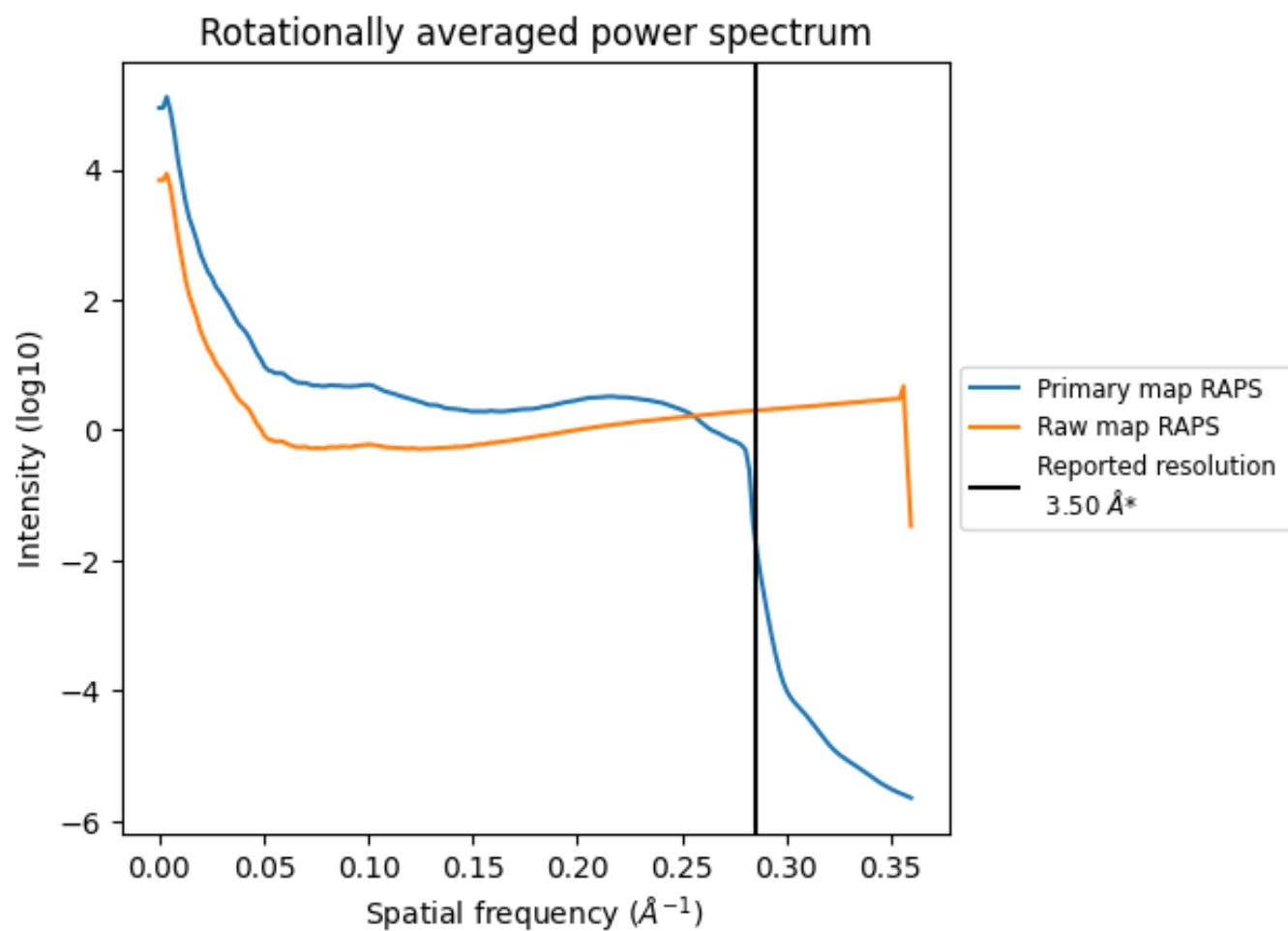
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 437 nm³; this corresponds to an approximate mass of 394 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 ⓘ

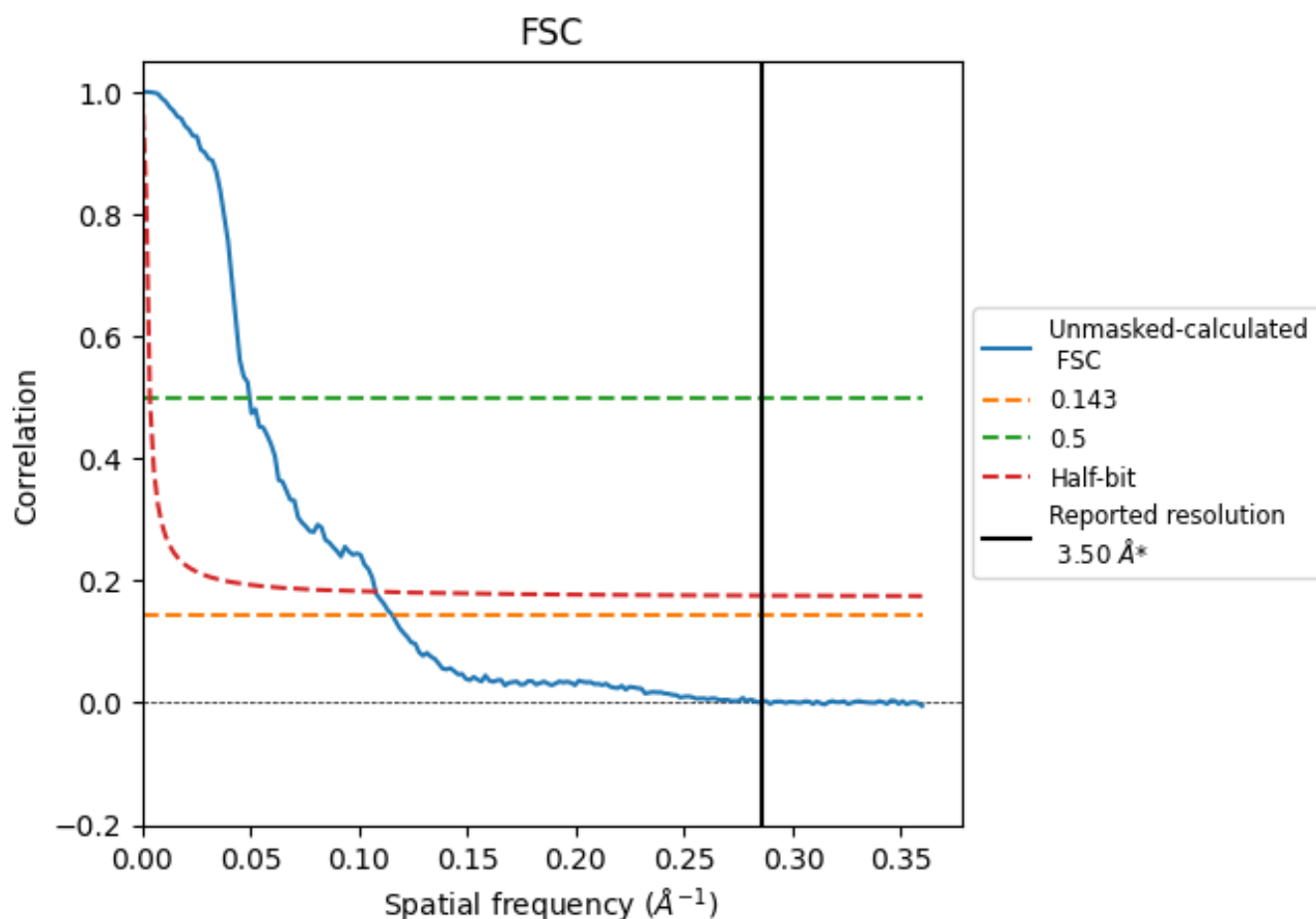


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

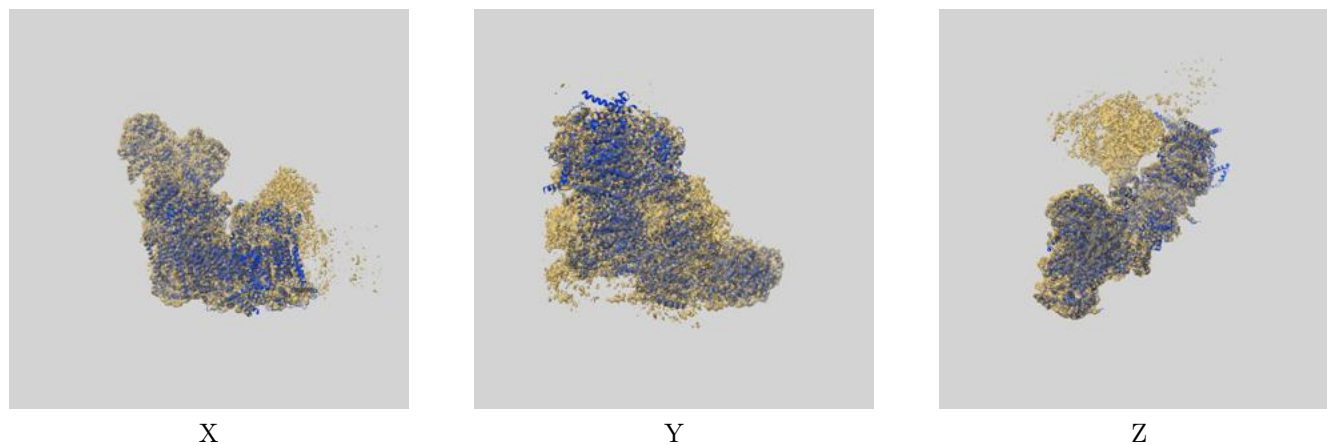
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	8.67	20.24	9.29

*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 8.67 differs from the reported value 3.5 by more than 10 %

9 Map-model fit [i](#)

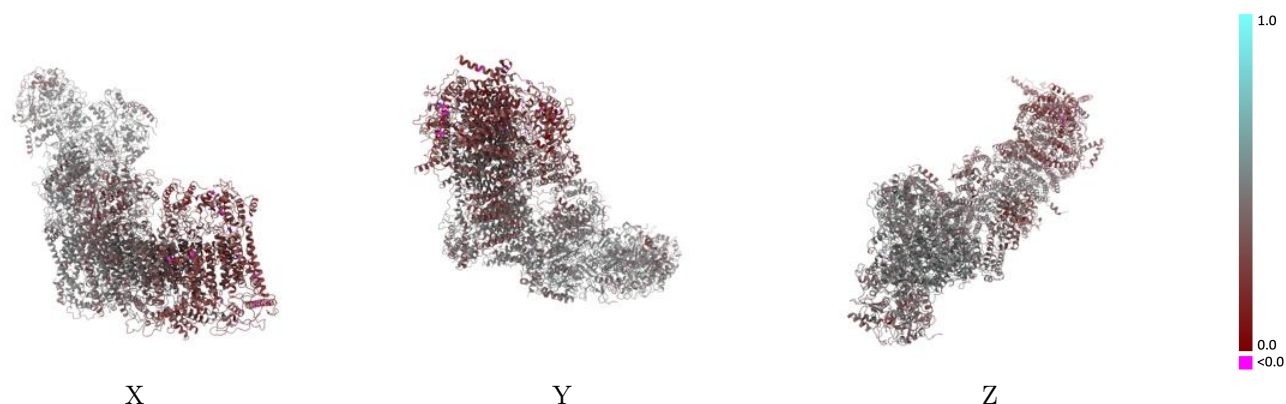
This section contains information regarding the fit between EMDB map EMD-42176 and PDB model 8UEZ. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



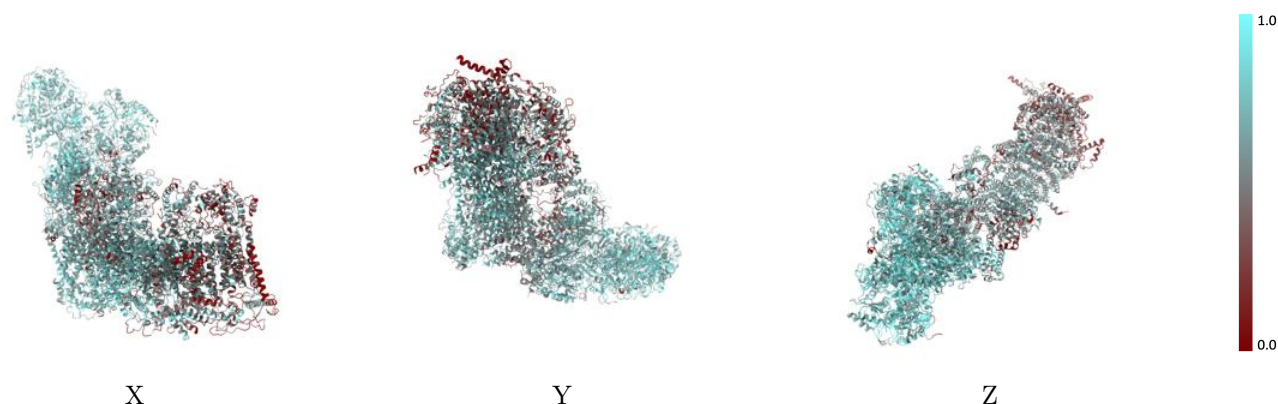
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



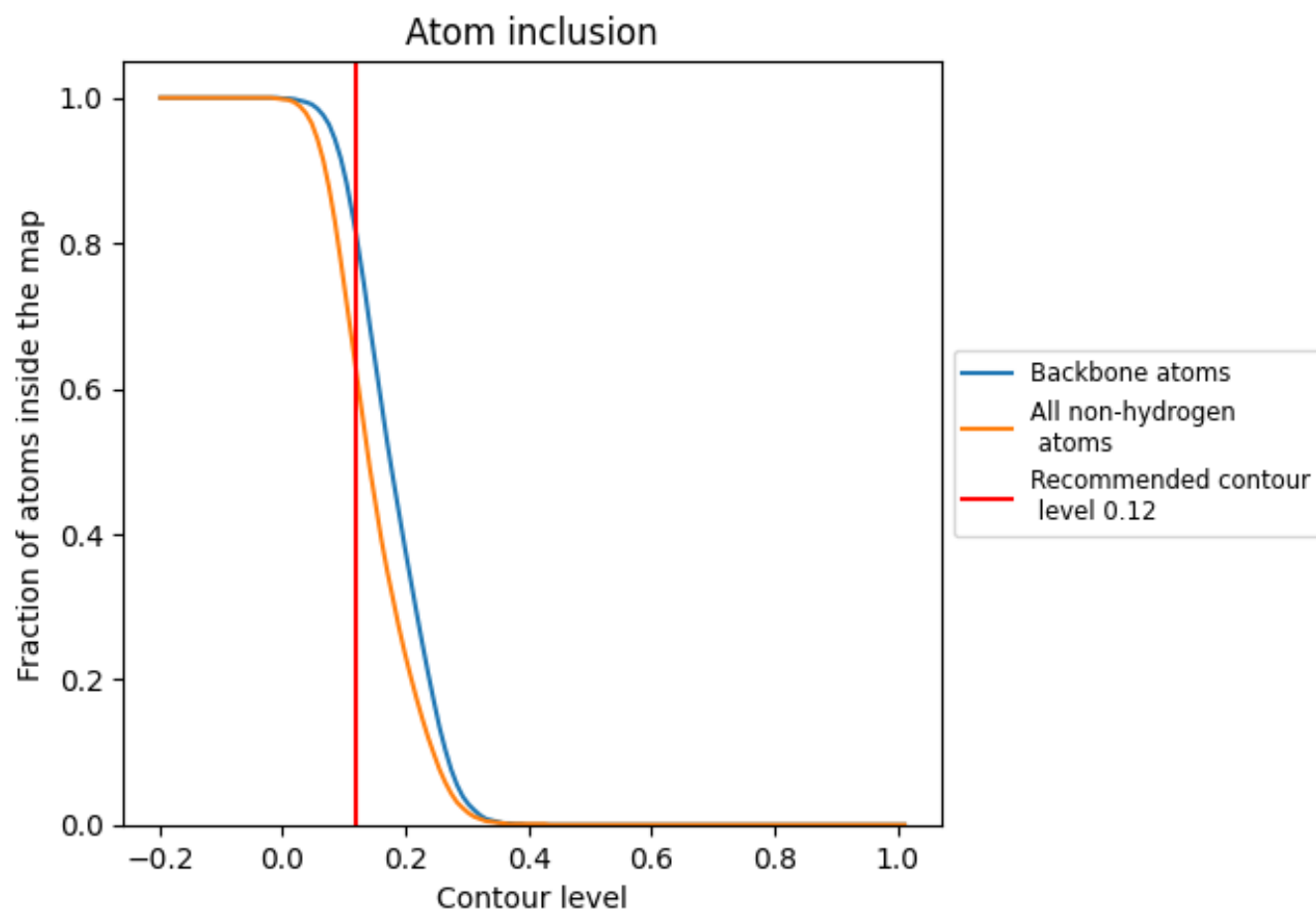
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 62% 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	 0.6230	 0.4010
1A	 0.5080	 0.4400
1B	 0.6810	 0.4650
1C	 0.7470	 0.4810
1D	 0.6960	 0.4630
1E	 0.7530	 0.4310
1F	 0.7600	 0.4330
1G	 0.7680	 0.4620
1H	 0.6370	 0.4520
1I	 0.7930	 0.4780
1J	 0.5660	 0.4110
1K	 0.6560	 0.4220
1L	 0.4650	 0.2850
1M	 0.6410	 0.3930
1N	 0.7170	 0.4480
1O	 0.4580	 0.3360
1P	 0.6340	 0.4620
1Q	 0.6640	 0.4610
1R	 0.7260	 0.4720
1S	 0.7300	 0.4200
1T	 0.4410	 0.3560
1U	 0.3490	 0.2370
1V	 0.6490	 0.4250
1W	 0.6380	 0.4360
1X	 0.7470	 0.4320
1Y	 0.6080	 0.3420
1Z	 0.7450	 0.4470
1a	 0.7460	 0.4700
1b	 0.6920	 0.4520
1c	 0.4900	 0.3690
1d	 0.6970	 0.4220
1e	 0.7200	 0.4420
1f	 0.4750	 0.3600
1g	 0.5180	 0.3530
1h	 0.6120	 0.3860



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
1i	 0.2920	 0.2750
1j	 0.2660	 0.2590
1k	 0.2150	 0.2400
1l	 0.4720	 0.2970
1m	 0.4870	 0.2980
1n	 0.4540	 0.2740
1o	 0.4030	 0.2470
1p	 0.5130	 0.3290
1q	 0.7440	 0.4730
1r	 0.7510	 0.4730
1s	 0.7090	 0.4110