



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 08:31 PM EDT

PDB ID : 8UER / pdb_00008uer
EMDB ID : EMD-42168
Title : In-situ complex I with Q10 (State-gamma)
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

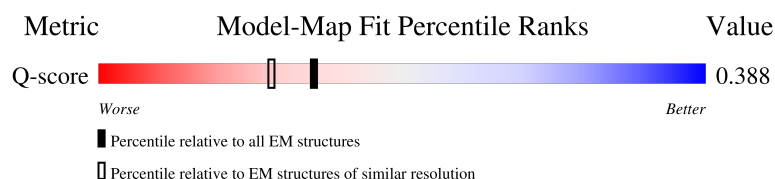
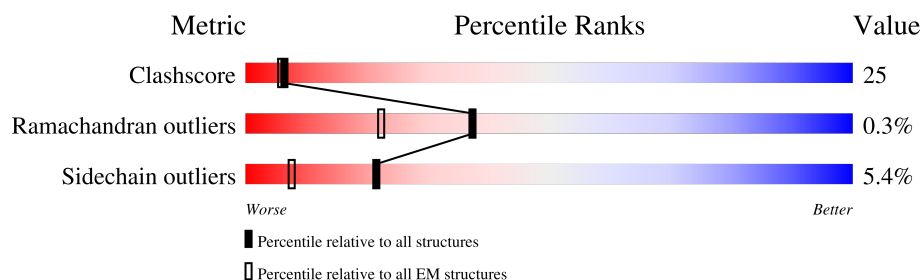
1 Overall quality at a glance i

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	43% 45% 50% .
2	1B	255	8% 33% 25% . 39%
3	1C	264	11% 52% 25% . 21%
4	1D	476	17% 51% 36% . 10%

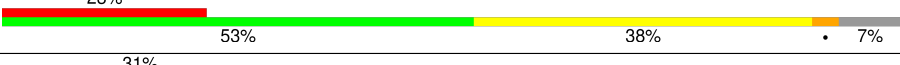
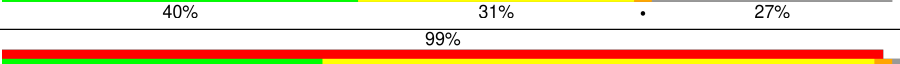
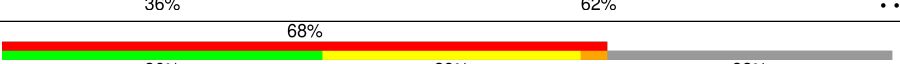
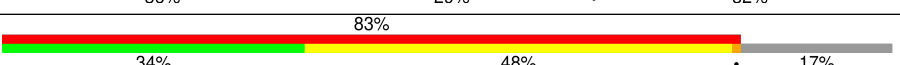
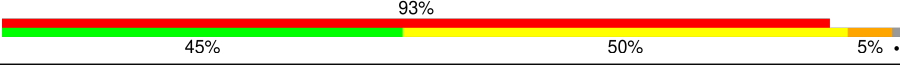
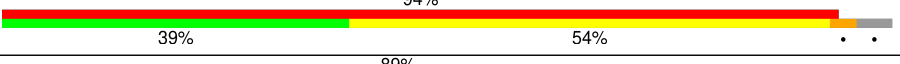
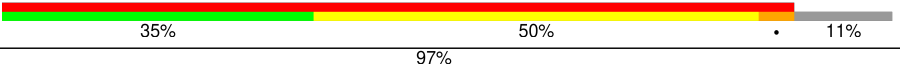
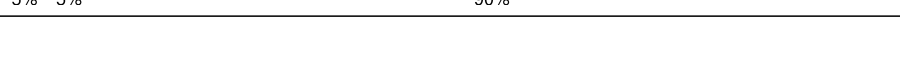
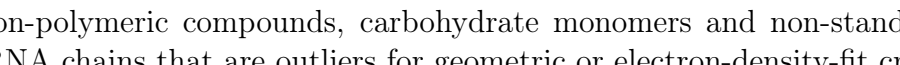
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24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

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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	-
45	SF4	1G	801	-	-	X	-
45	SF4	1G	802	-	-	X	-
45	SF4	1I	201	-	-	X	-
45	SF4	1I	202	-	-	X	-

2 Entry composition [i](#)

There are 58 unique types of molecules in this entry. The entry contains 67436 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		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1B	?	-	PRO	deletion	UNP A0A4X1VVS8
1B	?	-	SER	deletion	UNP A0A4X1VVS8
1B	?	-	SER	deletion	UNP A0A4X1VVS8

- 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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	S	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		

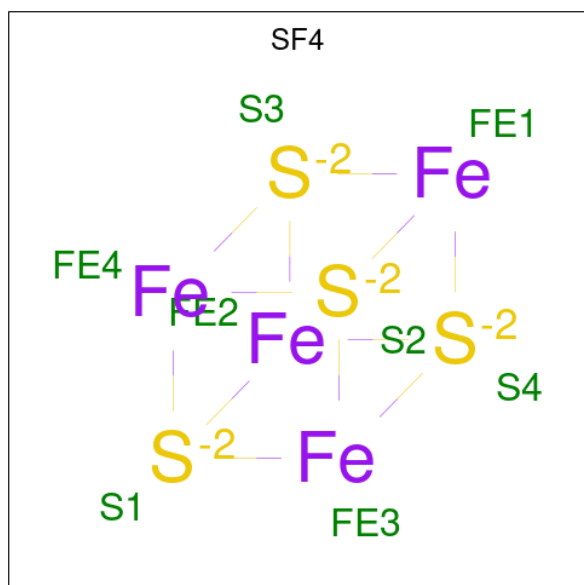
There is a discrepancy between the modelled and reference sequences:

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: Fe_4S_4).



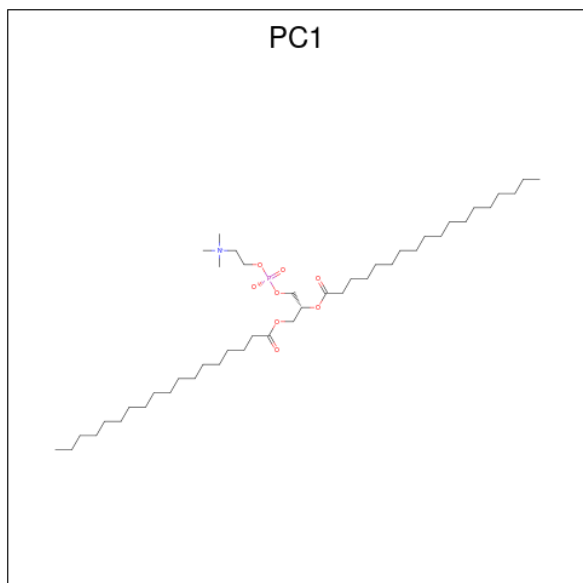
Mol	Chain	Residues	Atoms			AltConf
45	1B	1	Total	Fe	S	0
			8	4	4	
45	1F	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	

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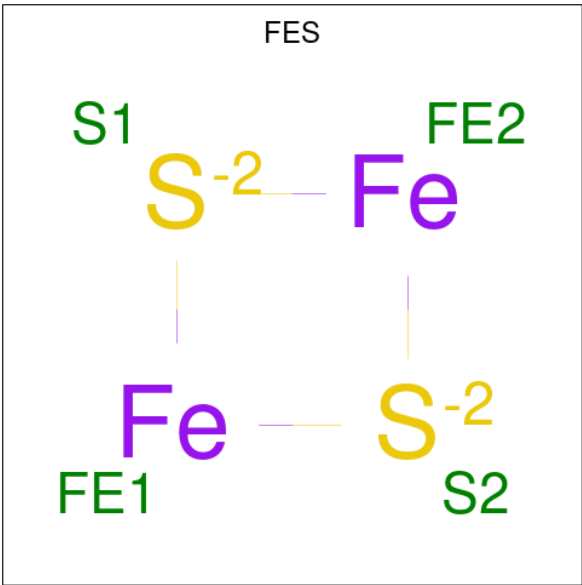
Mol	Chain	Residues	Atoms			AltConf
45	1I	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	

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



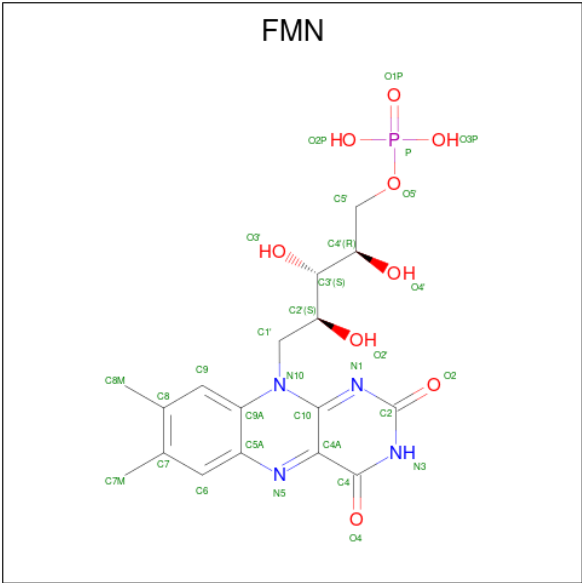
Mol	Chain	Residues	Atoms					AltConf
46	1B	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1h	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1m	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1q	1	Total	C	N	O	P	0
			48	38	1	8	1	

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



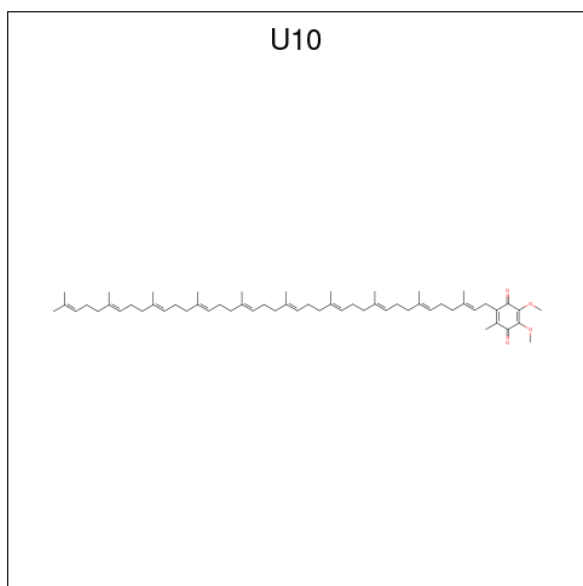
Mol	Chain	Residues	Atoms			AltConf
47	1E	1	Total	Fe	S	0
			4	2	2	
47	1G	1	Total	Fe	S	0
			4	2	2	

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



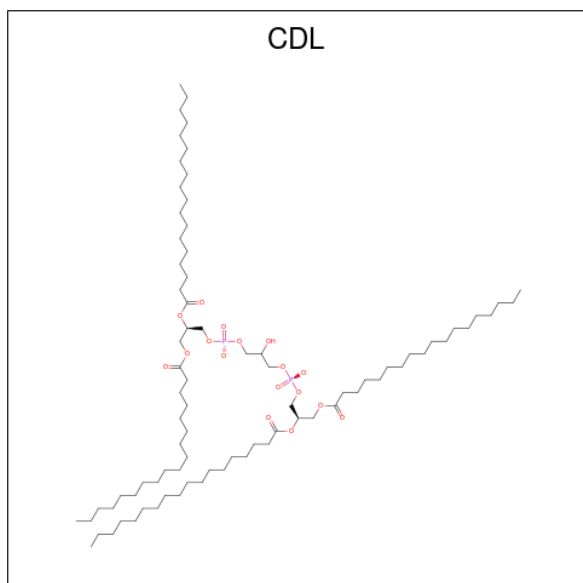
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

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



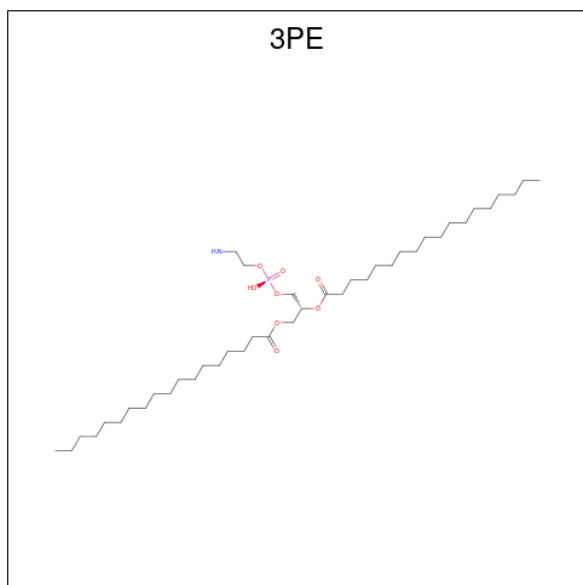
Mol	Chain	Residues	Atoms			AltConf
50	1H	1	Total	C	O	0
			63	59	4	

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



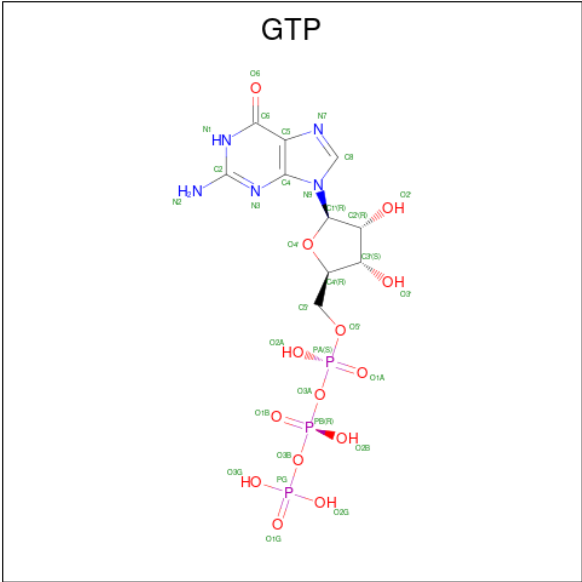
Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total	C	O	P	0
			51	32	17	2	
51	1O	1	Total	C	O	P	0
			67	48	17	2	
51	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
52	1N	1	Total	C	N	O	P	0
			38	28	1	8	1	
52	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
52	1g	1	Total	C	N	O	P	0
			51	41	1	8	1	
52	1n	1	Total	C	N	O	P	0
			42	32	1	8	1	

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

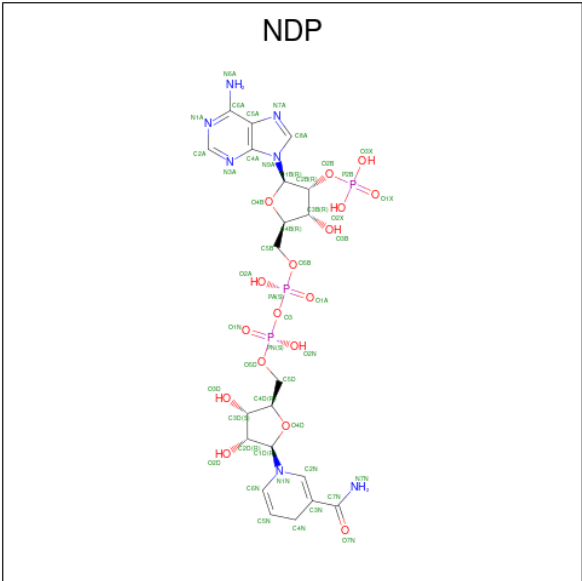


Mol	Chain	Residues	Atoms					AltConf
53	10	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

Mol	Chain	Residues	Atoms		AltConf
54	10	1	Total	Mg	0
			1	1	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

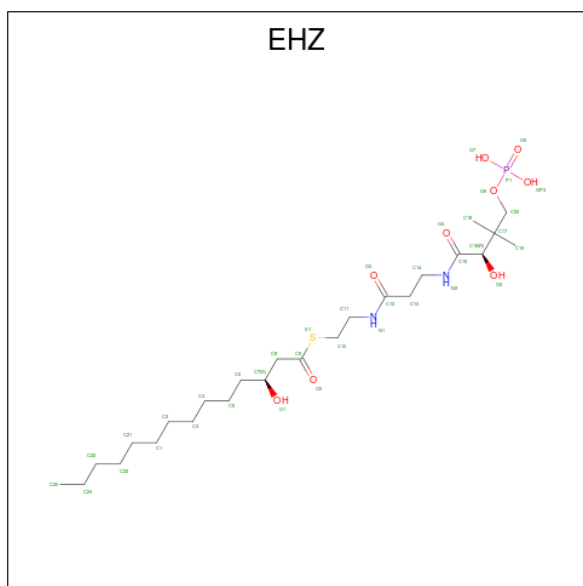


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

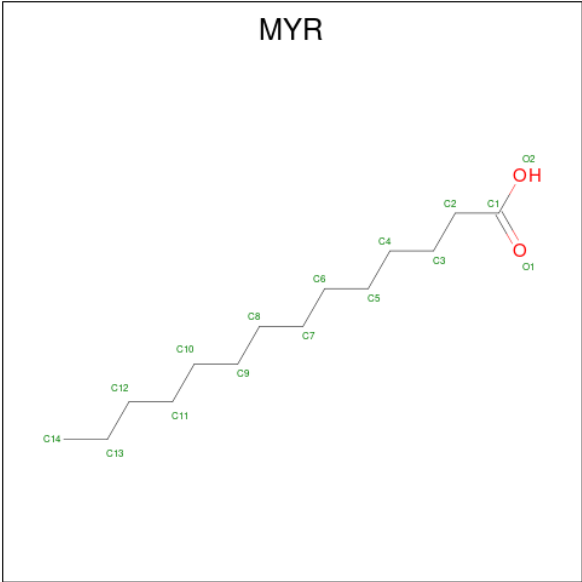
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

- Molecule 57 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).



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

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

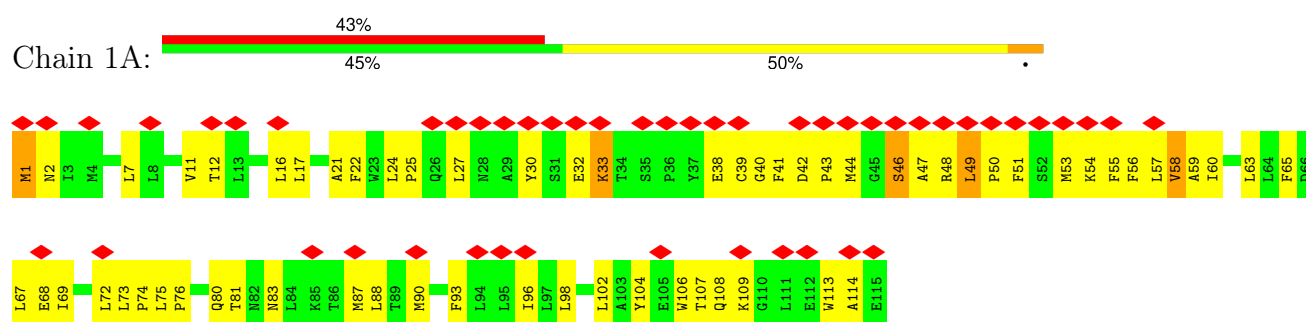


Mol	Chain	Residues	Atoms			AltConf
58	1l	1	Total	C	O	0
			15	14	1	

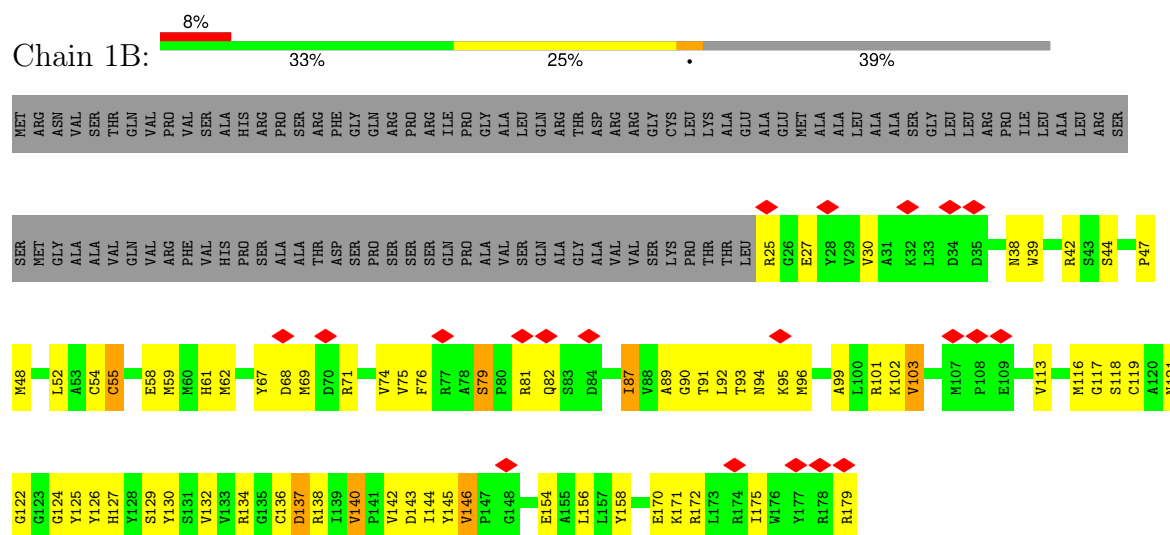
3 Residue-property plots

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

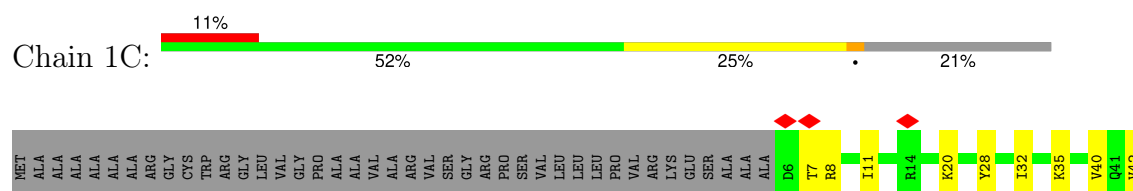
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

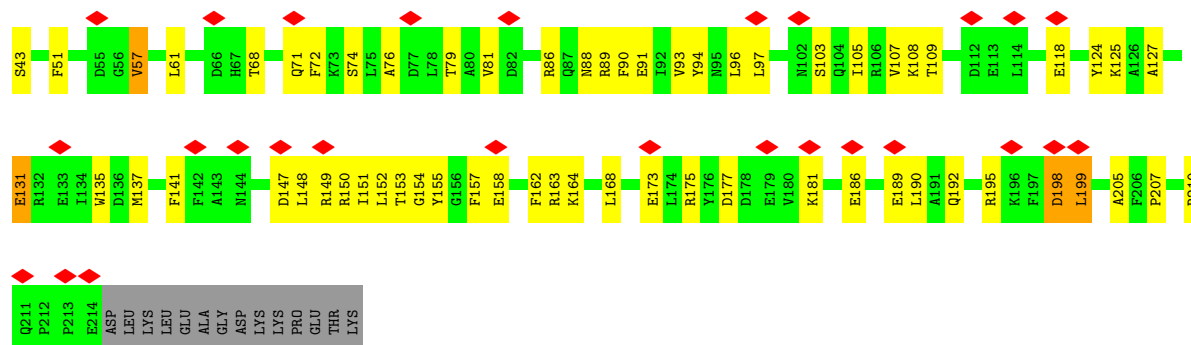


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

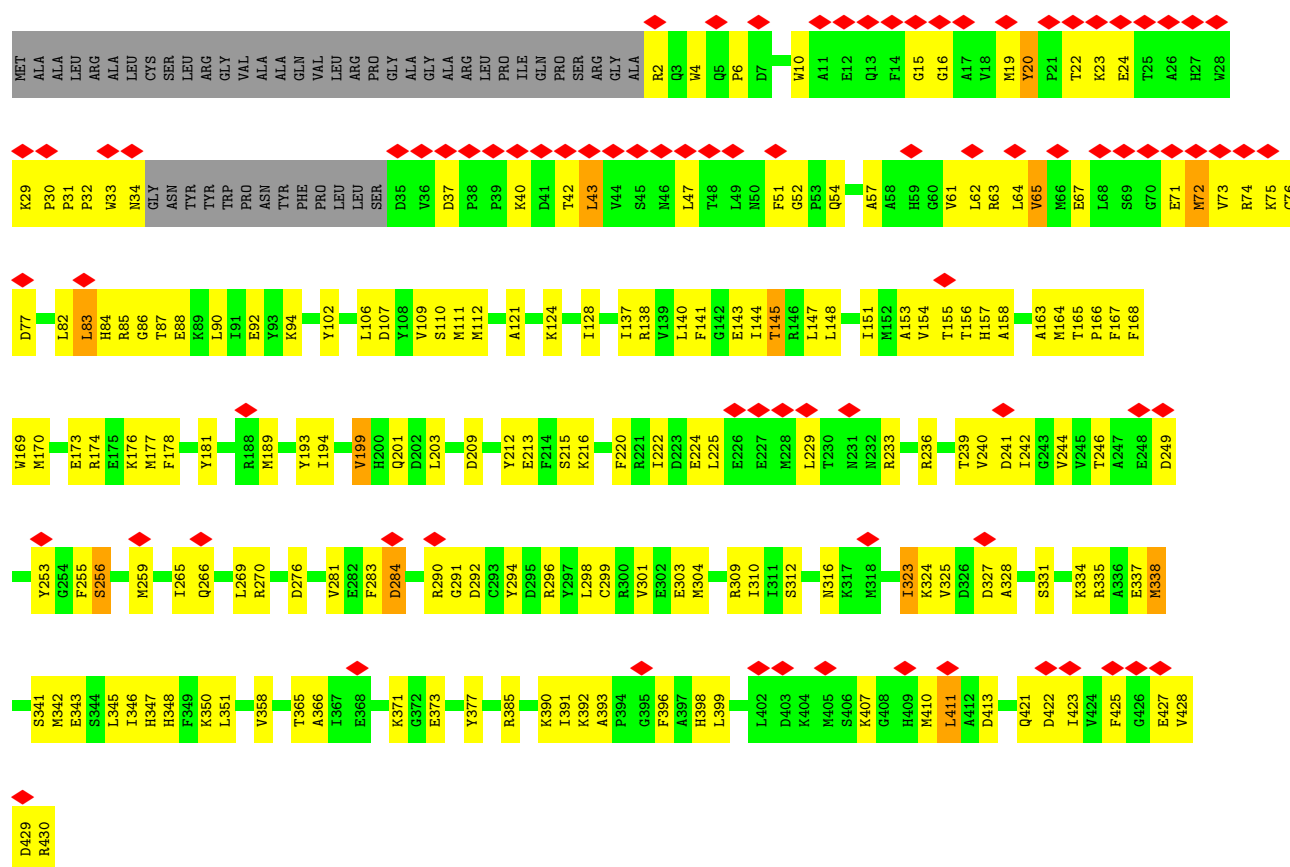


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

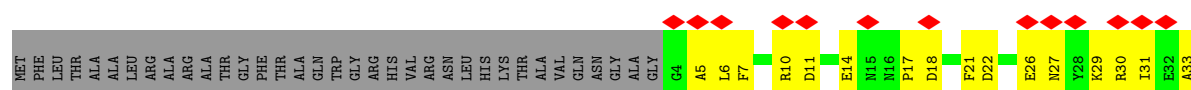


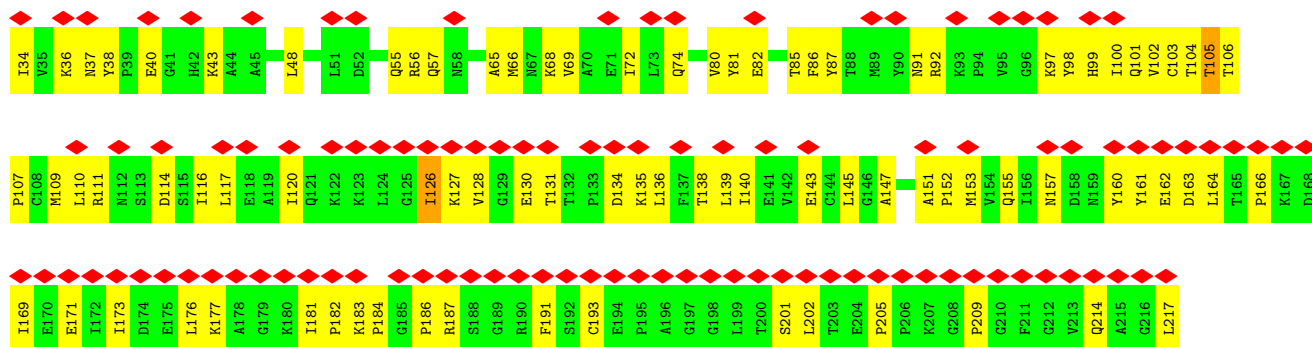


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

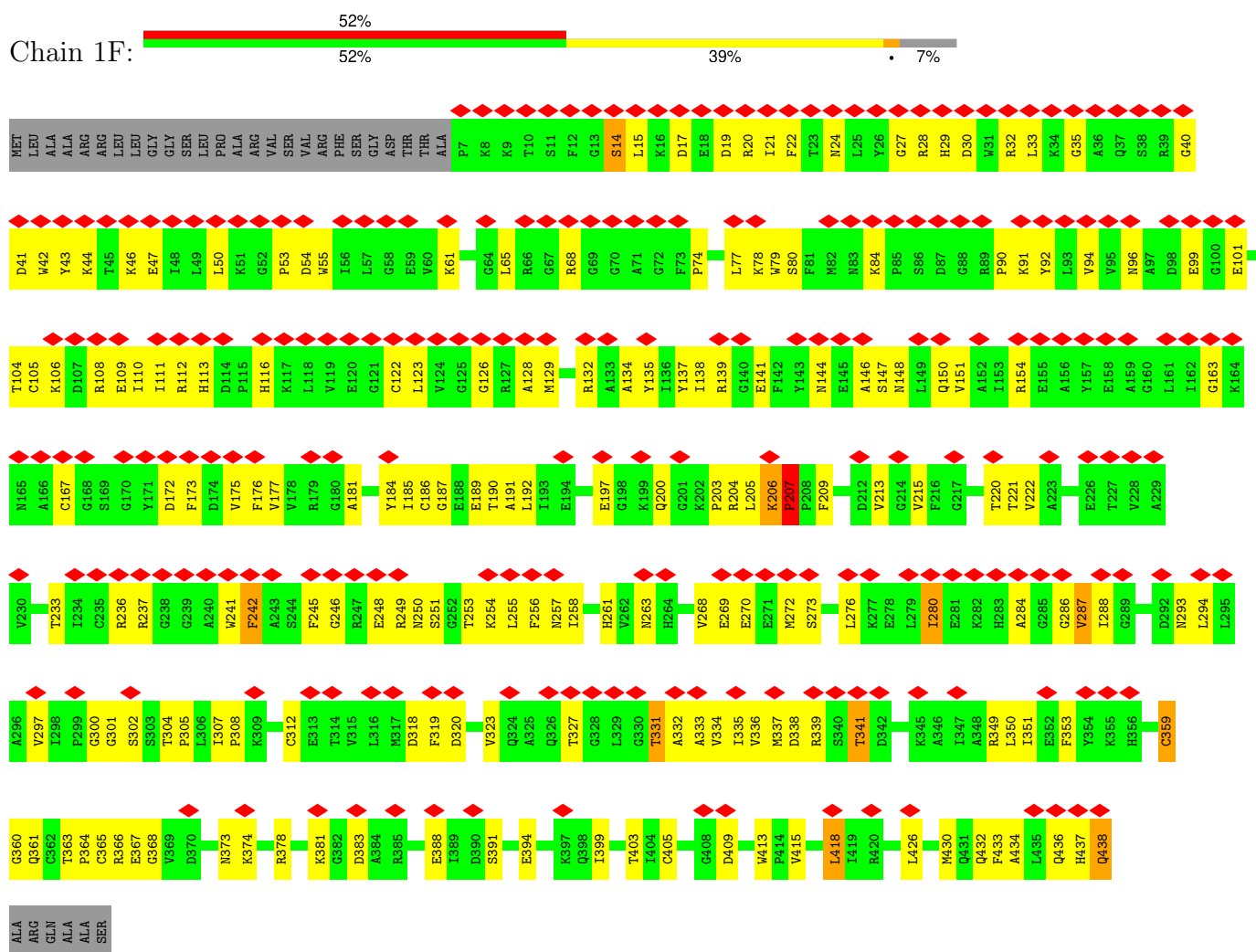


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

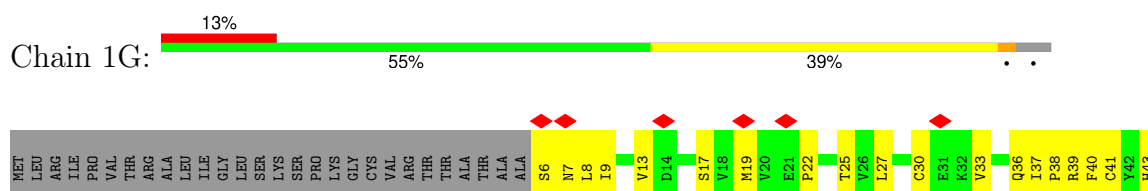


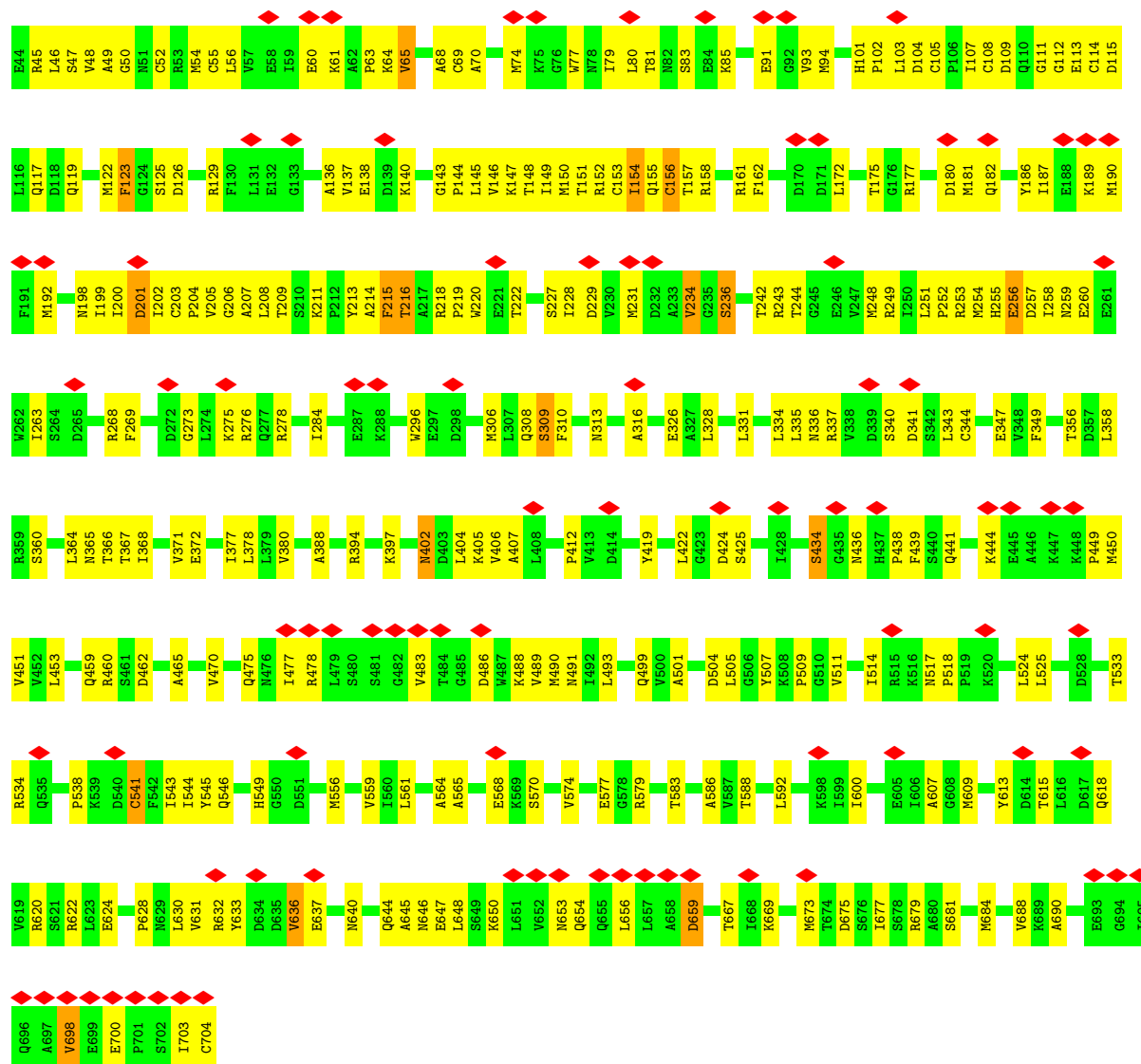


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

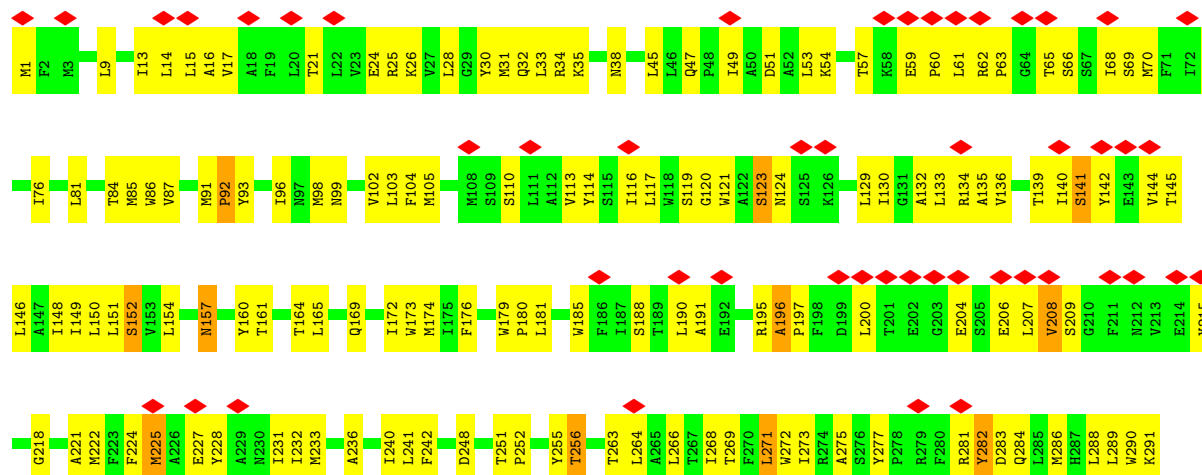


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



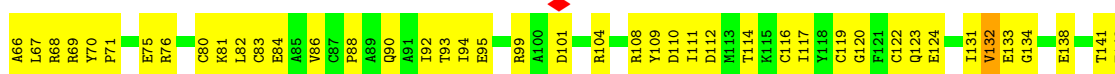
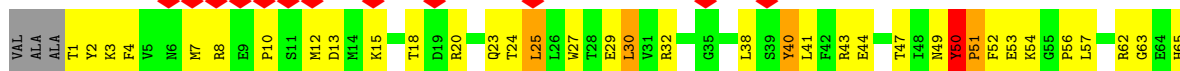
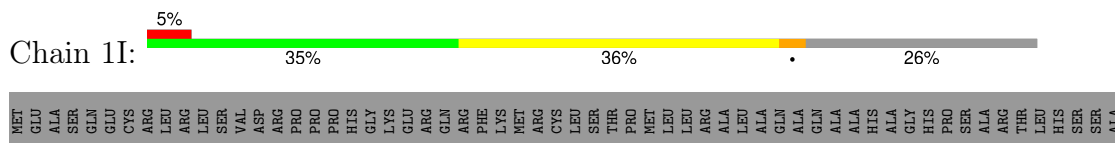


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

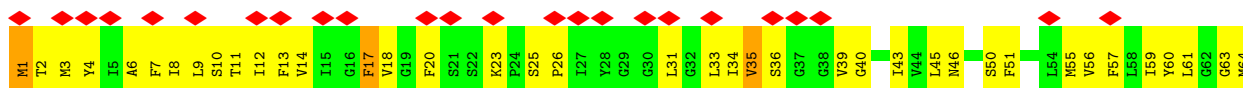




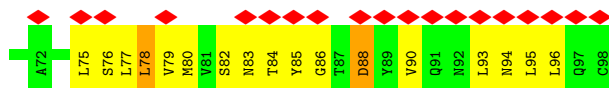
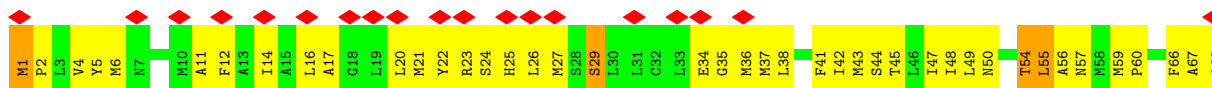
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



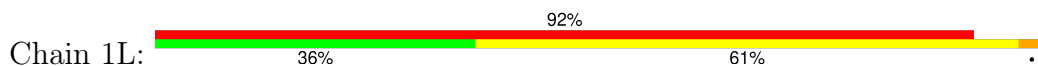
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

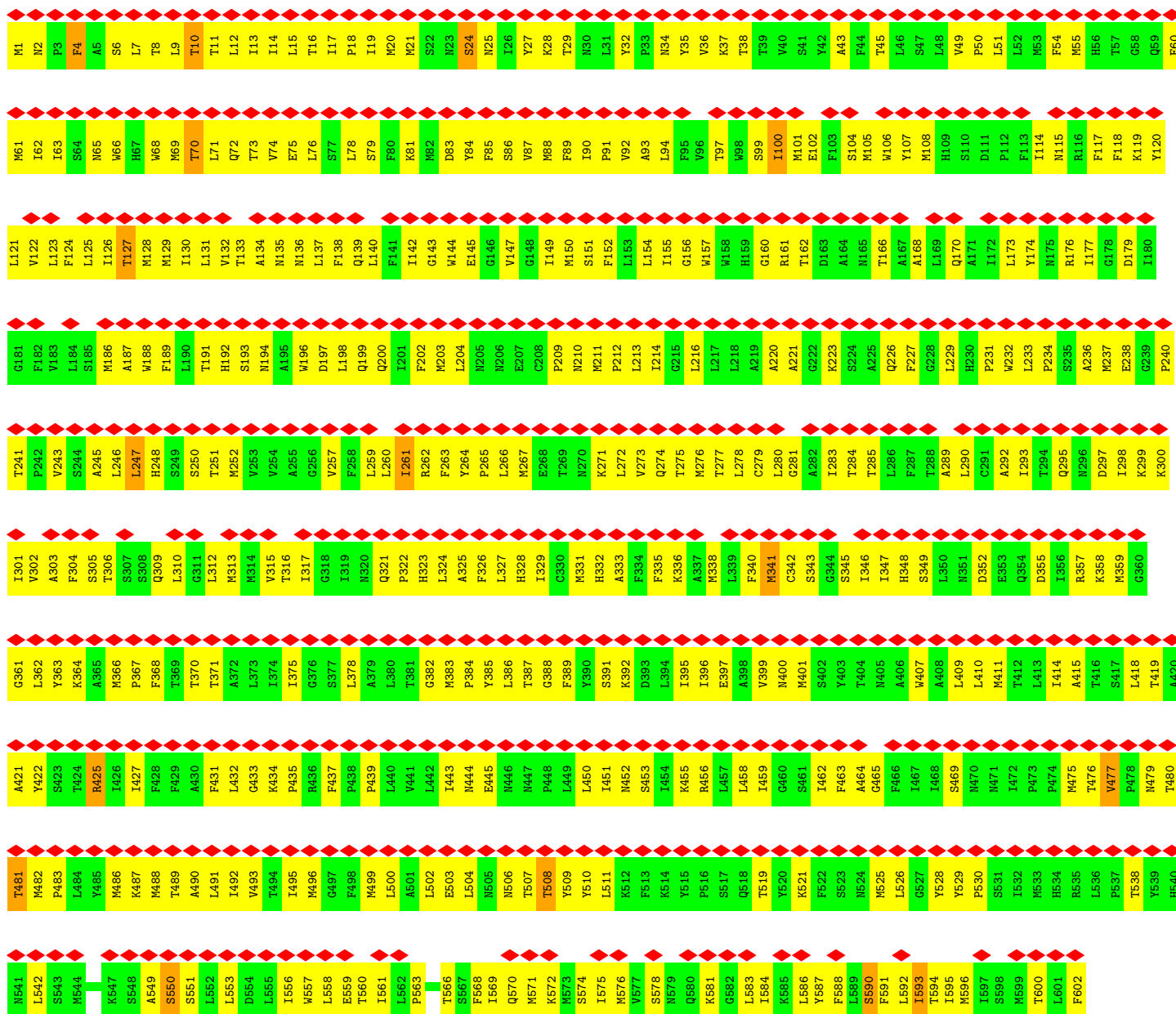


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

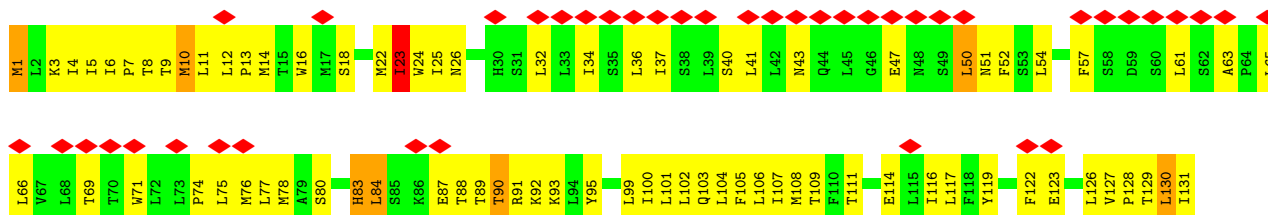


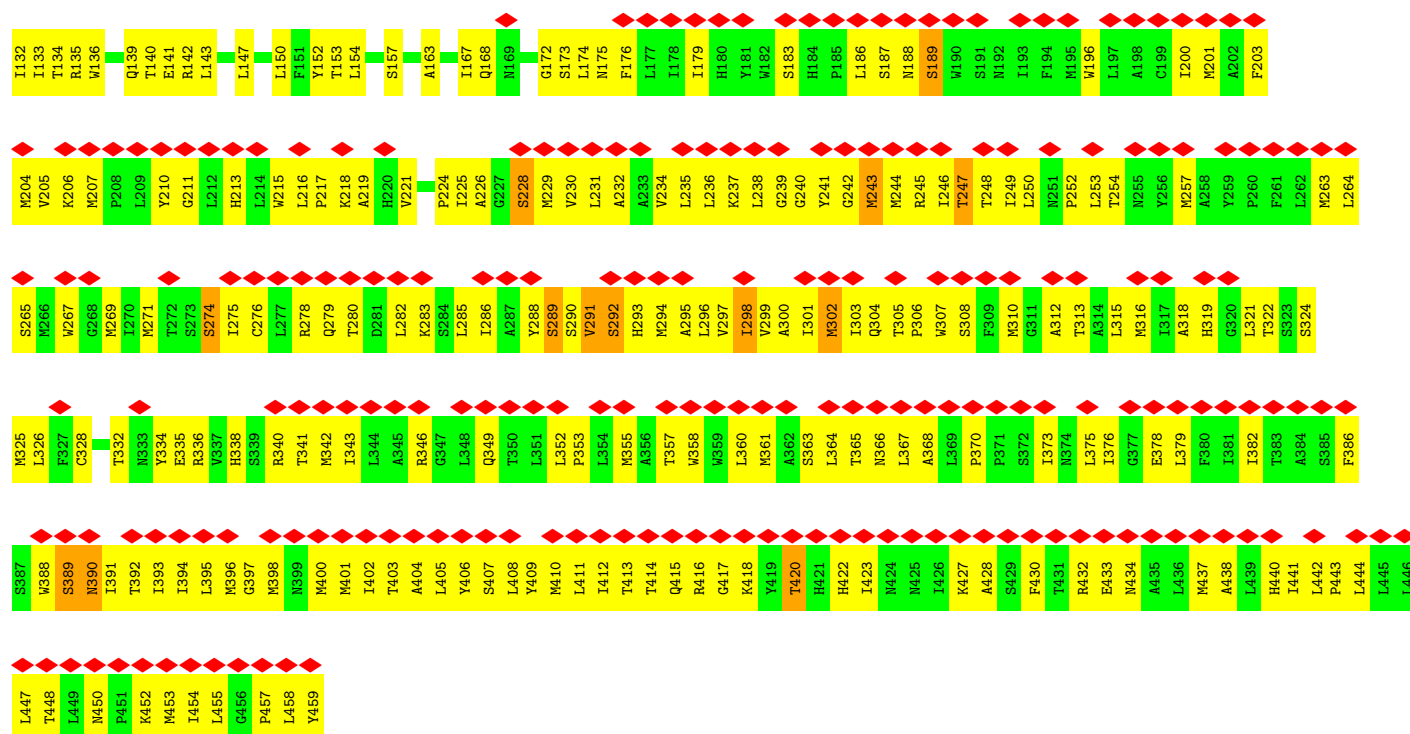
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5



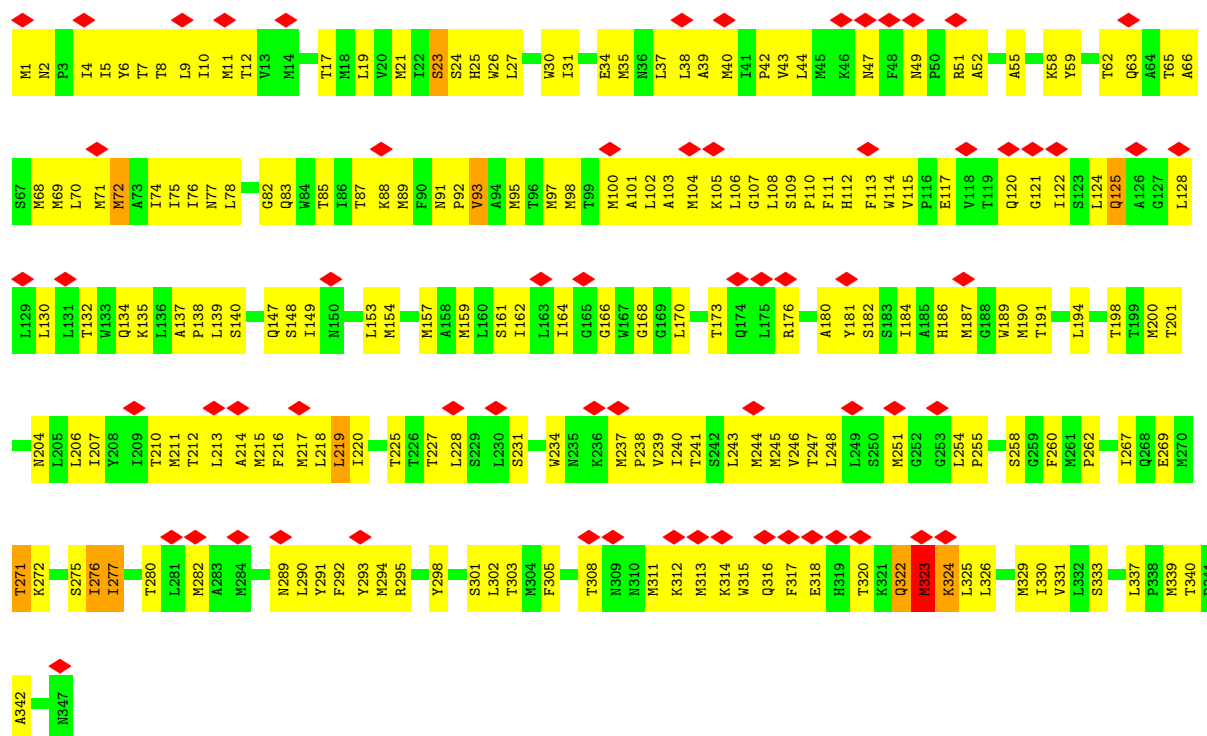


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

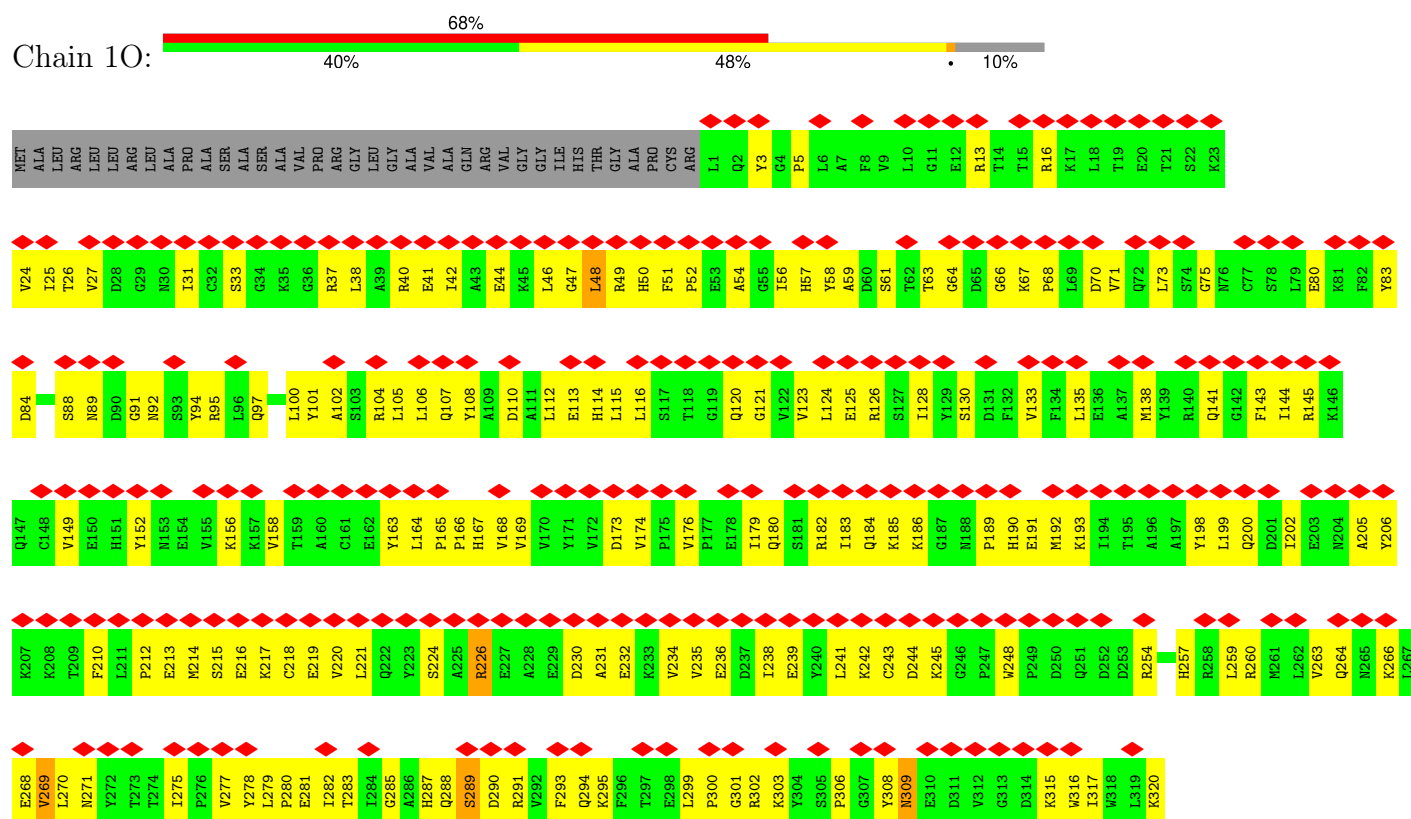




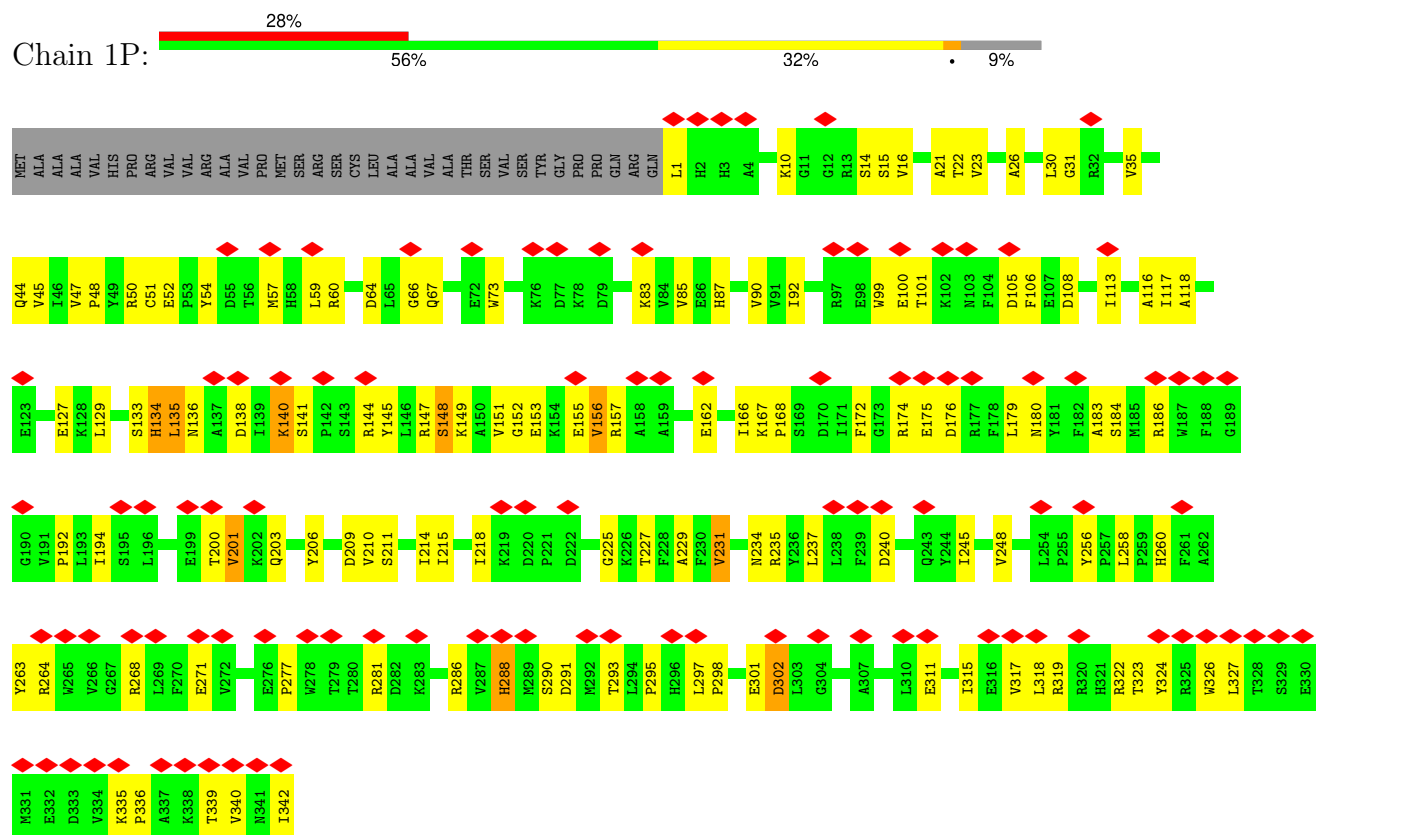
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



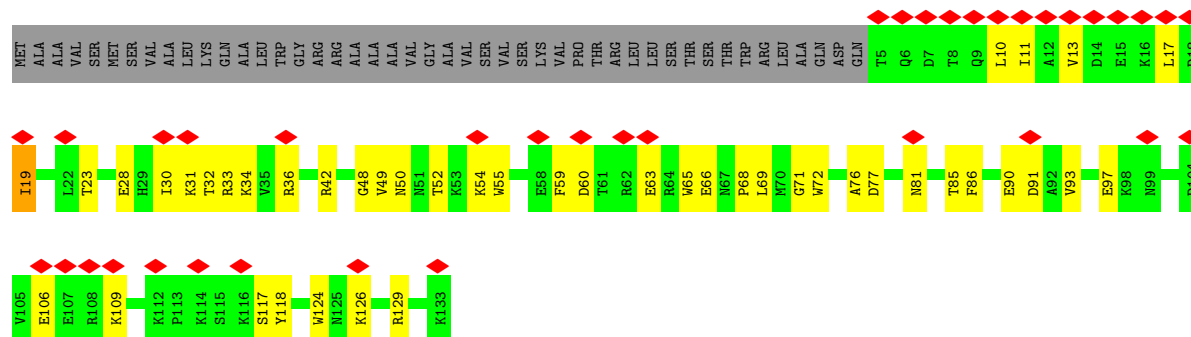
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



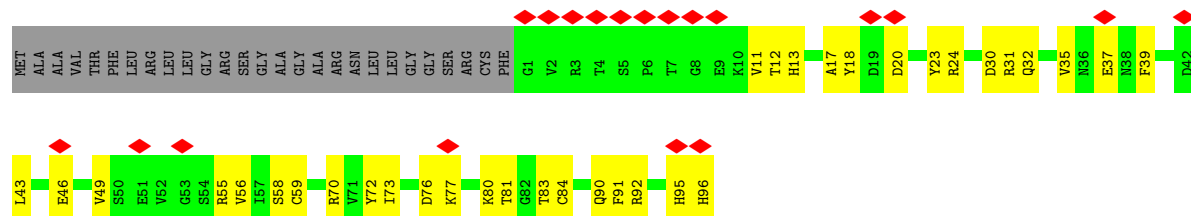
• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



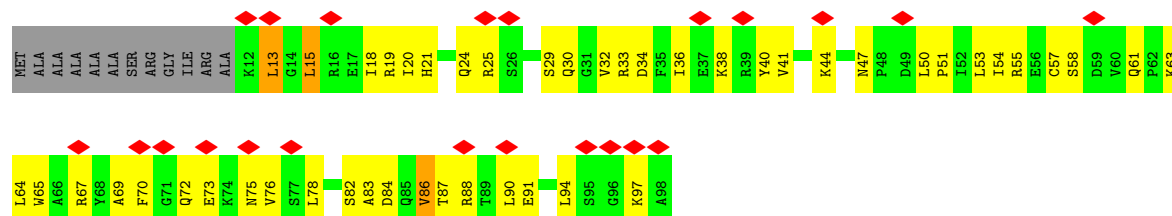
• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



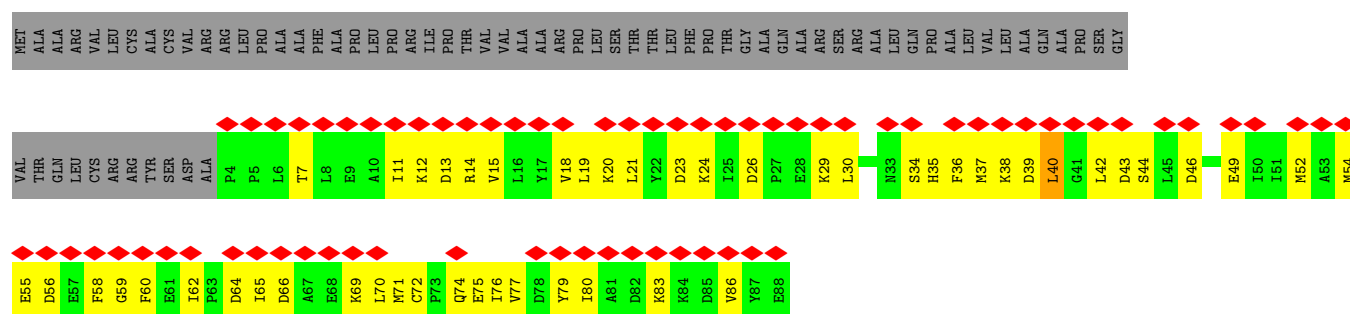
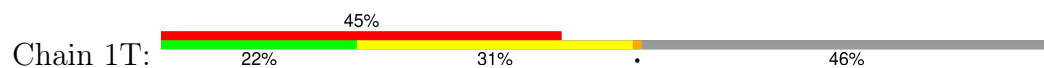
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



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



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



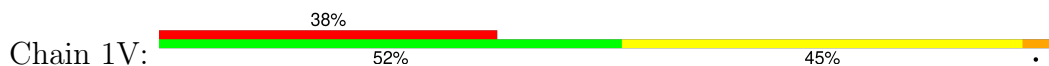
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



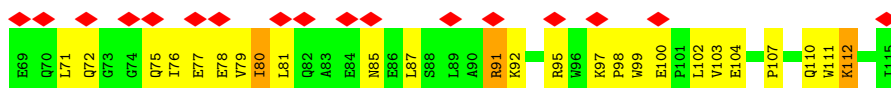
MET ALA ARG LEU CYS VAL ARG VAL ARG LEU PRO ALA PHE ALA PRO LEU PRO ARG ILE PRO THR VAL VAL ALA ALA PRO LEU THR THR LEU PHE PRO THR GLY ALA GLN ALA ARG SER ARG ALA LEU GLN PRO ALA VAL LEU LEU ALA GLN ALA PRO SER GLY



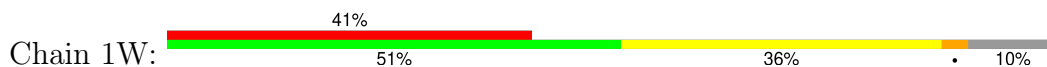
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



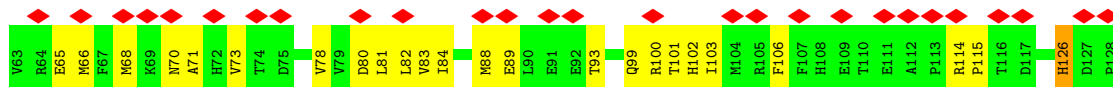
MET A1 G2 L3 L4 K5 K6 T7 T8 G9 L10 V11 G12 L13 A14 A15 V16 C16 E17 T18 R22 L23 K24 L25 L26 K29 I30 L31 D32 V33 L34 K39 Y43 R44 K45 Y46 T47 Q48 Q49 I50 T51 N52 E53 K54 M57 V58 K59 A60 E61 P62 P63 D63 V64 K65 K66 L67 E68



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



MET ALA SER GLY LEU PRO ARG ALA ALA ALA ALA G14 T15 S16 V17 K18 P19 P21 S22 R23 D24 M25 N26 E27 A28 K29 R30 R31 V32 R33 E34 R37 Y40 R41 E42 V43 P44 M45 T46 V47 H48 L49 F50 Q51 L52 D53 I54 S55 V56 K57 Q58 G59 R60 D61 K62



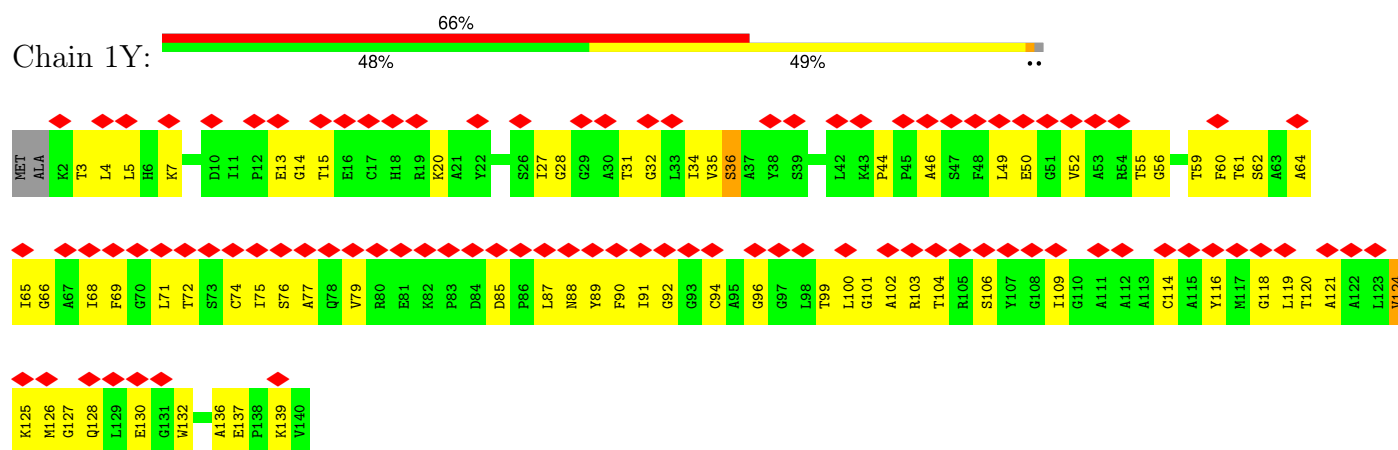
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



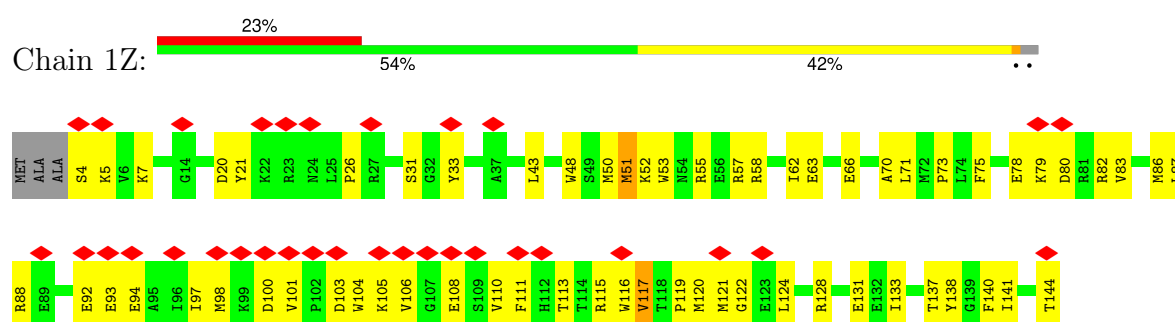
MET P1 G2 I3 V4 E5 L6 P7 T8 L9 D11 L12 K13 V14 Q15 E16 V17 K18 K25 H29 A33 Q34 P38 N39 K40 M43 L44 C45 R46 W47 E48 E49 K50 D51 P52 R53 R54 E58 G59 K60 L61 Q64 L67 D68 F69 F70 R71 Q72 I73 K74 R75



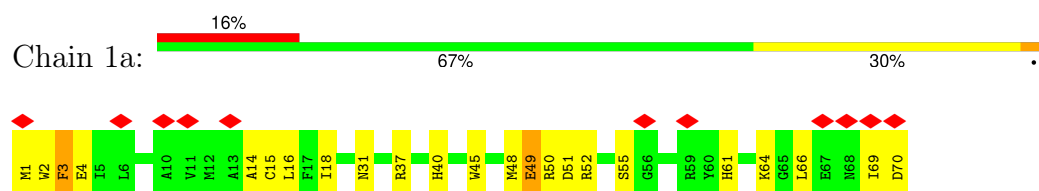
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



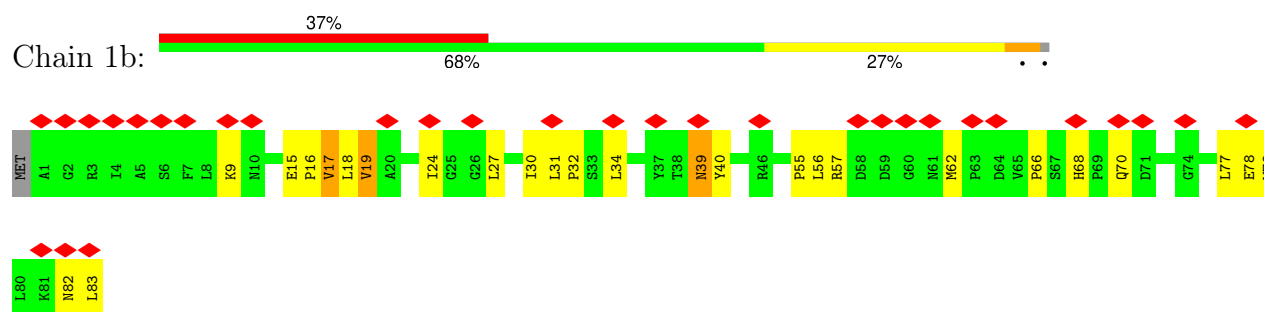
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



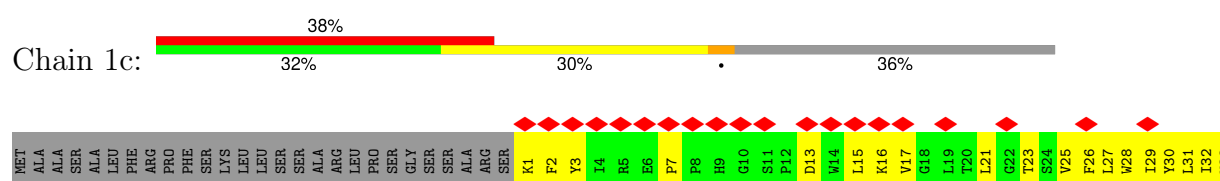
• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

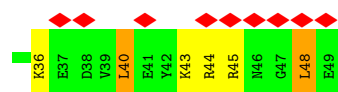


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

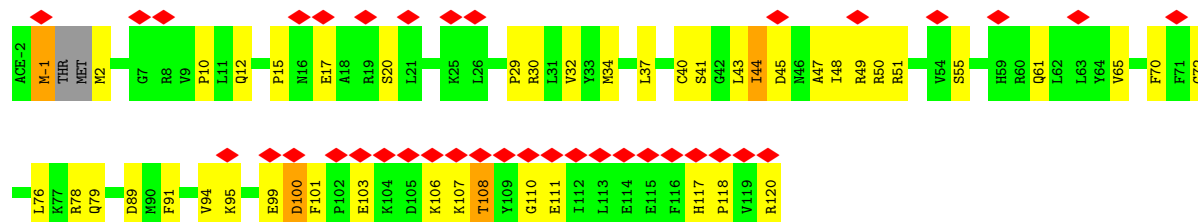


• Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

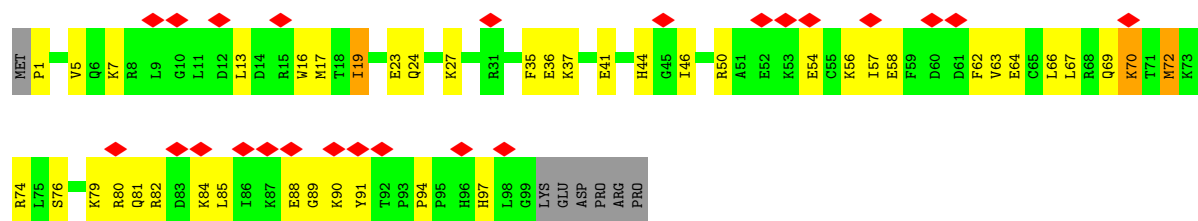




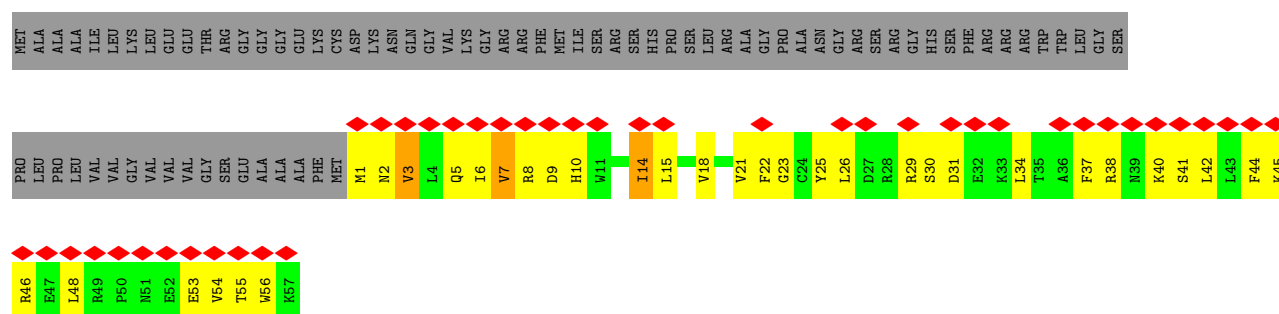
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



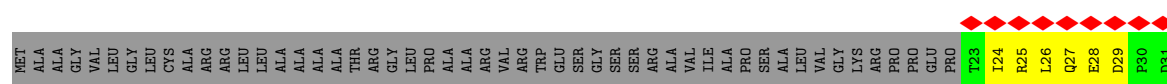
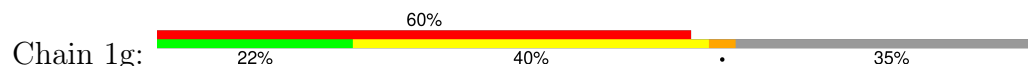
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

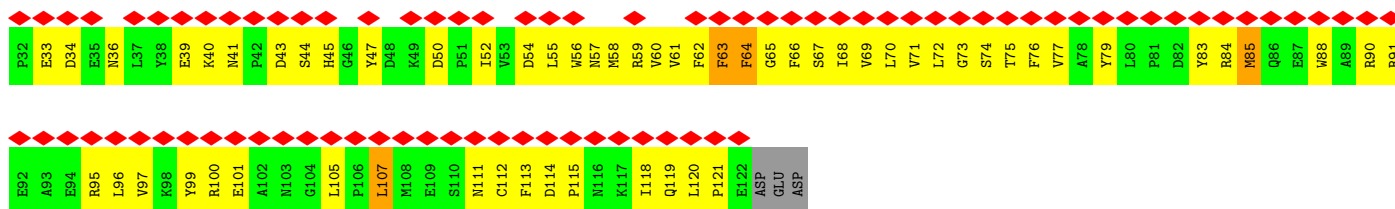


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



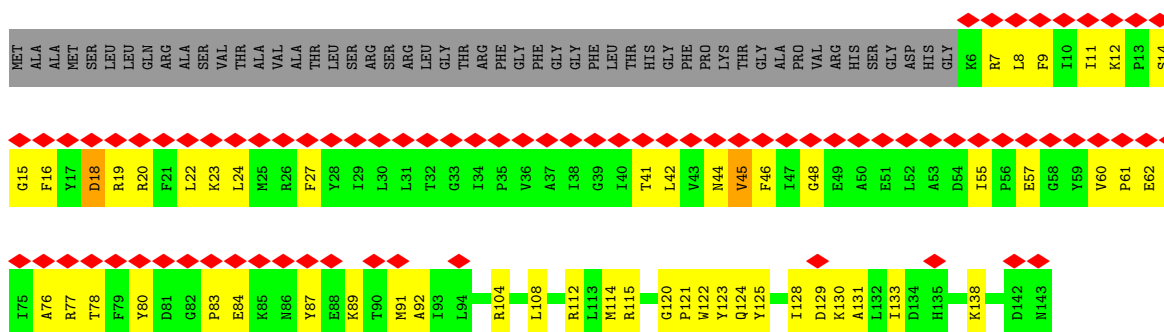
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial





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

Chain 1h:



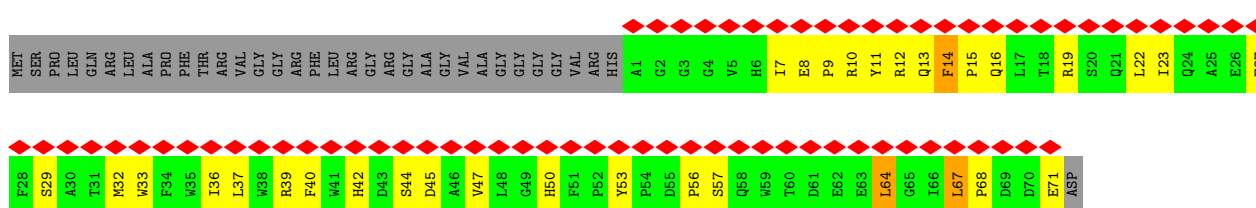
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain 1i:

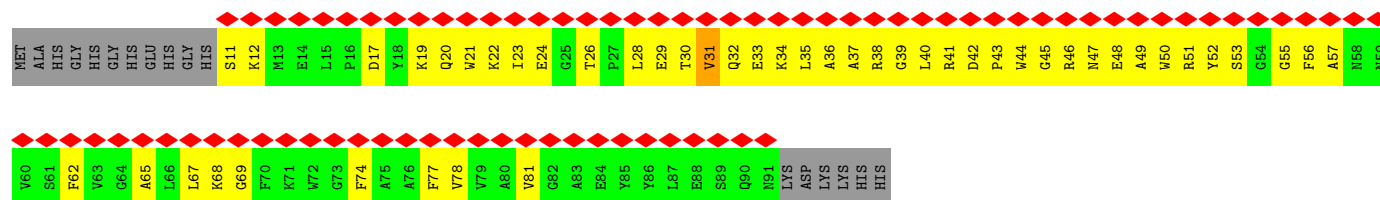
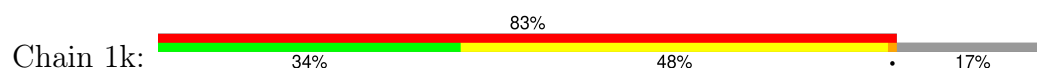


- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

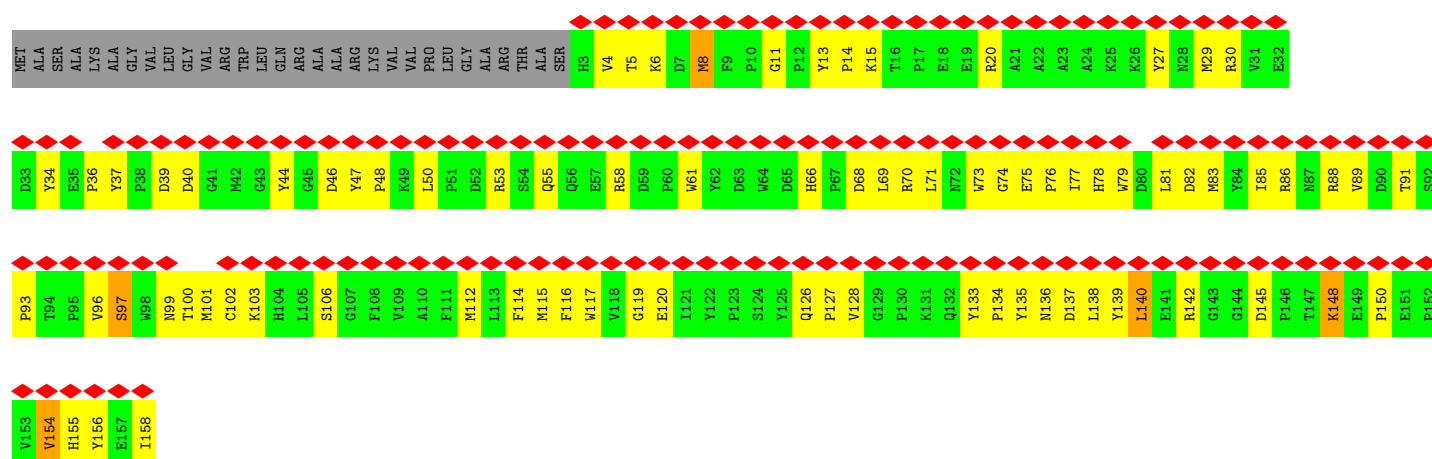
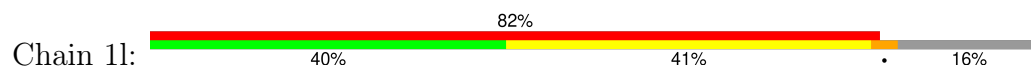
Chain 1j:



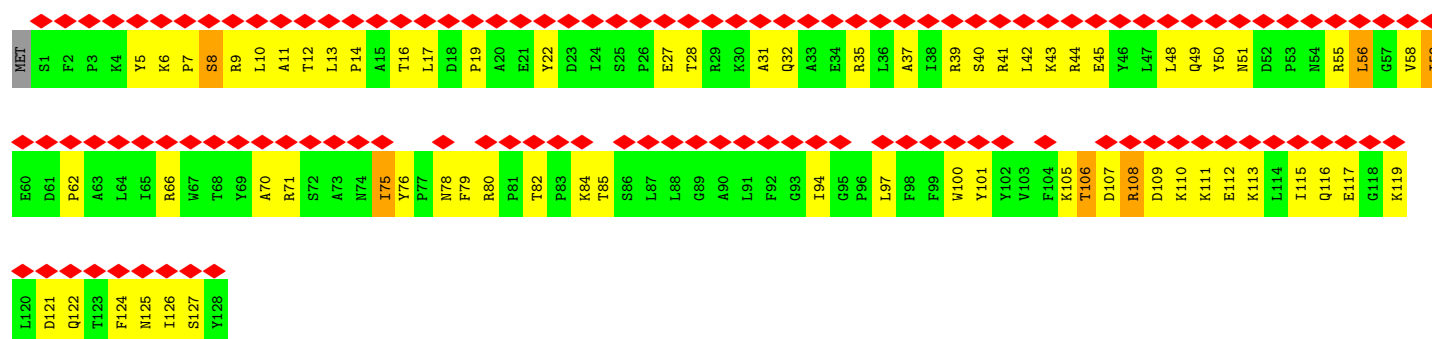
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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

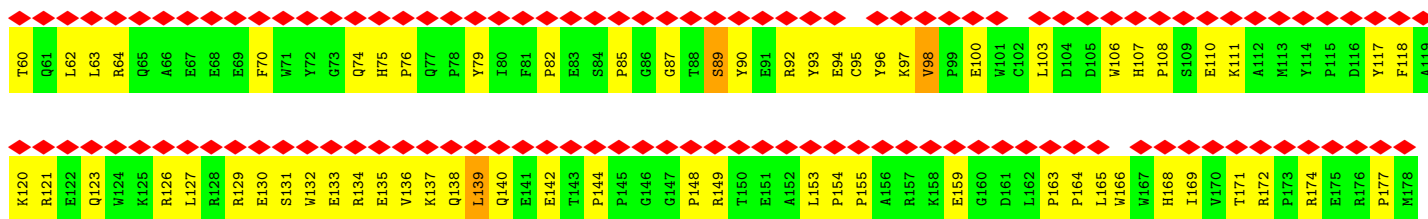


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

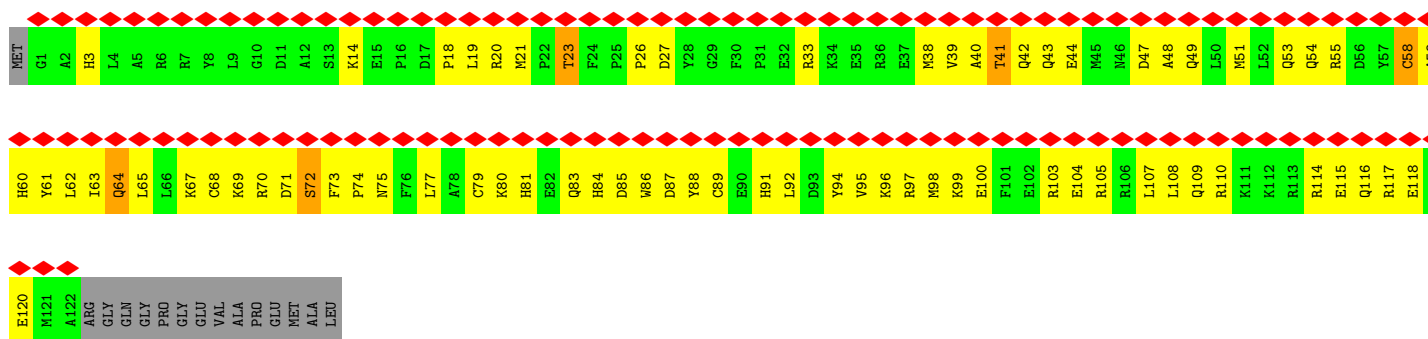
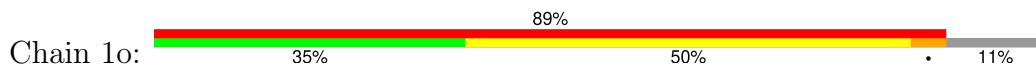


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

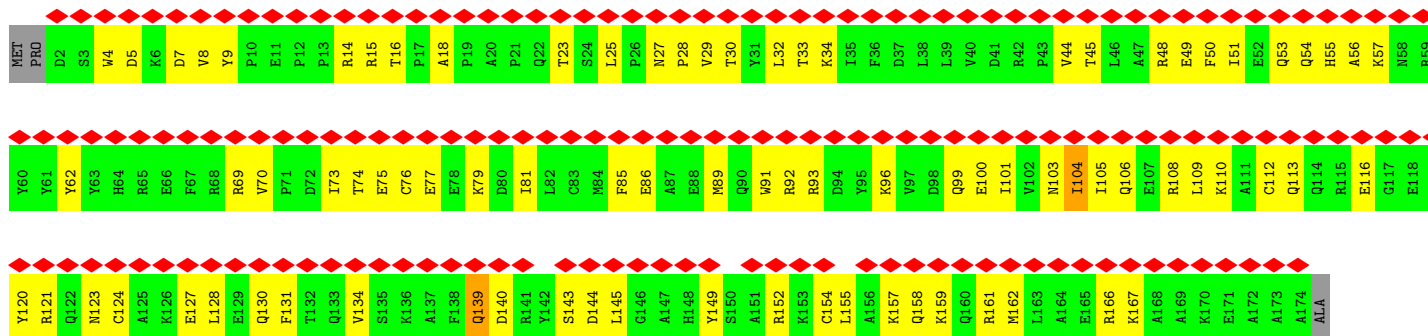




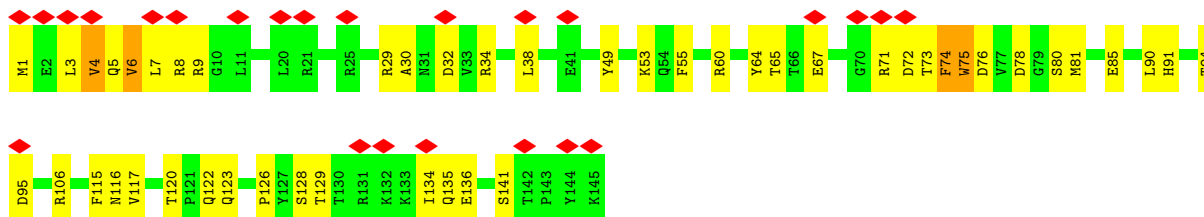
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



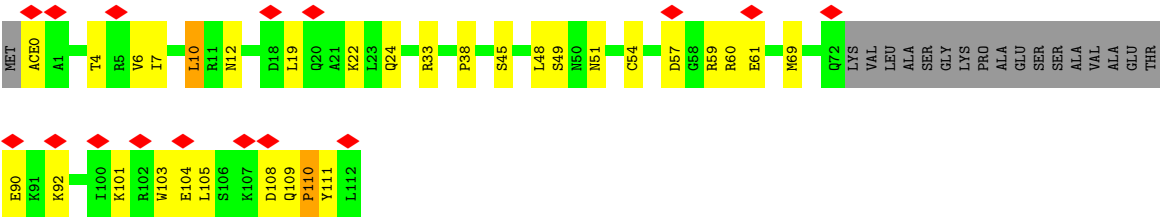
• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



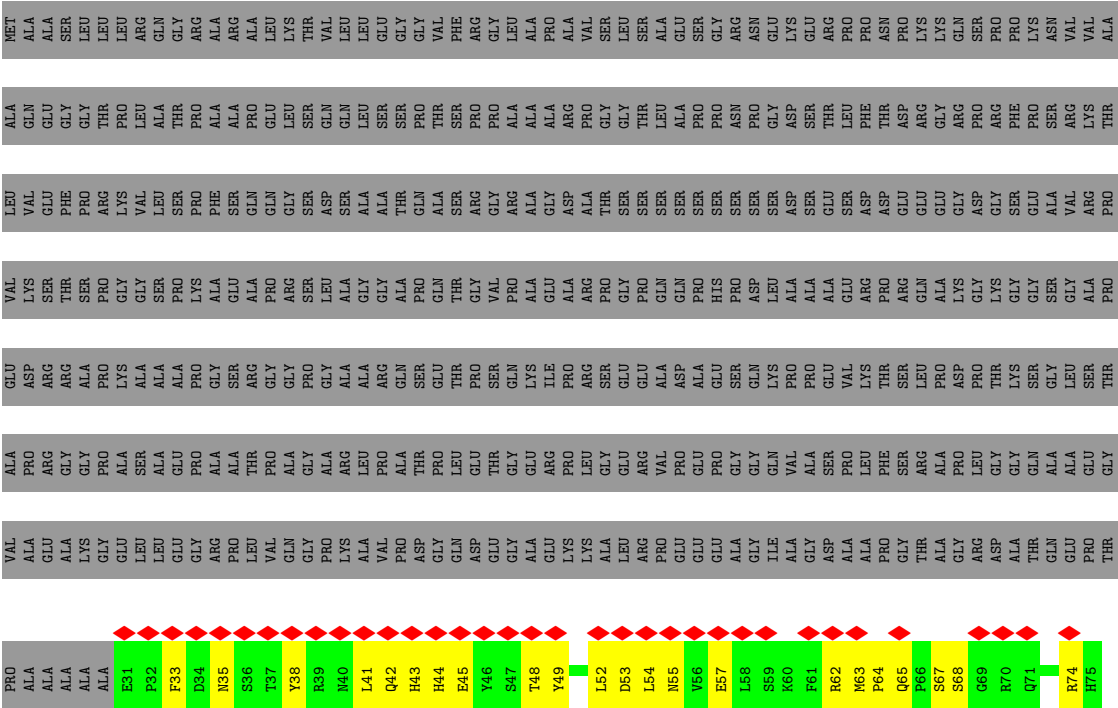
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.924	Depositor
Minimum map value	-0.272	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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, GTP, SAC, PC1, CDL, FES, U10, K, MYR, NDP, FME, FMN, 3PE, SF4, MG, ACE, ZN

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	0.20	0/930	0.55	1/1271 (0.1%)
2	1B	0.21	0/1273	0.44	0/1722
3	1C	0.17	0/1791	0.38	0/2439
4	1D	0.17	0/3545	0.36	1/4806 (0.0%)
5	1E	0.16	0/1698	0.40	0/2311
6	1F	0.15	0/3401	0.38	0/4595
7	1G	0.16	0/5451	0.39	0/7387
8	1H	0.19	0/2566	0.43	0/3509
9	1I	0.19	0/1443	0.39	0/1952
10	1J	0.18	0/1364	0.49	0/1850
11	1K	0.21	0/751	0.57	0/1018
12	1L	0.18	0/4939	0.52	2/6718 (0.0%)
13	1M	0.18	0/3713	0.51	1/5063 (0.0%)
14	1N	0.22	0/2765	0.53	2/3758 (0.1%)
15	1O	0.17	0/2650	0.47	1/3588 (0.0%)
16	1P	0.14	0/2828	0.33	0/3834
17	1Q	0.17	0/1070	0.43	0/1446
18	1R	0.15	0/755	0.43	0/1018
19	1S	0.17	0/711	0.45	0/956
20	1T	0.22	0/701	0.67	0/946
20	1U	0.24	0/706	0.68	2/954 (0.2%)
21	1V	0.17	0/946	0.43	0/1281
22	1W	0.19	0/995	0.52	0/1340
23	1X	0.13	0/1436	0.34	0/1938
24	1Y	0.16	0/1037	0.47	0/1404
25	1Z	0.17	0/1199	0.41	0/1617
26	1a	0.17	0/577	0.32	0/777
27	1b	0.14	0/664	0.42	0/912
28	1c	0.19	0/430	0.56	0/581
29	1d	0.17	0/1024	0.39	0/1383
30	1e	0.19	0/836	0.47	0/1118
31	1f	0.21	0/499	0.60	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.23	0/858	0.66	1/1165 (0.1%)
33	1h	0.15	0/1184	0.40	0/1603
34	1i	0.19	0/1131	0.55	0/1541
35	1j	0.20	0/627	0.54	0/858
36	1k	0.14	0/668	0.40	0/903
37	1l	0.17	0/1365	0.50	0/1867
38	1m	0.16	0/1092	0.41	0/1481
39	1n	0.17	0/1549	0.50	0/2098
40	1o	0.25	1/1069 (0.1%)	0.61	3/1430 (0.2%)
41	1p	0.14	0/1481	0.37	0/1997
42	1q	0.16	0/1253	0.40	0/1704
43	1r	0.21	0/782	0.54	1/1057 (0.1%)
44	1s	0.17	0/394	0.55	0/533
All	All	0.18	1/68147 (0.0%)	0.46	15/92402 (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
6	1F	0	2
8	1H	0	1
9	1I	0	1
14	1N	0	1
42	1q	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	1o	26	PRO	CG-CD	-6.25	1.29	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	1o	26	PRO	N-CD-CG	-10.96	86.76	103.20
43	1r	110	PRO	CA-N-CD	-8.22	100.48	112.00
32	1g	85	MET	CB-CG-SD	7.28	134.54	112.70
40	1o	26	PRO	CA-CB-CG	-6.67	91.84	104.50
40	1o	26	PRO	CA-N-CD	-6.28	103.21	112.00
14	1N	323	MET	N-CA-CB	6.22	121.00	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1O	226	ARG	CB-CG-CD	5.65	124.29	111.30
13	1M	84	LEU	CA-CB-CG	5.51	135.59	116.30
1	1A	50	PRO	CA-N-CD	-5.29	104.60	112.00
4	1D	276	ASP	CB-CA-C	-5.18	110.61	116.63
20	1U	21	LEU	CA-CB-CG	5.18	134.42	116.30
20	1U	4	PRO	CA-N-CD	-5.14	104.81	112.00
12	1L	382	GLY	CA-C-N	-5.14	107.47	122.21
12	1L	382	GLY	C-N-CA	-5.14	107.47	122.21
14	1N	323	MET	CA-CB-CG	5.05	124.20	114.10

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
6	1F	207	PRO	Peptide
8	1H	141	SER	Peptide
9	1I	50	TYR	Peptide
14	1N	322	GLN	Peptide
42	1q	74	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	62	0
2	1B	1242	0	1249	70	0
3	1C	1740	0	1691	56	0
4	1D	3452	0	3389	169	0
5	1E	1658	0	1662	94	0
6	1F	3325	0	3288	162	0
7	1G	5362	0	5388	243	0
8	1H	2504	0	2602	144	0
9	1I	1412	0	1366	94	0
10	1J	1339	0	1337	93	0
11	1K	750	0	798	65	0
12	1L	4818	0	4953	386	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	1M	3632	0	3836	300	0
14	1N	2712	0	2868	199	0
15	1O	2590	0	2556	160	0
16	1P	2751	0	2776	86	0
17	1Q	1047	0	1042	35	0
18	1R	741	0	704	22	0
19	1S	700	0	719	40	0
20	1T	689	0	687	58	0
20	1U	694	0	691	78	0
21	1V	927	0	972	47	0
22	1W	971	0	975	56	0
23	1X	1398	0	1378	58	0
24	1Y	1016	0	1020	55	0
25	1Z	1168	0	1161	77	0
26	1a	562	0	557	24	0
27	1b	643	0	645	25	0
28	1c	417	0	425	28	0
29	1d	996	0	989	46	0
30	1e	816	0	823	52	0
31	1f	487	0	498	35	0
32	1g	835	0	795	69	0
33	1h	1151	0	1164	72	0
34	1i	1100	0	1106	95	0
35	1j	601	0	546	41	0
36	1k	649	0	626	62	0
37	1l	1310	0	1204	100	0
38	1m	1062	0	1075	85	0
39	1n	1495	0	1434	128	0
40	1o	1045	0	1018	89	0
41	1p	1449	0	1416	97	0
42	1q	1212	0	1174	40	0
43	1r	767	0	791	26	0
44	1s	382	0	351	24	0
45	1B	8	0	0	1	0
45	1F	8	0	0	3	0
45	1G	16	0	0	8	0
45	1I	16	0	0	4	0
46	1B	34	0	42	1	0
46	1Y	35	0	44	2	0
46	1d	39	0	50	9	0
46	1h	34	0	42	2	0
46	1m	46	0	64	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1q	48	0	68	2	0
47	1E	4	0	0	1	0
47	1G	4	0	0	1	0
48	1F	31	0	19	2	0
49	1G	1	0	0	0	0
50	1H	63	0	90	11	0
51	1H	51	0	46	2	0
51	1O	67	0	78	8	0
51	1a	61	0	64	4	0
52	1N	38	0	50	6	0
52	1Y	35	0	43	2	0
52	1g	51	0	81	5	0
52	1n	42	0	52	4	0
53	1O	32	0	12	3	0
54	1O	1	0	0	0	0
55	1P	48	0	26	1	0
56	1R	1	0	0	0	0
57	1W	37	0	0	1	0
57	1n	37	0	0	0	0
58	1l	15	0	27	1	0
All	All	67436	0	67593	3425	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 (3425) 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)
14:1N:217:MET:HE3	51:1O:403:CDL:H711	1.36	1.04
10:1J:172:THR:HA	11:1K:80:MET:HE1	1.45	0.94
13:1M:450:ASN:HB3	13:1M:453:MET:HE1	1.50	0.93
7:1G:156:CYS:HB2	45:1G:802:SF4:S4	2.09	0.91
23:1X:6:LEU:HB2	25:1Z:88:ARG:HH21	1.34	0.90
7:1G:105:CYS:HA	7:1G:108:CYS:HB3	1.53	0.89
12:1L:359:MET:HE1	12:1L:362:LEU:HB2	1.55	0.89
7:1G:153:CYS:HB2	45:1G:802:SF4:S3	2.12	0.89
25:1Z:83:VAL:HG23	25:1Z:124:LEU:HD11	1.53	0.89
25:1Z:94:GLU:HA	25:1Z:97:ILE:HD12	1.54	0.88
7:1G:155:GLN:HG3	7:1G:181:MET:HE1	1.54	0.88
23:1X:146:ARG:HH22	30:1e:41:GLU:HG3	1.39	0.88
12:1L:123:LEU:HB2	12:1L:150:MET:HE1	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:94:CYS:HB2	24:1Y:114:CYS:HA	1.55	0.88
25:1Z:108:GLU:H	30:1e:74:ARG:HH22	1.23	0.86
7:1G:54:MET:HE1	7:1G:94:MET:HB2	1.55	0.86
1:1A:42:ASP:H	22:1W:99:GLN:HE22	1.21	0.86
2:1B:69:MET:HG3	2:1B:74:VAL:HG21	1.58	0.85
5:1E:104:THR:HG23	6:1F:349:ARG:HE	1.40	0.84
7:1G:41:CYS:SG	7:1G:52:CYS:HB2	2.16	0.83
20:1U:36:PHE:H	20:1U:71:MET:HE1	1.42	0.83
5:1E:101:GLN:HE22	5:1E:140:ILE:HG23	1.44	0.83
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.60	0.83
8:1H:31:MET:HE1	8:1H:272:TRP:HA	1.60	0.83
14:1N:112:HIS:HB2	14:1N:184:ILE:HD13	1.59	0.83
12:1L:486:MET:HE3	12:1L:486:MET:H	1.44	0.82
35:1j:14:PHE:HD2	35:1j:15:PRO:HD2	1.44	0.82
6:1F:205:LEU:HD11	7:1G:50:GLY:HA3	1.60	0.82
15:1O:61:SER:HA	15:1O:66:GLY:HA2	1.60	0.81
5:1E:214:GLN:HE21	5:1E:217:LEU:HD21	1.45	0.81
22:1W:70:ASN:HD21	22:1W:82:LEU:HD22	1.45	0.81
39:1n:14:LYS:HD3	39:1n:63:LEU:HD11	1.61	0.80
34:1i:42:MET:HE3	34:1i:42:MET:H	1.46	0.80
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.63	0.80
12:1L:305:SER:OG	12:1L:336:LYS:NZ	2.14	0.80
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.64	0.80
32:1g:107:LEU:HD11	41:1p:134:VAL:HG22	1.62	0.79
12:1L:500:LEU:HD22	52:1n:202:3PE:H362	1.65	0.79
34:1i:100:LYS:HB2	41:1p:14:ARG:HH22	1.46	0.79
37:1l:36:PRO:HA	37:1l:48:PRO:HA	1.66	0.78
15:1O:37:ARG:HA	15:1O:40:ARG:HG2	1.66	0.78
29:1d:78:ARG:HH22	46:1d:201:PC1:H251	1.49	0.78
12:1L:328:HIS:ND1	12:1L:391:SER:OG	2.16	0.77
13:1M:412:ILE:HA	13:1M:416:ARG:HB3	1.64	0.77
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.67	0.77
4:1D:106:LEU:HD11	4:1D:391:ILE:HD13	1.66	0.77
37:1l:85:ILE:HD12	37:1l:88:ARG:H	1.49	0.77
14:1N:215:MET:HA	14:1N:215:MET:HE2	1.66	0.77
27:1b:24:ILE:HA	27:1b:27:LEU:HD12	1.66	0.77
10:1J:127:ILE:HD12	11:1K:2:PRO:HG3	1.66	0.77
7:1G:534:ARG:HH11	7:1G:543:ILE:HD13	1.50	0.77
8:1H:62:ARG:HG3	8:1H:68:ILE:HD11	1.67	0.77
12:1L:483:PRO:HB2	12:1L:486:MET:HE1	1.66	0.77
13:1M:176:PHE:HB3	13:1M:245:ARG:HH21	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:73:ILE:HA	41:1p:76:CYS:HB3	1.66	0.77
11:1K:59:MET:HG2	14:1N:27:LEU:HD22	1.66	0.77
17:1Q:30:ILE:HG23	17:1Q:31:LYS:HD3	1.68	0.76
5:1E:27:ASN:HA	5:1E:30:ARG:HD2	1.68	0.76
12:1L:542:LEU:HB2	37:1l:83:MET:HE1	1.67	0.76
12:1L:114:ILE:HD12	12:1L:114:ILE:H	1.51	0.76
13:1M:87:GLU:O	13:1M:92:LYS:NZ	2.15	0.76
2:1B:179:ARG:HG3	16:1P:50:ARG:HH12	1.50	0.76
22:1W:57:LYS:O	22:1W:57:LYS:NZ	2.18	0.76
15:1O:309:ASN:ND2	28:1c:3:TYR:OH	2.18	0.75
4:1D:281:VAL:HG11	4:1D:310:ILE:HG23	1.67	0.75
12:1L:274:GLN:O	12:1L:277:THR:OG1	2.04	0.75
34:1i:119:MET:HE1	40:1o:63:ILE:HG12	1.67	0.75
35:1j:67:LEU:HD12	40:1o:110:ARG:HH12	1.51	0.75
32:1g:56:TRP:HZ2	52:1g:201:3PE:H322	1.52	0.75
10:1J:64:MET:HA	10:1J:64:MET:HE3	1.68	0.75
20:1U:54:MET:HE1	20:1U:76:ILE:HG21	1.68	0.75
35:1j:8:GLU:O	35:1j:16:GLN:NE2	2.18	0.75
7:1G:112:GLY:HA3	7:1G:219:PRO:HG2	1.68	0.75
14:1N:312:LYS:HD2	15:1O:75:GLY:H	1.52	0.75
10:1J:163:ILE:HG12	14:1N:12:THR:HG21	1.69	0.75
12:1L:121:LEU:HD12	12:1L:246:LEU:HD23	1.69	0.75
13:1M:410:MET:HE3	13:1M:410:MET:H	1.51	0.75
37:1l:53:ARG:HE	37:1l:58:ARG:HG2	1.52	0.75
7:1G:27:LEU:HD21	7:1G:39:ARG:HH21	1.50	0.74
6:1F:101:GLU:O	6:1F:104:THR:OG1	2.05	0.74
10:1J:9:LEU:HD12	10:1J:39:VAL:HG23	1.68	0.74
31:1f:37:PHE:HA	31:1f:40:LYS:HE2	1.68	0.74
34:1i:100:LYS:O	40:1o:49:GLN:NE2	2.21	0.74
14:1N:68:MET:HA	14:1N:68:MET:HE3	1.70	0.74
13:1M:294:MET:HA	13:1M:294:MET:HE3	1.70	0.74
12:1L:234:PRO:HG3	12:1L:304:PHE:HE1	1.50	0.74
13:1M:247:THR:HA	13:1M:250:LEU:HD12	1.70	0.74
29:1d:17:GLU:N	29:1d:17:GLU:OE2	2.21	0.74
3:1C:40:VAL:HG22	43:1r:69:MET:HE3	1.68	0.74
35:1j:9:PRO:HA	35:1j:16:GLN:HE22	1.50	0.74
37:1l:112:MET:O	37:1l:116:PHE:N	2.17	0.74
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.70	0.73
38:1m:43:LYS:HA	38:1m:43:LYS:HE2	1.68	0.73
38:1m:48:LEU:HD23	39:1n:165:LEU:HD21	1.70	0.73
7:1G:41:CYS:SG	7:1G:52:CYS:CB	2.76	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:256:GLU:O	7:1G:394:ARG:NH2	2.22	0.73
13:1M:334:TYR:O	13:1M:338:HIS:N	2.18	0.73
39:1n:23:LEU:HA	39:1n:26:LEU:HB2	1.70	0.73
29:1d:107:LYS:HE2	29:1d:107:LYS:HA	1.69	0.73
22:1W:23:ARG:NH1	22:1W:23:ARG:HA	2.03	0.73
12:1L:525:MET:N	12:1L:525:MET:SD	2.61	0.73
7:1G:60:GLU:HG3	7:1G:61:LYS:HG3	1.69	0.73
10:1J:167:VAL:HG23	14:1N:42:PRO:HG3	1.69	0.73
2:1B:71:ARG:HH21	8:1H:38:ASN:HD21	1.37	0.73
5:1E:97:LYS:HD2	5:1E:136:LEU:HD22	1.70	0.73
10:1J:55:MET:HA	10:1J:55:MET:HE3	1.69	0.73
35:1j:45:ASP:HB2	35:1j:50:HIS:HB3	1.69	0.73
5:1E:30:ARG:NH1	44:1s:53:ASP:OD1	2.22	0.73
9:1I:27:TRP:HB3	9:1I:30:LEU:HD23	1.69	0.73
51:1H:402:CDL:H722	51:1H:402:CDL:H521	1.71	0.72
30:1e:44:HIS:HD2	33:1h:129:ASP:HA	1.54	0.72
14:1N:272:LYS:HG2	33:1h:108:LEU:HD11	1.70	0.72
40:1o:48:ALA:HB2	40:1o:63:ILE:HD12	1.70	0.72
4:1D:72:MET:N	4:1D:72:MET:SD	2.63	0.72
40:1o:14:LYS:HB2	40:1o:109:GLN:HE22	1.52	0.72
12:1L:421:ALA:HB1	52:1n:202:3PE:H351	1.71	0.72
5:1E:68:LYS:HD3	5:1E:72:ILE:HD11	1.71	0.72
32:1g:85:MET:HE2	32:1g:85:MET:O	1.89	0.72
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	1.72	0.72
15:1O:52:PRO:O	15:1O:107:GLN:NE2	2.22	0.72
8:1H:24:GLU:HG3	8:1H:271:LEU:HD22	1.72	0.72
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.71	0.72
35:1j:10:ARG:HD3	35:1j:13:GLN:HB2	1.72	0.72
1:1A:90:MET:HA	1:1A:90:MET:HE3	1.72	0.71
7:1G:36:GLN:HG2	7:1G:39:ARG:HH22	1.56	0.71
12:1L:508:THR:O	39:1n:35:LYS:NZ	2.16	0.71
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.71	0.71
32:1g:64:PHE:HB3	32:1g:68:ILE:HD11	1.70	0.71
34:1i:13:GLN:HB3	39:1n:163:PRO:HG3	1.72	0.71
39:1n:153:LEU:HD12	39:1n:154:PRO:HD2	1.70	0.71
41:1p:89:MET:HA	41:1p:89:MET:HE3	1.71	0.71
33:1h:76:ALA:HA	33:1h:80:TYR:HB2	1.73	0.71
19:1S:19:ARG:HG3	19:1S:53:LEU:HB2	1.70	0.71
20:1T:52:MET:HE1	22:1W:37:ARG:HD2	1.72	0.71
4:1D:64:LEU:HD21	4:1D:76:CYS:HB3	1.72	0.71
15:1O:301:GLY:O	15:1O:309:ASN:ND2	2.23	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:50:HIS:HB2	15:1O:123:VAL:HB	1.73	0.71
1:1A:40:GLY:HA2	2:1B:103:VAL:HG23	1.73	0.71
9:1I:62:ARG:NH1	9:1I:119:CYS:O	2.24	0.71
11:1K:44:SER:HB2	11:1K:59:MET:HE1	1.72	0.71
12:1L:156:GLY:O	13:1M:416:ARG:NH2	2.24	0.71
23:1X:134:ARG:O	27:1b:57:ARG:NH1	2.24	0.71
4:1D:170:MET:HE1	4:1D:225:LEU:HB2	1.72	0.70
11:1K:20:LEU:HB3	12:1L:588:PHE:HB3	1.73	0.70
20:1T:26:ASP:HB3	20:1T:29:LYS:HD3	1.72	0.70
43:1r:104:GLU:N	43:1r:104:GLU:OE2	2.23	0.70
3:1C:94:TYR:HB2	3:1C:107:VAL:HG23	1.72	0.70
38:1m:113:LYS:O	38:1m:119:LYS:NZ	2.25	0.70
7:1G:347:GLU:HA	7:1G:459:GLN:HE22	1.56	0.70
7:1G:377:ILE:HG13	7:1G:450:MET:HG2	1.74	0.70
36:1k:28:LEU:HD22	36:1k:45:GLY:HA2	1.73	0.70
13:1M:411:LEU:HB3	13:1M:415:GLN:HE21	1.55	0.70
12:1L:386:LEU:HD23	12:1L:462:ILE:HA	1.73	0.70
15:1O:242:LYS:HD2	15:1O:244:ASP:H	1.56	0.70
17:1Q:28:GLU:O	17:1Q:32:THR:OG1	2.10	0.70
4:1D:19:MET:SD	14:1N:295:ARG:NH2	2.64	0.70
5:1E:111:ARG:HB2	5:1E:152:PRO:HD3	1.72	0.70
12:1L:14:ILE:HD11	12:1L:43:ALA:HB2	1.74	0.70
12:1L:357:ARG:HB3	39:1n:31:VAL:HG22	1.74	0.70
18:1R:46:GLU:OE1	18:1R:46:GLU:N	2.21	0.70
23:1X:7:PRO:O	25:1Z:88:ARG:NH2	2.25	0.70
40:1o:69:LYS:HA	40:1o:72:SER:HB3	1.74	0.70
13:1M:40:SER:O	13:1M:43:ASN:ND2	2.24	0.70
4:1D:151:ILE:O	4:1D:155:THR:OG1	2.08	0.70
11:1K:90:VAL:HG23	11:1K:93:LEU:HD21	1.74	0.70
12:1L:439:PRO:HB3	35:1j:12:ARG:HE	1.57	0.70
22:1W:25:MET:HE2	22:1W:25:MET:H	1.56	0.69
12:1L:499:MET:HA	12:1L:502:LEU:HB2	1.72	0.69
39:1n:63:LEU:HD12	39:1n:64:ARG:HH21	1.56	0.69
1:1A:57:LEU:HD23	10:1J:172:THR:HG21	1.74	0.69
13:1M:370:PRO:HD3	13:1M:375:LEU:HG	1.74	0.69
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.10	0.69
7:1G:105:CYS:HB3	45:1G:801:SF4:S4	2.31	0.69
13:1M:346:ARG:NE	37:1l:68:ASP:OD2	2.26	0.69
7:1G:358:LEU:HD22	7:1G:645:ALA:HB2	1.74	0.69
14:1N:339:MET:HA	14:1N:339:MET:HE3	1.74	0.69
15:1O:108:TYR:HD2	15:1O:128:ILE:HD12	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:26:LEU:HA	31:1f:29:ARG:HB3	1.75	0.69
6:1F:433:PHE:HA	6:1F:436:GLN:HE21	1.58	0.69
11:1K:5:TYR:HD1	11:1K:43:MET:HE1	1.57	0.69
6:1F:349:ARG:NH1	6:1F:349:ARG:O	2.26	0.69
6:1F:368:GLY:HA3	6:1F:399:ILE:HD11	1.74	0.69
14:1N:34:GLU:HA	14:1N:37:LEU:HB3	1.75	0.69
20:1U:78:ASP:OD1	34:1i:15:ARG:NH2	2.26	0.69
29:1d:106:LYS:HD2	41:1p:77:GLU:HG3	1.75	0.69
34:1i:71:VAL:HA	34:1i:75:LEU:HB3	1.75	0.69
6:1F:61:LYS:NZ	6:1F:80:SER:OG	2.25	0.69
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.58	0.69
9:1I:7:MET:SD	9:1I:8:ARG:NH1	2.66	0.69
15:1O:104:ARG:NH2	53:1O:401:GTP:N7	2.41	0.69
16:1P:175:GLU:OE2	16:1P:175:GLU:N	2.23	0.69
29:1d:100:ASP:OD1	29:1d:100:ASP:N	2.21	0.69
14:1N:69:MET:HB3	14:1N:97:MET:HE1	1.75	0.69
15:1O:299:LEU:HD22	15:1O:300:PRO:HD2	1.75	0.69
20:1U:44:SER:HB2	39:1n:16:LEU:HD11	1.75	0.69
40:1o:74:PRO:HG3	41:1p:27:ASN:HA	1.74	0.69
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.25	0.68
14:1N:159:MET:O	14:1N:159:MET:HE3	1.93	0.68
20:1T:55:GLU:OE2	20:1T:55:GLU:N	2.23	0.68
3:1C:89:ARG:HH12	3:1C:163:ARG:HD2	1.57	0.68
12:1L:221:ALA:HA	12:1L:226:GLN:HB2	1.74	0.68
14:1N:269:GLU:HA	14:1N:272:LYS:HD3	1.75	0.68
15:1O:40:ARG:NH1	15:1O:40:ARG:HA	2.08	0.68
37:1l:8:MET:SD	37:1l:8:MET:N	2.60	0.68
37:1l:14:PRO:O	37:1l:20:ARG:NH2	2.26	0.68
15:1O:165:PRO:O	15:1O:248:TRP:NE1	2.22	0.68
13:1M:335:GLU:N	13:1M:335:GLU:OE2	2.27	0.68
32:1g:70:LEU:O	32:1g:74:SER:OG	2.10	0.68
9:1I:50:TYR:O	9:1I:52:PHE:N	2.27	0.68
15:1O:102:ALA:HA	15:1O:105:LEU:HD12	1.75	0.68
20:1U:36:PHE:N	20:1U:71:MET:HE1	2.08	0.68
7:1G:372:GLU:O	7:1G:402:ASN:ND2	2.27	0.68
12:1L:29:THR:O	12:1L:115:ASN:ND2	2.27	0.68
12:1L:338:MET:HE1	12:1L:458:LEU:HD23	1.75	0.68
13:1M:418:LYS:HE3	37:1l:68:ASP:HA	1.75	0.68
22:1W:34:GLU:OE2	22:1W:34:GLU:N	2.23	0.68
25:1Z:97:ILE:HG22	25:1Z:98:MET:HE3	1.76	0.68
33:1h:129:ASP:OD1	33:1h:131:ALA:N	2.25	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:13:LEU:HD11	38:1m:17:LEU:HD22	1.76	0.68
5:1E:202:LEU:O	44:1s:35:ASN:ND2	2.27	0.68
7:1G:615:THR:HG22	7:1G:618:GLN:HE21	1.58	0.68
13:1M:24:TRP:HE1	13:1M:92:LYS:HG2	1.57	0.68
17:1Q:33:ARG:NH2	17:1Q:60:ASP:O	2.27	0.68
38:1m:7:PRO:HD3	38:1m:13:LEU:HD13	1.76	0.68
1:1A:53:MET:HE1	1:1A:56:PHE:HB3	1.76	0.68
7:1G:213:TYR:O	7:1G:216:THR:OG1	2.11	0.67
12:1L:89:PHE:HE2	12:1L:329:ILE:HD12	1.59	0.67
17:1Q:66:GLU:N	17:1Q:66:GLU:OE2	2.28	0.67
8:1H:157:ASN:HD21	8:1H:164:THR:HG23	1.59	0.67
7:1G:13:VAL:HG23	7:1G:79:ILE:HB	1.76	0.67
20:1U:23:ASP:N	20:1U:23:ASP:OD1	2.27	0.67
10:1J:130:THR:HG22	25:1Z:121:MET:HB2	1.77	0.67
12:1L:104:SER:O	12:1L:108:MET:N	2.27	0.67
13:1M:263:MET:SD	38:1m:101:TYR:HB2	2.34	0.67
34:1i:70:ALA:O	34:1i:75:LEU:N	2.20	0.67
3:1C:205:ALA:HA	7:1G:122:MET:HE2	1.76	0.67
4:1D:335:ARG:HG3	9:1I:176:ARG:HG3	1.76	0.67
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.76	0.67
8:1H:283:ASP:OD1	8:1H:284:GLN:N	2.28	0.67
14:1N:106:LEU:HD22	14:1N:187:MET:HE2	1.77	0.67
20:1T:12:LYS:HE2	20:1T:77:VAL:HG11	1.75	0.67
20:1U:35:HIS:HB2	20:1U:72:CYS:SG	2.35	0.67
7:1G:187:ILE:HD11	7:1G:189:LYS:HE2	1.77	0.67
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.77	0.67
8:1H:24:GLU:OE1	8:1H:228:TYR:OH	2.13	0.67
12:1L:99:SER:O	12:1L:453:SER:OG	2.12	0.67
19:1S:64:LEU:HB2	19:1S:78:LEU:HD11	1.76	0.67
39:1n:136:VAL:O	39:1n:140:GLN:NE2	2.28	0.67
8:1H:76:ILE:HD13	8:1H:222:MET:HE1	1.77	0.66
10:1J:1:FME:SD	10:1J:2:THR:N	2.67	0.66
32:1g:90:ARG:NH1	41:1p:100:GLU:OE1	2.28	0.66
37:1l:102:CYS:O	37:1l:106:SER:OG	2.10	0.66
40:1o:87:ASP:O	40:1o:91:HIS:N	2.28	0.66
43:1r:90:GLU:OE2	43:1r:92:LYS:NZ	2.28	0.66
2:1B:125:TYR:HD2	9:1I:117:ILE:HG12	1.60	0.66
7:1G:337:ARG:HE	7:1G:609:MET:HB2	1.60	0.66
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.27	0.66
17:1Q:10:LEU:HB3	22:1W:16:SER:HB2	1.76	0.66
39:1n:159:GLU:N	39:1n:159:GLU:OE2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:96:LEU:HD12	14:1N:51:ARG:HH21	1.60	0.66
12:1L:596:MET:O	12:1L:600:THR:N	2.21	0.66
18:1R:37:GLU:N	18:1R:37:GLU:OE2	2.28	0.66
1:1A:67:LEU:HD11	11:1K:68:ALA:HB3	1.76	0.66
7:1G:308:GLN:NE2	7:1G:607:ALA:O	2.28	0.66
12:1L:558:LEU:HG	13:1M:211:GLY:HA2	1.77	0.66
15:1O:224:SER:HB2	15:1O:226:ARG:NH2	2.10	0.66
16:1P:297:LEU:HD12	16:1P:298:PRO:HD2	1.77	0.66
7:1G:356:THR:O	19:1S:55:ARG:NH2	2.26	0.66
13:1M:393:ILE:O	13:1M:397:GLY:N	2.23	0.66
15:1O:38:LEU:HD11	15:1O:234:VAL:HG11	1.78	0.66
20:1U:19:LEU:HB2	20:1U:30:LEU:HD11	1.78	0.66
2:1B:137:ASP:OD1	2:1B:137:ASP:N	2.29	0.66
6:1F:132:ARG:NH2	44:1s:64:PRO:O	2.28	0.66
10:1J:130:THR:O	10:1J:130:THR:OG1	2.14	0.66
12:1L:62:ILE:HD11	12:1L:81:LYS:HD3	1.78	0.66
12:1L:200:GLN:NE2	41:1p:106:GLN:OE1	2.27	0.66
28:1c:40:LEU:HA	28:1c:43:LYS:HG2	1.78	0.66
4:1D:393:ALA:HB1	4:1D:427:GLU:HG3	1.78	0.66
20:1T:43:ASP:OD1	20:1T:44:SER:N	2.29	0.66
6:1F:287:VAL:HG11	6:1F:294:LEU:HB2	1.78	0.66
7:1G:648:LEU:HD21	19:1S:44:LYS:HG2	1.77	0.66
12:1L:142:ILE:HG12	13:1M:370:PRO:HB2	1.76	0.66
12:1L:161:ARG:NH1	12:1L:238:GLU:OE1	2.29	0.66
16:1P:90:VAL:HG11	16:1P:218:ILE:HG12	1.77	0.66
34:1i:18:ARG:NH1	39:1n:172:ARG:O	2.28	0.66
34:1i:26:GLU:OE1	34:1i:26:GLU:N	2.29	0.66
5:1E:116:ILE:HD12	5:1E:152:PRO:HB2	1.79	0.65
13:1M:286:ILE:HG12	13:1M:326:LEU:HB3	1.76	0.65
36:1k:46:ARG:HE	36:1k:46:ARG:H	1.42	0.65
39:1n:82:PRO:HA	39:1n:87:GLY:HA3	1.78	0.65
40:1o:95:VAL:O	40:1o:99:LYS:N	2.26	0.65
7:1G:45:ARG:NH1	7:1G:260:GLU:OE1	2.30	0.65
14:1N:294:MET:HE2	14:1N:294:MET:HA	1.78	0.65
2:1B:52:LEU:HG	2:1B:96:MET:HE1	1.78	0.65
6:1F:32:ARG:NH1	44:1s:42:GLN:OE1	2.29	0.65
11:1K:80:MET:HA	11:1K:83:ASN:HB2	1.78	0.65
13:1M:126:LEU:HD11	14:1N:254:LEU:HD22	1.77	0.65
14:1N:44:LEU:HD13	14:1N:122:ILE:HG21	1.77	0.65
20:1U:82:ASP:OD1	34:1i:19:ARG:NH2	2.28	0.65
3:1C:150:ARG:NH2	3:1C:157:PHE:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.13	0.65
7:1G:190:MET:HE2	7:1G:190:MET:HA	1.77	0.65
10:1J:35:VAL:O	10:1J:39:VAL:HG12	1.96	0.65
12:1L:83:ASP:H	12:1L:86:SER:HB2	1.61	0.65
14:1N:59:TYR:HE2	14:1N:63:GLN:HE21	1.42	0.65
4:1D:15:GLY:HA2	14:1N:228:LEU:HD21	1.78	0.65
20:1U:80:ILE:H	20:1U:80:ILE:HD12	1.60	0.65
40:1o:59:ALA:HA	40:1o:62:LEU:HD12	1.78	0.65
11:1K:37:MET:HG3	11:1K:67:ALA:HB1	1.78	0.65
12:1L:20:MET:O	12:1L:24:SER:OG	2.15	0.65
13:1M:102:LEU:HD11	13:1M:235:LEU:HD11	1.77	0.65
24:1Y:85:ASP:O	24:1Y:88:ASN:ND2	2.29	0.65
40:1o:100:GLU:OE2	40:1o:103:ARG:NH2	2.27	0.65
8:1H:47:GLN:NE2	8:1H:51:ASP:OD2	2.29	0.65
13:1M:318:ALA:O	13:1M:322:THR:OG1	2.13	0.65
14:1N:320:THR:O	14:1N:322:GLN:NE2	2.30	0.65
34:1i:107:ASP:OD1	40:1o:70:ARG:NH1	2.30	0.65
5:1E:103:CYS:SG	5:1E:105:THR:OG1	2.54	0.65
7:1G:255:HIS:ND1	7:1G:255:HIS:O	2.30	0.65
12:1L:213:LEU:HD23	12:1L:216:LEU:HD12	1.79	0.65
22:1W:89:GLU:O	22:1W:93:THR:OG1	2.15	0.65
5:1E:22:ASP:O	5:1E:57:GLN:NE2	2.30	0.65
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.78	0.65
32:1g:95:ARG:HH12	32:1g:99:TYR:HB2	1.60	0.65
42:1q:5:GLN:HA	42:1q:8:ARG:HE	1.60	0.65
6:1F:381:LYS:O	6:1F:381:LYS:NZ	2.30	0.65
14:1N:316:GLN:OE1	15:1O:63:THR:OG1	2.14	0.65
16:1P:301:GLU:OE1	16:1P:301:GLU:N	2.29	0.65
36:1k:74:PHE:HA	36:1k:77:PHE:HD1	1.62	0.65
14:1N:255:PRO:HG3	14:1N:260:PHE:CG	2.31	0.64
19:1S:63:LYS:NZ	19:1S:64:LEU:O	2.22	0.64
31:1f:14:ILE:HG22	52:1g:201:3PE:H3H1	1.78	0.64
34:1i:116:ILE:HD12	34:1i:117:PRO:HD2	1.77	0.64
12:1L:279:CYS:HA	37:1l:116:PHE:CE1	2.32	0.64
7:1G:347:GLU:HB2	7:1G:499:GLN:HG3	1.80	0.64
16:1P:302:ASP:N	16:1P:302:ASP:OD1	2.30	0.64
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.14	0.64
2:1B:125:TYR:CD2	9:1I:117:ILE:HG12	2.31	0.64
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.14	0.64
4:1D:43:LEU:HD22	11:1K:86:GLY:HA3	1.78	0.64
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:155:ILE:HD11	12:1L:168:ALA:HB2	1.79	0.64
7:1G:55:CYS:HB3	47:1G:803:FES:S2	2.36	0.64
12:1L:132:VAL:O	12:1L:262:ARG:NH2	2.27	0.64
15:1O:3:TYR:HE2	15:1O:257:HIS:HA	1.62	0.64
22:1W:25:MET:HE2	22:1W:25:MET:N	2.12	0.64
33:1h:7:ARG:HH11	34:1i:27:LEU:HD23	1.61	0.64
38:1m:125:ASN:O	41:1p:139:GLN:NE2	2.31	0.64
13:1M:22:MET:O	13:1M:24:TRP:N	2.30	0.64
1:1A:38:GLU:HG2	1:1A:43:PRO:HA	1.80	0.64
13:1M:89:THR:HA	13:1M:92:LYS:HE2	1.80	0.64
13:1M:452:LYS:HG3	13:1M:453:MET:HE2	1.78	0.64
14:1N:251:MET:HB3	14:1N:293:TYR:CE2	2.32	0.64
20:1T:66:ASP:HA	20:1T:69:LYS:HZ2	1.62	0.64
12:1L:313:MET:HG3	12:1L:328:HIS:HB3	1.80	0.64
15:1O:101:TYR:HE1	15:1O:128:ILE:HG23	1.62	0.64
15:1O:176:VAL:HG11	15:1O:200:GLN:HG2	1.80	0.64
33:1h:24:LEU:HA	33:1h:27:PHE:HB3	1.80	0.64
2:1B:125:TYR:HE1	4:1D:102:TYR:CZ	2.16	0.64
8:1H:96:ILE:HG23	25:1Z:144:THR:HG21	1.79	0.64
11:1K:43:MET:HE2	11:1K:43:MET:HA	1.80	0.64
12:1L:60:GLU:H	34:1i:99:ARG:HD3	1.62	0.64
12:1L:363:TYR:HB2	12:1L:431:PHE:HB3	1.79	0.64
37:1l:96:VAL:HG13	37:1l:101:MET:HE1	1.79	0.64
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.16	0.64
23:1X:148:GLU:O	30:1e:50:ARG:NH2	2.30	0.64
30:1e:54:GLU:N	30:1e:54:GLU:OE2	2.30	0.64
40:1o:75:ASN:OD1	41:1p:23:THR:OG1	2.13	0.64
8:1H:316:PRO:HA	25:1Z:58:ARG:HH11	1.63	0.63
12:1L:70:THR:HA	12:1L:75:GLU:HA	1.80	0.63
12:1L:160:GLY:H	39:1n:95:CYS:HB3	1.63	0.63
20:1T:49:GLU:OE2	20:1T:49:GLU:N	2.21	0.63
25:1Z:105:LYS:HD2	25:1Z:108:GLU:HB2	1.80	0.63
5:1E:14:GLU:N	5:1E:14:GLU:OE2	2.30	0.63
5:1E:162:GLU:OE2	6:1F:108:ARG:NH2	2.31	0.63
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.32	0.63
40:1o:107:LEU:HD23	40:1o:110:ARG:HD2	1.80	0.63
7:1G:704:CYS:SG	9:1I:104:ARG:NH1	2.71	0.63
14:1N:217:MET:HB2	14:1N:326:LEU:HD13	1.80	0.63
20:1U:60:PHE:HE2	20:1U:62:ILE:HB	1.61	0.63
5:1E:69:VAL:HA	5:1E:72:ILE:HD12	1.80	0.63
6:1F:338:ASP:OD1	6:1F:341:THR:OG1	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:133:LEU:HD21	10:1J:72:THR:HG21	1.79	0.63
12:1L:154:LEU:HB3	12:1L:243:VAL:HG21	1.80	0.63
13:1M:230:VAL:HG12	13:1M:235:LEU:HD13	1.79	0.63
15:1O:24:VAL:HG23	15:1O:115:LEU:HD22	1.80	0.63
20:1U:24:LYS:H	20:1U:24:LYS:HD2	1.63	0.63
58:1L:201:MYR:H52	58:1L:201:MYR:H92	1.80	0.63
12:1L:100:ILE:HD12	12:1L:246:LEU:HB2	1.80	0.63
12:1L:216:LEU:HD22	12:1L:259:LEU:HD11	1.80	0.63
15:1O:242:LYS:HD3	15:1O:244:ASP:HB2	1.80	0.63
40:1o:68:CYS:O	40:1o:72:SER:N	2.31	0.63
4:1D:107:ASP:OD1	4:1D:371:LYS:NZ	2.30	0.63
12:1L:331:MET:HB3	12:1L:387:THR:HB	1.80	0.63
13:1M:236:LEU:HB3	13:1M:237:LYS:HD3	1.80	0.63
13:1M:263:MET:HE3	38:1m:97:LEU:HB3	1.79	0.63
38:1m:80:ARG:HE	38:1m:82:THR:HG22	1.64	0.63
42:1q:74:PHE:O	42:1q:76:ASP:N	2.31	0.63
7:1G:438:PRO:O	7:1G:441:GLN:NE2	2.32	0.63
8:1H:196:ALA:HB3	8:1H:197:PRO:HD3	1.81	0.63
14:1N:108:LEU:HD11	14:1N:191:THR:HG21	1.80	0.63
39:1n:126:ARG:HG2	39:1n:129:ARG:HH22	1.64	0.63
6:1F:78:LYS:HG2	6:1F:79:TRP:HD1	1.63	0.63
10:1J:71:THR:HA	10:1J:75:ALA:HB3	1.80	0.63
16:1P:153:GLU:OE2	16:1P:167:LYS:NZ	2.32	0.63
22:1W:61:ASP:OD1	22:1W:61:ASP:N	2.31	0.63
1:1A:48:ARG:NH1	8:1H:124:ASN:OD1	2.31	0.63
8:1H:190:LEU:HD21	8:1H:273:ILE:HG21	1.79	0.63
12:1L:549:ALA:HB1	13:1M:275:ILE:HB	1.81	0.63
14:1N:83:GLN:NE2	30:1e:36:GLU:OE1	2.32	0.63
14:1N:187:MET:HA	14:1N:187:MET:HE3	1.81	0.63
20:1T:36:PHE:HA	20:1T:40:LEU:HB2	1.80	0.63
43:1r:108:ASP:OD2	43:1r:109:GLN:N	2.32	0.63
15:1O:67:LYS:HA	15:1O:67:LYS:HE2	1.80	0.62
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.31	0.62
39:1n:70:PHE:O	39:1n:74:GLN:N	2.32	0.62
6:1F:138:ILE:HG21	6:1F:146:ALA:HB2	1.82	0.62
7:1G:227:SER:O	7:1G:253:ARG:NH2	2.32	0.62
7:1G:284:ILE:HG22	7:1G:559:VAL:HG22	1.81	0.62
10:1J:120:ASN:HD21	30:1e:76:SER:HB3	1.63	0.62
13:1M:275:ILE:HG13	13:1M:279:GLN:NE2	2.14	0.62
15:1O:84:ASP:HA	15:1O:193:LYS:HD3	1.81	0.62
16:1P:264:ARG:HG2	16:1P:281:ARG:HG2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:81:LEU:O	21:1V:85:ASN:ND2	2.32	0.62
2:1B:126:TYR:OH	4:1D:85:ARG:NH2	2.32	0.62
8:1H:142:TYR:CZ	8:1H:191:ALA:HB1	2.34	0.62
12:1L:65:ASN:HA	34:1i:89:VAL:HG11	1.81	0.62
12:1L:72:GLN:O	41:1p:103:ASN:ND2	2.23	0.62
15:1O:105:LEU:HA	15:1O:128:ILE:HD11	1.81	0.62
30:1e:37:LYS:O	30:1e:41:GLU:HG2	1.99	0.62
34:1i:24:ASP:HB3	39:1n:120:LYS:HD3	1.80	0.62
40:1o:39:VAL:HB	40:1o:60:HIS:HB3	1.81	0.62
6:1F:112:ARG:HB2	6:1F:148:ASN:HD22	1.64	0.62
15:1O:138:MET:O	15:1O:143:PHE:HB2	1.99	0.62
8:1H:134:ARG:NH1	8:1H:206:GLU:OE1	2.32	0.62
34:1i:109:ILE:HD13	41:1p:16:THR:H	1.64	0.62
37:1l:154:VAL:O	40:1o:33:ARG:NH2	2.32	0.62
4:1D:350:LYS:HD2	7:1G:117:GLN:HB3	1.82	0.62
13:1M:71:TRP:CH2	13:1M:443:PRO:HB3	2.35	0.62
14:1N:125:GLN:NE2	51:1O:403:CDL:OB5	2.33	0.62
25:1Z:98:MET:HG3	25:1Z:104:TRP:CD2	2.33	0.62
30:1e:81:GLN:HG2	30:1e:84:LYS:HE3	1.82	0.62
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.30	0.62
7:1G:609:MET:SD	7:1G:609:MET:N	2.69	0.62
8:1H:252:PRO:O	8:1H:256:THR:OG1	2.18	0.62
12:1L:561:ILE:HD12	46:1m:201:PC1:H281	1.80	0.62
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.32	0.62
14:1N:211:MET:HE3	14:1N:212:THR:N	2.15	0.62
16:1P:134:HIS:O	16:1P:167:LYS:NZ	2.33	0.62
33:1h:9:PHE:O	39:1n:174:ARG:NH1	2.29	0.62
50:1H:401:U10:H1M1	50:1H:401:U10:H112	1.82	0.62
16:1P:21:ALA:HB3	16:1P:45:VAL:HG12	1.82	0.62
6:1F:22:PHE:CD2	6:1F:255:LEU:HD21	2.34	0.62
7:1G:43:HIS:HB3	7:1G:46:LEU:HB2	1.79	0.62
12:1L:313:MET:HE3	12:1L:329:ILE:HG22	1.82	0.62
20:1U:47:GLN:HG3	20:1U:71:MET:SD	2.40	0.62
32:1g:68:ILE:HG22	32:1g:72:LEU:HD12	1.81	0.62
38:1m:5:TYR:HE2	38:1m:13:LEU:HA	1.65	0.62
2:1B:130:TYR:HH	4:1D:84:HIS:HE2	1.46	0.62
7:1G:40:PHE:N	7:1G:52:CYS:SG	2.73	0.62
11:1K:54:THR:OG1	30:1e:24:GLN:OE1	2.16	0.61
12:1L:6:SER:O	12:1L:10:THR:OG1	2.17	0.61
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.34	0.61
13:1M:245:ARG:HA	13:1M:245:ARG:HH11	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:107:HIS:O	39:1n:111:LYS:N	2.33	0.61
16:1P:194:ILE:HB	16:1P:288:HIS:CE1	2.35	0.61
1:1A:102:LEU:HD22	8:1H:294:LEU:HD12	1.82	0.61
9:1I:71:PRO:HB3	42:1q:106:ARG:HH21	1.64	0.61
9:1I:109:TYR:OH	45:1I:202:SF4:S2	2.54	0.61
13:1M:91:ARG:HB3	13:1M:136:TRP:HH2	1.65	0.61
27:1b:78:GLU:OE1	27:1b:78:GLU:N	2.28	0.61
31:1f:18:VAL:HA	31:1f:21:VAL:HG12	1.80	0.61
37:1l:83:MET:HA	37:1l:83:MET:HE3	1.82	0.61
39:1n:133:GLU:N	39:1n:133:GLU:OE2	2.31	0.61
4:1D:290:ARG:NH1	4:1D:290:ARG:HB2	2.16	0.61
7:1G:444:LYS:HD3	7:1G:477:ILE:HG22	1.83	0.61
15:1O:164:LEU:HD12	15:1O:165:PRO:HD2	1.81	0.61
5:1E:74:GLN:OE1	5:1E:74:GLN:N	2.34	0.61
6:1F:246:GLY:HA3	6:1F:251:SER:HA	1.82	0.61
5:1E:120:ILE:HG13	5:1E:169:ILE:HD13	1.82	0.61
6:1F:41:ASP:OD1	6:1F:42:TRP:N	2.33	0.61
13:1M:336:ARG:HH12	13:1M:352:LEU:HD11	1.66	0.61
30:1e:85:LEU:O	30:1e:89:GLY:N	2.33	0.61
34:1i:20:ARG:HA	34:1i:23:LYS:HB3	1.82	0.61
4:1D:148:LEU:HD22	4:1D:174:ARG:HH11	1.65	0.61
5:1E:82:GLU:HB3	6:1F:200:GLN:HE21	1.65	0.61
6:1F:263:ASN:ND2	6:1F:286:GLY:O	2.32	0.61
13:1M:343:ILE:O	13:1M:346:ARG:NH1	2.32	0.61
13:1M:410:MET:O	13:1M:414:THR:N	2.32	0.61
28:1c:1:LYS:HE2	28:1c:3:TYR:HB2	1.82	0.61
36:1k:35:LEU:HG	36:1k:40:LEU:HB3	1.82	0.61
38:1m:107:ASP:N	38:1m:107:ASP:OD1	2.33	0.61
15:1O:268:GLU:OE1	15:1O:268:GLU:N	2.33	0.61
6:1F:365:CYS:HB2	45:1F:502:SF4:S3	2.38	0.61
7:1G:249:ARG:HH21	7:1G:251:LEU:HD11	1.64	0.61
7:1G:434:SER:OG	7:1G:436:ASN:ND2	2.34	0.61
12:1L:233:LEU:HD22	12:1L:248:HIS:HB3	1.82	0.61
13:1M:18:SER:HB3	13:1M:26:ASN:HD22	1.65	0.61
13:1M:210:TYR:HB3	13:1M:264:LEU:HG	1.83	0.61
20:1T:35:HIS:CD2	20:1T:38:LYS:H	2.19	0.61
20:1U:42:LEU:HB3	20:1U:46:ASP:HB3	1.83	0.61
36:1k:35:LEU:O	36:1k:39:GLY:N	2.34	0.61
42:1q:117:VAL:HG23	42:1q:123:GLN:HA	1.83	0.61
12:1L:267:MET:O	12:1L:267:MET:HE3	2.01	0.61
12:1L:407:TRP:NE1	37:1l:115:MET:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:126:ARG:NH1	15:1O:206:TYR:OH	2.34	0.61
20:1U:36:PHE:HA	20:1U:40:LEU:HB3	1.82	0.61
25:1Z:97:ILE:HG23	30:1e:82:ARG:HH12	1.66	0.61
37:1l:91:THR:HG22	38:1m:10:LEU:HA	1.81	0.61
38:1m:40:SER:OG	39:1n:148:PRO:O	2.19	0.61
5:1E:101:GLN:HA	5:1E:101:GLN:HE21	1.66	0.60
12:1L:9:LEU:HA	12:1L:12:LEU:HD13	1.83	0.60
15:1O:13:ARG:HB2	15:1O:16:ARG:HG3	1.83	0.60
18:1R:11:VAL:HG12	18:1R:17:ALA:HB2	1.82	0.60
18:1R:32:GLN:NE2	42:1q:122:GLN:O	2.31	0.60
32:1g:76:PHE:HD1	46:1h:201:PC1:H3A2	1.66	0.60
8:1H:92:PRO:HD3	8:1H:255:TYR:HD1	1.65	0.60
12:1L:189:PHE:O	12:1L:194:ASN:N	2.33	0.60
12:1L:399:VAL:HG22	12:1L:409:LEU:HD13	1.82	0.60
41:1p:51:ILE:HA	41:1p:54:GLN:HE21	1.65	0.60
6:1F:144:ASN:HB3	44:1s:43:HIS:HB2	1.82	0.60
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.34	0.60
15:1O:58:TYR:HE1	15:1O:106:LEU:HG	1.66	0.60
17:1Q:36:ARG:NH1	17:1Q:106:GLU:OE2	2.32	0.60
24:1Y:65:ILE:H	24:1Y:65:ILE:HD12	1.66	0.60
2:1B:116:MET:HA	2:1B:146:VAL:HG13	1.82	0.60
4:1D:158:ALA:HB1	4:1D:163:ALA:HB3	1.83	0.60
14:1N:214:ALA:HA	14:1N:217:MET:HG3	1.83	0.60
20:1U:74:GLN:OE1	20:1U:74:GLN:N	2.33	0.60
27:1b:78:GLU:O	27:1b:82:ASN:ND2	2.33	0.60
31:1f:38:ARG:HD2	31:1f:54:VAL:HG11	1.84	0.60
4:1D:137:ILE:HG21	4:1D:203:LEU:HD11	1.84	0.60
6:1F:92:TYR:HB2	6:1F:220:THR:HG22	1.83	0.60
8:1H:225:MET:N	8:1H:225:MET:SD	2.75	0.60
9:1I:112:ASP:OD1	9:1I:114:THR:OG1	2.19	0.60
10:1J:173:ARG:HH12	15:1O:254:ARG:HH21	1.50	0.60
24:1Y:127:GLY:HA2	24:1Y:132:TRP:HB2	1.83	0.60
3:1C:86:ARG:NH1	3:1C:91:GLU:OE1	2.35	0.60
12:1L:283:ILE:HD13	37:1l:112:MET:HG2	1.83	0.60
13:1M:252:PRO:HG3	29:1d:117:HIS:CE1	2.37	0.60
34:1i:93:PRO:HB3	41:1p:4:TRP:CD2	2.36	0.60
36:1k:41:ARG:O	36:1k:41:ARG:NH1	2.34	0.60
39:1n:19:TYR:CE1	39:1n:23:LEU:HD23	2.37	0.60
40:1o:43:GLN:OE1	40:1o:43:GLN:N	2.34	0.60
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.84	0.60
13:1M:10:MET:O	13:1M:10:MET:HG2	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:58:ARG:HD3	37:1l:70:ARG:HB2	1.82	0.60
12:1L:81:LYS:N	12:1L:133:THR:O	2.35	0.60
13:1M:221:VAL:O	13:1M:340:ARG:NH1	2.35	0.60
35:1j:37:LEU:HA	35:1j:40:PHE:HB2	1.84	0.60
37:1l:112:MET:N	37:1l:112:MET:SD	2.74	0.60
3:1C:90:PHE:HZ	3:1C:163:ARG:HH11	1.49	0.60
12:1L:584:ILE:HG23	12:1L:588:PHE:HE2	1.67	0.60
13:1M:206:LYS:O	13:1M:206:LYS:NZ	2.27	0.60
20:1U:35:HIS:CE1	20:1U:38:LYS:HG2	2.36	0.60
27:1b:30:ILE:HG13	27:1b:31:LEU:N	2.16	0.60
30:1e:35:PHE:HB3	30:1e:62:PHE:HB2	1.84	0.60
39:1n:144:PRO:HB2	39:1n:149:ARG:HH11	1.66	0.60
8:1H:25:ARG:HD3	50:1H:401:U10:H312	1.84	0.59
17:1Q:71:GLY:H	42:1q:128:SER:HB2	1.67	0.59
18:1R:70:ARG:NH1	18:1R:72:TYR:OH	2.35	0.59
23:1X:152:GLU:N	23:1X:152:GLU:OE2	2.31	0.59
40:1o:47:ASP:OD1	41:1p:15:ARG:NH2	2.31	0.59
2:1B:58:GLU:HB3	4:1D:189:MET:HE3	1.84	0.59
4:1D:312:SER:O	4:1D:316:ASN:ND2	2.33	0.59
12:1L:128:MET:SD	12:1L:252:MET:HB3	2.41	0.59
12:1L:292:ALA:HB1	12:1L:301:ILE:HG23	1.84	0.59
13:1M:14:MET:O	13:1M:18:SER:OG	2.18	0.59
15:1O:219:GLU:OE1	15:1O:245:LYS:NZ	2.35	0.59
34:1i:69:PHE:HA	34:1i:73:HIS:HD1	1.66	0.59
35:1j:68:PRO:O	40:1o:114:ARG:NH2	2.34	0.59
37:1l:15:LYS:NZ	37:1l:39:ASP:OD2	2.35	0.59
37:1l:55:GLN:HG3	37:1l:69:LEU:HB3	1.84	0.59
4:1D:4:TRP:CG	13:1M:140:THR:HG1	2.20	0.59
7:1G:38:PRO:HB2	7:1G:54:MET:HG2	1.84	0.59
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.35	0.59
20:1U:17:TYR:HA	20:1U:20:LYS:HG2	1.85	0.59
20:1U:68:GLU:HG2	39:1n:17:ARG:HH12	1.67	0.59
31:1f:53:GLU:OE2	31:1f:53:GLU:N	2.29	0.59
4:1D:165:THR:OG1	8:1H:275:ALA:O	2.19	0.59
6:1F:28:ARG:O	6:1F:29:HIS:ND1	2.31	0.59
6:1F:272:MET:O	6:1F:273:SER:OG	2.19	0.59
6:1F:437:HIS:O	6:1F:438:GLN:NE2	2.36	0.59
8:1H:65:THR:HA	16:1P:324:TYR:HB2	1.84	0.59
14:1N:128:LEU:HD13	14:1N:216:PHE:HB2	1.84	0.59
4:1D:23:LYS:O	4:1D:23:LYS:NZ	2.30	0.59
6:1F:150:GLN:HE21	44:1s:54:LEU:HG	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:111:ILE:HD12	9:1I:154:LEU:HD21	1.84	0.59
13:1M:243:MET:HG2	13:1M:301:ILE:HG21	1.84	0.59
14:1N:19:LEU:O	14:1N:23:SER:OG	2.17	0.59
16:1P:10:LYS:O	16:1P:15:SER:OG	2.13	0.59
20:1U:36:PHE:O	20:1U:41:GLY:N	2.35	0.59
21:1V:104:GLU:N	21:1V:104:GLU:OE2	2.35	0.59
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.36	0.59
36:1k:23:ILE:O	36:1k:26:THR:OG1	2.19	0.59
40:1o:14:LYS:HB2	40:1o:109:GLN:NE2	2.18	0.59
2:1B:76:PHE:HB2	50:1H:401:U10:H102	1.84	0.59
4:1D:65:VAL:HG23	4:1D:77:ASP:HB3	1.85	0.59
13:1M:355:MET:HA	13:1M:355:MET:HE2	1.84	0.59
37:1l:73:TRP:HE1	38:1m:45:GLU:HG3	1.67	0.59
13:1M:291:VAL:HA	13:1M:294:MET:HB2	1.84	0.59
32:1g:59:ARG:O	32:1g:63:PHE:HB2	2.02	0.59
43:1r:4:THR:HG22	43:1r:6:VAL:H	1.67	0.59
8:1H:148:ILE:O	8:1H:152:SER:OG	2.21	0.59
11:1K:45:THR:HA	11:1K:48:ILE:HD11	1.85	0.59
12:1L:11:THR:O	12:1L:15:LEU:HD23	2.03	0.59
12:1L:486:MET:O	12:1L:489:THR:OG1	2.21	0.59
16:1P:194:ILE:HD13	16:1P:260:HIS:HA	1.85	0.59
17:1Q:11:ILE:HB	22:1W:23:ARG:HH22	1.67	0.59
34:1i:81:ILE:O	34:1i:85:LEU:HD23	2.03	0.59
10:1J:126:VAL:HG13	25:1Z:122:GLY:HA3	1.84	0.59
12:1L:434:LYS:NZ	36:1k:56:PHE:O	2.36	0.59
14:1N:245:MET:HE1	52:1N:401:3PE:H371	1.85	0.59
15:1O:138:MET:HE1	15:1O:144:ILE:HG21	1.85	0.59
19:1S:63:LYS:HZ1	19:1S:75:ASN:HA	1.68	0.59
34:1i:64:TYR:HD2	34:1i:65:ARG:HH12	1.49	0.59
4:1D:342:MET:HE2	7:1G:103:LEU:HD13	1.85	0.59
6:1F:109:GLU:HA	6:1F:112:ARG:HE	1.68	0.59
10:1J:159:TRP:CE2	10:1J:163:ILE:HD11	2.37	0.59
12:1L:475:MET:SD	40:1o:53:GLN:NE2	2.76	0.59
13:1M:1:FME:HE1	13:1M:111:THR:HB	1.85	0.59
13:1M:116:ILE:HD12	13:1M:119:TYR:HB3	1.84	0.59
15:1O:26:THR:HB	15:1O:124:LEU:HB2	1.84	0.59
25:1Z:97:ILE:O	30:1e:81:GLN:NE2	2.35	0.59
7:1G:460:ARG:NH1	7:1G:659:ASP:O	2.34	0.58
12:1L:504:LEU:O	12:1L:507:THR:OG1	2.16	0.58
15:1O:189:PRO:HA	15:1O:192:MET:HG2	1.84	0.58
23:1X:17:VAL:O	26:1a:50:ARG:NH2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.03	0.58
38:1m:7:PRO:HB3	38:1m:13:LEU:HB2	1.83	0.58
4:1D:325:VAL:HG22	4:1D:327:ASP:H	1.67	0.58
7:1G:544:ILE:HG23	7:1G:559:VAL:HB	1.85	0.58
7:1G:646:ASN:OD1	7:1G:650:LYS:NZ	2.36	0.58
13:1M:47:GLU:OE1	13:1M:47:GLU:N	2.36	0.58
13:1M:143:LEU:HD21	14:1N:303:THR:HG21	1.84	0.58
4:1D:241:ASP:N	4:1D:292:ASP:OD2	2.36	0.58
14:1N:24:SER:HB3	30:1e:1:PRO:HG3	1.85	0.58
14:1N:239:VAL:HG11	29:1d:47:ALA:HB1	1.84	0.58
20:1T:74:GLN:HA	20:1T:77:VAL:HG23	1.84	0.58
20:1U:14:ARG:HH21	20:1U:57:GLU:HG2	1.68	0.58
20:1U:18:VAL:HA	20:1U:21:LEU:HD13	1.84	0.58
39:1n:135:GLU:OE1	39:1n:166:TRP:NE1	2.35	0.58
6:1F:189:GLU:HB2	6:1F:222:VAL:HG21	1.84	0.58
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.86	0.58
11:1K:25:HIS:ND1	11:1K:88:ASP:OD2	2.36	0.58
12:1L:407:TRP:HD1	37:1l:116:PHE:CD2	2.22	0.58
13:1M:40:SER:HB3	46:1h:201:PC1:H322	1.85	0.58
14:1N:324:LYS:O	14:1N:325:LEU:HB2	2.01	0.58
52:1N:401:3PE:H331	52:1N:401:3PE:H372	1.85	0.58
22:1W:43:VAL:HG11	22:1W:60:ARG:HD3	1.84	0.58
29:1d:94:VAL:HG23	29:1d:101:PHE:HD2	1.67	0.58
1:1A:109:LYS:HE2	1:1A:109:LYS:HA	1.85	0.58
2:1B:92:LEU:HD23	2:1B:136:CYS:HA	1.84	0.58
6:1F:215:VAL:HG12	6:1F:220:THR:HG21	1.83	0.58
6:1F:337:MET:H	6:1F:337:MET:HE2	1.68	0.58
7:1G:377:ILE:HG22	7:1G:406:VAL:HA	1.86	0.58
16:1P:26:ALA:HB3	16:1P:47:VAL:HG23	1.84	0.58
26:1a:1:MET:HB2	26:1a:3:PHE:CE1	2.39	0.58
33:1h:19:ARG:HA	33:1h:22:LEU:HD12	1.85	0.58
35:1j:10:ARG:HH11	35:1j:13:GLN:HB2	1.68	0.58
38:1m:116:GLN:OE1	38:1m:116:GLN:N	2.30	0.58
39:1n:23:LEU:HD13	39:1n:36:TYR:OH	2.03	0.58
4:1D:390:LYS:HZ2	4:1D:430:ARG:HH22	1.52	0.58
14:1N:271:THR:HG23	14:1N:276:ILE:HG22	1.86	0.58
20:1U:69:LYS:HD3	34:1i:1:SAC:H2A2	1.86	0.58
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	1.84	0.58
24:1Y:99:THR:O	24:1Y:103:ARG:N	2.36	0.58
3:1C:20:LYS:N	3:1C:20:LYS:HE2	2.18	0.58
8:1H:119:SER:O	8:1H:123:SER:OG	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:331:MET:N	12:1L:331:MET:SD	2.76	0.58
32:1g:115:PRO:HA	32:1g:118:ILE:HD11	1.86	0.58
12:1L:71:LEU:N	12:1L:74:VAL:O	2.34	0.58
13:1M:207:MET:HE2	13:1M:207:MET:HA	1.85	0.58
13:1M:257:MET:HA	13:1M:257:MET:HE3	1.86	0.58
14:1N:311:MET:SD	14:1N:315:TRP:NE1	2.76	0.58
40:1o:74:PRO:HG2	41:1p:25:LEU:HB3	1.84	0.58
3:1C:68:THR:HG21	21:1V:54:LYS:HE2	1.85	0.58
7:1G:60:GLU:O	7:1G:61:LYS:HD2	2.02	0.58
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.39	0.58
14:1N:30:TRP:HD1	14:1N:70:LEU:HD12	1.68	0.58
20:1U:8:LEU:HA	20:1U:11:ILE:HG22	1.86	0.58
20:1U:74:GLN:HA	20:1U:77:VAL:HG22	1.86	0.58
37:1l:135:TYR:HB3	37:1l:140:LEU:HD13	1.85	0.58
38:1m:39:ARG:HH21	38:1m:43:LYS:HD2	1.69	0.58
3:1C:175:ARG:NH2	3:1C:177:ASP:OD2	2.35	0.58
6:1F:17:ASP:HA	6:1F:20:ARG:HG3	1.86	0.58
7:1G:667:THR:HG22	7:1G:669:LYS:H	1.68	0.58
9:1I:65:HIS:CD2	9:1I:133:GLU:HG2	2.39	0.58
12:1L:397:GLU:OE2	12:1L:479:ASN:ND2	2.28	0.58
14:1N:276:ILE:O	14:1N:280:THR:OG1	2.21	0.58
15:1O:116:LEU:HB3	15:1O:260:ARG:HD2	1.84	0.58
29:1d:103:GLU:N	29:1d:103:GLU:OE2	2.36	0.58
36:1k:19:LYS:HA	36:1k:22:LYS:HE3	1.85	0.58
37:1l:138:LEU:O	37:1l:142:ARG:N	2.37	0.58
6:1F:106:LYS:HB2	6:1F:255:LEU:HD12	1.86	0.57
8:1H:13:ILE:O	8:1H:17:VAL:HG23	2.03	0.57
8:1H:207:LEU:O	8:1H:209:SER:N	2.37	0.57
12:1L:486:MET:HA	12:1L:489:THR:HG23	1.85	0.57
14:1N:207:ILE:HG21	14:1N:262:PRO:HG3	1.86	0.57
38:1m:113:LYS:HA	38:1m:116:GLN:HE22	1.68	0.57
40:1o:103:ARG:NH1	40:1o:107:LEU:HD12	2.18	0.57
7:1G:249:ARG:HE	7:1G:251:LEU:HD21	1.68	0.57
12:1L:338:MET:HA	12:1L:341:MET:HB2	1.87	0.57
12:1L:407:TRP:CD1	37:1l:116:PHE:HA	2.39	0.57
13:1M:224:PRO:O	13:1M:228:SER:OG	2.21	0.57
14:1N:342:ALA:HA	29:1d:79:GLN:HG3	1.86	0.57
20:1U:48:VAL:HG22	20:1U:52:MET:HE2	1.85	0.57
21:1V:17:GLU:OE2	21:1V:17:GLU:N	2.35	0.57
25:1Z:80:ASP:N	25:1Z:80:ASP:OD1	2.32	0.57
26:1a:3:PHE:CD2	51:1a:101:CDL:HB61	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:100:ARG:HB3	32:1g:105:LEU:HB2	1.85	0.57
41:1p:45:THR:O	41:1p:49:GLU:HG2	2.04	0.57
12:1L:105:MET:HB3	12:1L:118:PHE:HZ	1.69	0.57
12:1L:119:LYS:O	12:1L:123:LEU:HD12	2.04	0.57
14:1N:2:ASN:HB3	14:1N:5:ILE:HG13	1.85	0.57
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	1.85	0.57
16:1P:144:ARG:HB2	16:1P:144:ARG:NH1	2.18	0.57
23:1X:171:MET:HE3	29:1d:29:PRO:HG2	1.85	0.57
41:1p:14:ARG:NH2	41:1p:15:ARG:O	2.34	0.57
2:1B:48:MET:O	2:1B:87:ILE:HD11	2.05	0.57
9:1I:7:MET:N	9:1I:7:MET:HE3	2.20	0.57
11:1K:12:PHE:CE1	11:1K:36:MET:HB2	2.39	0.57
13:1M:74:PRO:HA	13:1M:77:LEU:HD12	1.86	0.57
23:1X:2:GLY:O	25:1Z:105:LYS:NZ	2.37	0.57
25:1Z:128:ARG:HD3	30:1e:97:HIS:HD2	1.68	0.57
31:1f:10:HIS:HE2	52:1g:201:3PE:H241	1.68	0.57
7:1G:242:THR:HG21	7:1G:586:ALA:HB1	1.86	0.57
7:1G:336:ASN:OD1	19:1S:67:ARG:NH1	2.36	0.57
9:1I:65:HIS:HA	9:1I:133:GLU:HA	1.87	0.57
32:1g:75:THR:O	32:1g:79:TYR:HB2	2.03	0.57
3:1C:118:GLU:OE2	3:1C:118:GLU:N	2.28	0.57
7:1G:156:CYS:O	7:1G:157:THR:OG1	2.22	0.57
7:1G:326:GLU:OE1	7:1G:326:GLU:N	2.36	0.57
8:1H:91:MET:O	8:1H:93:TYR:N	2.37	0.57
10:1J:12:ILE:H	10:1J:12:ILE:HD12	1.68	0.57
12:1L:538:THR:HG23	37:1l:89:VAL:HG12	1.85	0.57
12:1L:568:PHE:O	12:1L:572:LYS:N	2.30	0.57
13:1M:204:MET:HA	13:1M:204:MET:HE3	1.87	0.57
16:1P:162:GLU:N	16:1P:162:GLU:OE1	2.36	0.57
25:1Z:98:MET:HG3	25:1Z:104:TRP:CE3	2.40	0.57
29:1d:99:GLU:OE2	29:1d:99:GLU:N	2.26	0.57
32:1g:47:TYR:CD2	32:1g:57:ASN:HB3	2.40	0.57
4:1D:4:TRP:CD1	13:1M:140:THR:HA	2.40	0.57
6:1F:261:HIS:HB3	6:1F:288:ILE:HD11	1.86	0.57
11:1K:56:ALA:HA	30:1e:17:MET:HE2	1.87	0.57
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	1.87	0.57
13:1M:265:SER:OG	13:1M:295:ALA:O	2.21	0.57
14:1N:120:GLN:HA	14:1N:176:ARG:HE	1.70	0.57
19:1S:24:GLN:O	19:1S:25:ARG:NH1	2.38	0.57
32:1g:121:PRO:O	41:1p:166:ARG:NH2	2.38	0.57
39:1n:43:MET:HB3	39:1n:46:ARG:HH21	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:245:ARG:HA	13:1M:245:ARG:NH1	2.19	0.57
24:1Y:46:ALA:N	24:1Y:50:GLU:OE2	2.34	0.57
29:1d:110:GLY:HA3	41:1p:74:THR:HG23	1.86	0.57
8:1H:224:PHE:HE1	50:1H:401:U10:H352	1.70	0.57
10:1J:119:PHE:CG	11:1K:6:MET:HG3	2.39	0.57
13:1M:364:LEU:HA	13:1M:367:LEU:HG	1.87	0.57
23:1X:15:GLN:HE22	23:1X:67:LEU:HD21	1.69	0.57
33:1h:20:ARG:O	33:1h:24:LEU:HG	2.04	0.57
34:1i:67:SER:O	34:1i:71:VAL:HG13	2.05	0.57
35:1j:19:ARG:O	35:1j:23:ILE:HG13	2.05	0.57
5:1E:101:GLN:HA	5:1E:101:GLN:NE2	2.20	0.57
6:1F:94:VAL:HG12	6:1F:135:TYR:HB2	1.87	0.57
7:1G:74:MET:N	7:1G:74:MET:HE3	2.20	0.57
12:1L:303:ALA:O	12:1L:306:THR:OG1	2.18	0.57
12:1L:435:PRO:HB2	36:1k:51:ARG:HG2	1.87	0.57
12:1L:496:MET:HA	12:1L:499:MET:SD	2.45	0.57
14:1N:189:TRP:HB3	14:1N:204:ASN:HD21	1.70	0.57
25:1Z:103:ASP:N	25:1Z:103:ASP:OD2	2.37	0.57
32:1g:96:LEU:HD11	41:1p:101:ILE:HG21	1.87	0.57
34:1i:14:LEU:HD11	39:1n:169:ILE:HG12	1.87	0.57
37:1l:30:ARG:HH12	38:1m:31:ALA:HB1	1.69	0.57
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.38	0.56
7:1G:475:GLN:HA	7:1G:478:ARG:HB3	1.87	0.56
12:1L:174:TYR:HD2	12:1L:232:TRP:HB3	1.70	0.56
16:1P:22:THR:HG21	16:1P:85:VAL:HG12	1.86	0.56
37:1l:133:TYR:HB3	37:1l:137:ASP:HA	1.87	0.56
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.87	0.56
8:1H:113:VAL:HG21	8:1H:139:THR:HG21	1.87	0.56
13:1M:130:LEU:O	13:1M:134:THR:OG1	2.15	0.56
14:1N:115:VAL:HB	14:1N:184:ILE:HD11	1.86	0.56
15:1O:44:GLU:N	15:1O:44:GLU:OE2	2.38	0.56
20:1T:66:ASP:OD2	20:1T:66:ASP:N	2.34	0.56
24:1Y:32:GLY:O	24:1Y:36:SER:OG	2.22	0.56
29:1d:44:ILE:O	29:1d:48:ILE:HG12	2.05	0.56
40:1o:42:GLN:HG2	40:1o:43:GLN:OE1	2.05	0.56
5:1E:143:GLU:HB3	6:1F:353:PHE:HD1	1.70	0.56
6:1F:129:MET:HE1	6:1F:221:THR:HB	1.87	0.56
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.87	0.56
7:1G:486:ASP:OD2	7:1G:486:ASP:N	2.35	0.56
8:1H:102:VAL:HG11	8:1H:154:LEU:HD11	1.87	0.56
9:1I:4:PHE:HB3	9:1I:7:MET:HE2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:90:ILE:O	12:1L:94:LEU:HD23	2.06	0.56
12:1L:209:PRO:HG2	12:1L:213:LEU:HD11	1.87	0.56
12:1L:359:MET:HE3	12:1L:362:LEU:HD13	1.87	0.56
12:1L:396:ILE:HG21	12:1L:490:ALA:HB2	1.86	0.56
13:1M:285:LEU:HD11	13:1M:342:MET:HE1	1.85	0.56
14:1N:162:ILE:HD13	14:1N:282:MET:HB3	1.87	0.56
16:1P:176:ASP:OD1	16:1P:180:ASN:ND2	2.38	0.56
20:1T:70:LEU:HD21	20:1T:79:TYR:CG	2.39	0.56
20:1U:17:TYR:O	20:1U:21:LEU:N	2.33	0.56
26:1a:3:PHE:HD2	51:1a:101:CDL:HB61	1.70	0.56
35:1j:56:PRO:HD2	35:1j:57:SER:H	1.69	0.56
1:1A:81:THR:HG23	1:1A:83:ASN:H	1.70	0.56
11:1K:26:LEU:HD22	11:1K:78:LEU:HD23	1.88	0.56
12:1L:368:PHE:HD2	12:1L:451:ILE:HD12	1.71	0.56
18:1R:20:ASP:N	18:1R:20:ASP:OD2	2.36	0.56
20:1U:35:HIS:CE1	20:1U:38:LYS:H	2.23	0.56
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	1.86	0.56
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.87	0.56
32:1g:43:ASP:N	32:1g:43:ASP:OD1	2.38	0.56
40:1o:91:HIS:O	40:1o:95:VAL:HG22	2.06	0.56
1:1A:46:SER:HB2	1:1A:49:LEU:HD12	1.87	0.56
5:1E:33:ALA:O	5:1E:37:ASN:ND2	2.39	0.56
10:1J:127:ILE:HA	25:1Z:120:MET:HE1	1.86	0.56
20:1T:66:ASP:O	20:1T:70:LEU:HD13	2.05	0.56
6:1F:209:PHE:O	6:1F:213:VAL:N	2.33	0.56
7:1G:102:PRO:HG3	7:1G:151:THR:HG23	1.86	0.56
12:1L:8:THR:O	12:1L:12:LEU:HD12	2.06	0.56
12:1L:27:TYR:C	12:1L:28:LYS:HE2	2.31	0.56
12:1L:297:ASP:HA	12:1L:355:ASP:HA	1.87	0.56
12:1L:395:ILE:O	12:1L:399:VAL:HG12	2.05	0.56
14:1N:77:ASN:ND2	14:1N:89:MET:SD	2.79	0.56
22:1W:23:ARG:HA	22:1W:23:ARG:HH11	1.69	0.56
22:1W:34:GLU:HA	22:1W:37:ARG:HB2	1.88	0.56
25:1Z:119:PRO:HB2	25:1Z:124:LEU:HD21	1.86	0.56
39:1n:120:LYS:O	39:1n:123:GLN:NE2	2.38	0.56
4:1D:112:MET:HG2	4:1D:181:TYR:OH	2.05	0.56
6:1F:46:LYS:NZ	6:1F:167:CYS:O	2.29	0.56
7:1G:36:GLN:HE22	17:1Q:48:GLY:HA2	1.71	0.56
8:1H:142:TYR:OH	8:1H:191:ALA:HB1	2.06	0.56
12:1L:13:ILE:O	12:1L:16:THR:OG1	2.22	0.56
15:1O:285:GLY:O	15:1O:289:SER:OG	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:69:PHE:HA	34:1i:73:HIS:ND1	2.21	0.56
8:1H:269:THR:HG22	8:1H:272:TRP:HE3	1.70	0.56
9:1I:81:LYS:HG2	9:1I:94:ILE:HD11	1.88	0.56
14:1N:58:LYS:O	14:1N:62:THR:OG1	2.18	0.56
24:1Y:96:GLY:O	24:1Y:100:LEU:N	2.34	0.56
37:1I:158:ILE:HG23	40:1o:96:LYS:HE2	1.88	0.56
44:1s:45:GLU:OE2	44:1s:45:GLU:N	2.28	0.56
3:1C:88:ASN:HD22	21:1V:110:GLN:HE21	1.52	0.56
4:1D:4:TRP:O	13:1M:142:ARG:NH2	2.39	0.56
24:1Y:85:ASP:OD2	24:1Y:87:LEU:HG	2.06	0.56
32:1g:41:ASN:O	32:1g:44:SER:OG	2.24	0.56
3:1C:88:ASN:HB2	21:1V:110:GLN:HE22	1.70	0.56
7:1G:105:CYS:N	45:1G:801:SF4:S4	2.79	0.56
15:1O:144:ILE:HG13	15:1O:145:ARG:H	1.71	0.56
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	1.88	0.55
15:1O:224:SER:HB2	15:1O:226:ARG:CZ	2.36	0.55
16:1P:157:ARG:NH1	16:1P:225:GLY:O	2.39	0.55
16:1P:203:GLN:N	16:1P:291:ASP:OD1	2.28	0.55
34:1i:18:ARG:HH22	39:1n:174:ARG:HA	1.71	0.55
34:1i:82:HIS:CE1	34:1i:86:LYS:HD2	2.40	0.55
2:1B:116:MET:HE2	2:1B:156:LEU:HD13	1.87	0.55
12:1L:578:SER:HB3	14:1N:168:GLY:HA2	1.87	0.55
13:1M:69:THR:HG22	13:1M:234:VAL:HG21	1.88	0.55
19:1S:57:CYS:SG	19:1S:58:SER:N	2.80	0.55
19:1S:88:ARG:HH21	19:1S:91:GLU:HG2	1.72	0.55
20:1U:79:TYR:O	20:1U:83:LYS:N	2.29	0.55
34:1i:27:LEU:HD11	34:1i:31:GLU:HG3	1.88	0.55
42:1q:29:ARG:NH2	42:1q:64:TYR:O	2.40	0.55
2:1B:113:VAL:HG11	2:1B:140:VAL:HG11	1.88	0.55
4:1D:338:MET:HE1	4:1D:348:HIS:CE1	2.41	0.55
8:1H:190:LEU:HD11	8:1H:196:ALA:HB3	1.89	0.55
11:1K:37:MET:HE2	14:1N:68:MET:HE1	1.88	0.55
20:1T:35:HIS:HD2	20:1T:37:MET:H	1.54	0.55
21:1V:97:LYS:HD2	21:1V:99:TRP:HZ3	1.71	0.55
34:1i:109:ILE:HD13	41:1p:15:ARG:HA	1.89	0.55
42:1q:78:ASP:OD2	42:1q:80:SER:N	2.39	0.55
2:1B:121:ASN:HB3	9:1I:114:THR:HG22	1.88	0.55
4:1D:259:MET:HA	4:1D:259:MET:HE3	1.88	0.55
4:1D:345:LEU:HD12	7:1G:103:LEU:HD12	1.88	0.55
8:1H:99:ASN:OD1	26:1a:40:HIS:ND1	2.38	0.55
10:1J:128:TYR:O	25:1Z:121:MET:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:149:TYR:OH	30:1e:23:GLU:OE2	2.17	0.55
12:1L:506:ASN:HA	12:1L:509:TYR:HB2	1.87	0.55
13:1M:9:THR:HG22	13:1M:104:LEU:HD21	1.88	0.55
13:1M:153:THR:O	13:1M:157:SER:OG	2.20	0.55
13:1M:240:GLY:O	13:1M:244:MET:HE3	2.06	0.55
14:1N:248:LEU:HD12	14:1N:251:MET:HG3	1.88	0.55
15:1O:104:ARG:HH21	15:1O:126:ARG:HD2	1.71	0.55
33:1h:48:GLY:HA2	41:1p:55:HIS:CD2	2.42	0.55
39:1n:93:TYR:HB3	39:1n:177:PRO:HD2	1.89	0.55
39:1n:103:LEU:HD12	39:1n:121:ARG:HH11	1.72	0.55
12:1L:349:SER:HB2	12:1L:443:ILE:HG23	1.88	0.55
12:1L:362:LEU:HD23	12:1L:431:PHE:CE1	2.42	0.55
13:1M:206:LYS:O	13:1M:206:LYS:HG2	2.07	0.55
20:1T:29:LYS:HZ3	20:1T:40:LEU:HD13	1.72	0.55
20:1U:26:ASP:H	20:1U:29:LYS:HE2	1.71	0.55
20:1U:36:PHE:H	20:1U:71:MET:CE	2.15	0.55
23:1X:6:LEU:HD13	25:1Z:88:ARG:HE	1.70	0.55
23:1X:170:THR:HG23	23:1X:171:MET:SD	2.46	0.55
32:1g:62:PHE:HA	32:1g:66:PHE:CD1	2.41	0.55
7:1G:156:CYS:C	7:1G:158:ARG:H	2.15	0.55
12:1L:174:TYR:HB3	12:1L:229:LEU:HB3	1.88	0.55
13:1M:286:ILE:HD12	13:1M:286:ILE:H	1.71	0.55
20:1T:58:PHE:HB2	20:1T:60:PHE:CE2	2.41	0.55
20:1T:66:ASP:HA	20:1T:69:LYS:NZ	2.20	0.55
20:1U:52:MET:SD	39:1n:20:LYS:HA	2.47	0.55
34:1i:77:PRO:O	34:1i:81:ILE:HG22	2.07	0.55
36:1k:49:ALA:HA	36:1k:52:TYR:HD2	1.72	0.55
6:1F:258:ILE:HG21	6:1F:284:ALA:HB2	1.88	0.55
11:1K:23:ARG:HG3	11:1K:24:SER:H	1.72	0.55
12:1L:61:MET:HB3	34:1i:98:GLU:OE2	2.07	0.55
13:1M:275:ILE:HG13	13:1M:279:GLN:HE22	1.72	0.55
14:1N:17:THR:HG22	14:1N:21:MET:HE1	1.88	0.55
30:1e:56:LYS:C	30:1e:56:LYS:HD3	2.31	0.55
32:1g:64:PHE:O	32:1g:69:VAL:HG23	2.06	0.55
5:1E:5:ALA:O	18:1R:55:ARG:NH2	2.40	0.55
6:1F:434:ALA:O	6:1F:438:GLN:NE2	2.39	0.55
12:1L:278:LEU:HD12	12:1L:315:VAL:HG13	1.88	0.55
13:1M:196:TRP:CG	13:1M:253:LEU:HD12	2.41	0.55
13:1M:422:HIS:HB2	38:1m:59:ILE:HD11	1.89	0.55
16:1P:113:ILE:O	16:1P:117:ILE:HD12	2.06	0.55
20:1T:14:ARG:HH12	20:1T:58:PHE:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:65:PHE:O	1:1A:69:ILE:HG23	2.05	0.55
6:1F:222:VAL:HG23	48:1F:501:FMN:H5'2	1.87	0.55
7:1G:205:VAL:HG13	45:1G:801:SF4:S3	2.47	0.55
12:1L:170:GLN:HA	12:1L:173:LEU:HB3	1.89	0.55
13:1M:105:PHE:O	13:1M:109:THR:OG1	2.16	0.55
15:1O:308:TYR:CZ	15:1O:320:LYS:HG2	2.41	0.55
20:1U:72:CYS:O	20:1U:75:GLU:HG2	2.07	0.55
7:1G:412:PRO:O	7:1G:419:TYR:OH	2.22	0.55
12:1L:32:TYR:HA	12:1L:35:TYR:HB3	1.88	0.55
14:1N:244:MET:HE3	14:1N:244:MET:O	2.07	0.55
22:1W:68:MET:HE3	22:1W:68:MET:H	1.71	0.55
22:1W:80:ASP:O	22:1W:84:ILE:HG13	2.07	0.55
38:1m:19:PRO:HA	38:1m:22:TYR:HD2	1.72	0.55
6:1F:206:LYS:HB3	6:1F:207:PRO:HD3	1.88	0.54
7:1G:248:MET:H	7:1G:248:MET:HE2	1.71	0.54
8:1H:195:ARG:HD3	8:1H:231:ILE:HD11	1.89	0.54
12:1L:317:ILE:HG22	12:1L:322:PRO:HA	1.88	0.54
15:1O:293:PHE:HD2	15:1O:293:PHE:O	1.90	0.54
7:1G:74:MET:HE3	7:1G:74:MET:H	1.73	0.54
12:1L:364:LYS:HB2	35:1j:14:PHE:HZ	1.72	0.54
12:1L:586:LEU:H	12:1L:586:LEU:HD12	1.72	0.54
14:1N:258:SER:OG	14:1N:333:SER:O	2.23	0.54
16:1P:152:GLY:O	16:1P:156:VAL:HG12	2.07	0.54
24:1Y:14:GLY:HA3	24:1Y:77:ALA:HB3	1.88	0.54
37:1l:5:THR:OG1	37:1l:6:LYS:N	2.38	0.54
39:1n:25:HIS:CD2	39:1n:74:GLN:HA	2.43	0.54
4:1D:29:LYS:HD3	4:1D:30:PRO:HD2	1.89	0.54
5:1E:56:ARG:NH1	44:1s:48:THR:O	2.41	0.54
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.89	0.54
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.07	0.54
11:1K:17:ALA:O	11:1K:21:MET:HB3	2.06	0.54
12:1L:276:MET:N	12:1L:276:MET:SD	2.78	0.54
13:1M:76:MET:HB3	13:1M:226:ALA:HB1	1.90	0.54
13:1M:242:GLY:O	13:1M:246:ILE:HG13	2.07	0.54
15:1O:50:HIS:HE2	15:1O:125:GLU:CD	2.16	0.54
15:1O:165:PRO:HB3	15:1O:217:LYS:HD3	1.88	0.54
20:1T:35:HIS:HD2	20:1T:37:MET:N	2.05	0.54
20:1T:35:HIS:HB3	20:1T:39:ASP:H	1.72	0.54
25:1Z:104:TRP:HZ3	25:1Z:106:VAL:HA	1.71	0.54
34:1i:105:PRO:HG2	34:1i:119:MET:HE2	1.89	0.54
38:1m:50:TYR:HA	38:1m:55:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.88	0.54
40:1o:94:TYR:HA	40:1o:97:ARG:HH11	1.72	0.54
40:1o:98:MET:O	40:1o:98:MET:HE3	2.06	0.54
5:1E:126:ILE:HG23	5:1E:130:GLU:HG2	1.90	0.54
7:1G:27:LEU:HA	7:1G:37:ILE:HD13	1.89	0.54
8:1H:117:LEU:HD11	8:1H:136:VAL:HG23	1.89	0.54
11:1K:5:TYR:OH	11:1K:50:ASN:ND2	2.40	0.54
12:1L:86:SER:OG	12:1L:262:ARG:NH2	2.40	0.54
12:1L:246:LEU:O	12:1L:251:THR:OG1	2.24	0.54
12:1L:581:LYS:HG3	24:1Y:44:PRO:HD3	1.88	0.54
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.90	0.54
15:1O:80:GLU:HG3	15:1O:190:HIS:CD2	2.43	0.54
16:1P:293:THR:HG22	16:1P:295:PRO:HD3	1.89	0.54
20:1T:11:ILE:O	20:1T:15:VAL:HG12	2.07	0.54
20:1T:56:ASP:N	20:1T:56:ASP:OD1	2.39	0.54
38:1m:5:TYR:CE2	38:1m:14:PRO:HD3	2.43	0.54
6:1F:237:ARG:CB	6:1F:241:TRP:HE3	2.21	0.54
11:1K:37:MET:HE3	11:1K:67:ALA:HA	1.88	0.54
15:1O:169:VAL:HG11	15:1O:210:PHE:HZ	1.72	0.54
15:1O:180:GLN:O	15:1O:184:GLN:HG2	2.06	0.54
21:1V:111:TRP:O	21:1V:112:LYS:HB3	2.08	0.54
29:1d:12:GLN:H	46:1d:201:PC1:H232	1.72	0.54
33:1h:16:PHE:HB3	39:1n:107:HIS:CE1	2.42	0.54
34:1i:43:GLU:O	34:1i:47:ASN:ND2	2.41	0.54
41:1p:48:ARG:O	41:1p:51:ILE:HG13	2.07	0.54
41:1p:99:GLN:O	41:1p:103:ASN:ND2	2.41	0.54
1:1A:48:ARG:NH2	8:1H:121:TRP:O	2.41	0.54
12:1L:220:ALA:HB2	12:1L:260:LEU:HD11	1.89	0.54
14:1N:217:MET:HE3	51:1O:403:CDL:C71	2.23	0.54
16:1P:138:ASP:OD1	16:1P:140:LYS:NZ	2.41	0.54
20:1T:52:MET:CE	22:1W:37:ARG:HD2	2.38	0.54
20:1U:22:TYR:HB3	20:1U:25:ILE:HB	1.88	0.54
30:1e:91:TYR:OH	30:1e:94:PRO:HD3	2.08	0.54
33:1h:115:ARG:NH1	33:1h:123:TYR:OH	2.39	0.54
42:1q:78:ASP:OD2	42:1q:81:MET:HG3	2.08	0.54
7:1G:316:ALA:HB1	7:1G:514:ILE:HD12	1.89	0.54
8:1H:21:THR:HG21	50:1H:401:U10:H372	1.90	0.54
8:1H:116:ILE:HD12	8:1H:135:ALA:HB1	1.90	0.54
13:1M:361:MET:HA	13:1M:364:LEU:HG	1.90	0.54
14:1N:87:THR:HG22	14:1N:88:LYS:H	1.72	0.54
14:1N:88:LYS:HB2	14:1N:148:SER:HB3	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:135:LYS:NZ	14:1N:187:MET:SD	2.78	0.54
16:1P:194:ILE:HD12	16:1P:288:HIS:HE2	1.72	0.54
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.89	0.54
20:1U:24:LYS:HD2	20:1U:24:LYS:N	2.23	0.54
20:1U:37:MET:HB3	20:1U:43:ASP:HA	1.90	0.54
31:1f:3:VAL:O	31:1f:6:ILE:HG13	2.07	0.54
36:1k:41:ARG:H	36:1k:41:ARG:HD3	1.73	0.54
36:1k:77:PHE:O	36:1k:81:VAL:HG22	2.07	0.54
39:1n:23:LEU:HB2	39:1n:36:TYR:HE1	1.73	0.54
40:1o:80:LYS:H	40:1o:80:LYS:HD2	1.73	0.54
14:1N:206:LEU:O	14:1N:210:THR:HG23	2.08	0.54
14:1N:342:ALA:HB3	46:1d:201:PC1:H3D1	1.90	0.54
16:1P:179:LEU:HB2	16:1P:317:VAL:HG11	1.90	0.54
21:1V:43:TYR:O	21:1V:47:THR:OG1	2.20	0.54
28:1c:28:TRP:O	28:1c:32:ILE:HD12	2.08	0.54
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.73	0.54
1:1A:106:TRP:CZ2	8:1H:291:LYS:HG2	2.43	0.54
6:1F:21:ILE:HG23	6:1F:233:THR:HG21	1.90	0.54
6:1F:68:ARG:O	6:1F:106:LYS:NZ	2.40	0.54
6:1F:250:ASN:HD21	6:1F:320:ASP:CG	2.16	0.54
10:1J:127:ILE:HD11	30:1e:72:MET:HE2	1.88	0.54
13:1M:306:PRO:HB3	13:1M:458:LEU:HD12	1.89	0.54
15:1O:64:GLY:HA2	28:1c:3:TYR:HD1	1.73	0.54
15:1O:89:ASN:HD21	32:1g:24:ILE:HB	1.73	0.54
25:1Z:58:ARG:O	25:1Z:62:ILE:HD12	2.08	0.54
28:1c:36:LYS:O	28:1c:40:LEU:HG	2.08	0.54
3:1C:164:LYS:NZ	4:1D:92:GLU:OE2	2.36	0.53
4:1D:224:GLU:OE1	9:1I:40:TYR:OH	2.24	0.53
6:1F:300:GLY:HA2	6:1F:333:ALA:H	1.73	0.53
7:1G:175:THR:OG1	7:1G:182:GLN:O	2.23	0.53
12:1L:9:LEU:HA	12:1L:12:LEU:CD1	2.37	0.53
12:1L:459:ILE:O	12:1L:463:PHE:HB2	2.08	0.53
13:1M:102:LEU:HD13	13:1M:106:LEU:HD23	1.90	0.53
22:1W:18:LYS:HD2	22:1W:19:PRO:HD2	1.91	0.53
39:1n:85:PRO:HA	39:1n:90:TYR:CG	2.42	0.53
6:1F:14:SER:O	6:1F:14:SER:OG	2.25	0.53
7:1G:69:CYS:SG	7:1G:70:ALA:N	2.80	0.53
7:1G:470:VAL:HG13	7:1G:490:MET:HE1	1.90	0.53
8:1H:31:MET:HG3	9:1I:41:LEU:HD23	1.91	0.53
10:1J:98:MET:C	10:1J:98:MET:HE2	2.34	0.53
12:1L:313:MET:HB3	12:1L:325:ALA:HB1	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:361:GLY:N	12:1L:433:GLY:O	2.41	0.53
13:1M:71:TRP:O	13:1M:71:TRP:HD1	1.91	0.53
13:1M:76:MET:N	13:1M:76:MET:SD	2.81	0.53
14:1N:314:LYS:HD3	15:1O:270:LEU:HD13	1.89	0.53
20:1U:14:ARG:NH1	35:1j:11:TYR:OH	2.41	0.53
32:1g:112:CYS:H	41:1p:158:GLN:HE22	1.54	0.53
4:1D:34:ASN:HB3	15:1O:158:VAL:HG13	1.91	0.53
5:1E:106:THR:HA	5:1E:109:MET:HG3	1.90	0.53
12:1L:528:TYR:HB3	37:1l:101:MET:HG3	1.89	0.53
13:1M:278:ARG:O	38:1m:71:ARG:NH2	2.41	0.53
13:1M:282:LEU:HA	13:1M:285:LEU:HG	1.91	0.53
20:1T:72:CYS:HB2	20:1T:75:GLU:HG3	1.90	0.53
4:1D:220:PHE:CD2	43:1r:22:LYS:HD2	2.44	0.53
7:1G:364:LEU:HD12	7:1G:491:ASN:HB3	1.88	0.53
12:1L:419:THR:HA	12:1L:422:TYR:CE1	2.43	0.53
13:1M:78:MET:O	13:1M:432:ARG:HD3	2.08	0.53
13:1M:135:ARG:NH2	14:1N:301:SER:O	2.32	0.53
13:1M:154:LEU:HD11	14:1N:254:LEU:HD21	1.89	0.53
29:1d:94:VAL:HG23	29:1d:101:PHE:CD2	2.43	0.53
37:1l:145:ASP:O	37:1l:148:LYS:NZ	2.40	0.53
39:1n:44:ARG:NE	39:1n:48:ASP:OD2	2.41	0.53
3:1C:198:ASP:OD1	3:1C:198:ASP:N	2.42	0.53
9:1I:51:PRO:HB2	42:1q:64:TYR:HE2	1.74	0.53
12:1L:366:MET:HE1	12:1L:445:GLU:HG2	1.89	0.53
20:1U:77:VAL:HA	20:1U:80:ILE:HD13	1.90	0.53
26:1a:49:GLU:OE1	26:1a:52:ARG:NH2	2.39	0.53
37:1l:69:LEU:HB2	37:1l:71:LEU:HD21	1.91	0.53
39:1n:159:GLU:CD	39:1n:159:GLU:H	2.15	0.53
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.43	0.53
4:1D:34:ASN:ND2	15:1O:158:VAL:HG22	2.22	0.53
5:1E:143:GLU:OE1	6:1F:349:ARG:NH2	2.39	0.53
13:1M:388:TRP:O	38:1m:111:LYS:NZ	2.42	0.53
15:1O:49:ARG:HE	15:1O:114:HIS:CE1	2.25	0.53
28:1c:29:ILE:O	28:1c:33:LYS:HB2	2.09	0.53
2:1B:59:MET:HE1	50:1H:401:U10:H4M1	1.90	0.53
7:1G:365:ASN:HB3	7:1G:488:LYS:HE3	1.90	0.53
12:1L:105:MET:HB3	12:1L:118:PHE:CZ	2.44	0.53
12:1L:192:HIS:HE1	13:1M:386:PHE:HE1	1.56	0.53
12:1L:506:ASN:O	12:1L:510:TYR:N	2.41	0.53
12:1L:569:ILE:HD12	46:1m:201:PC1:H352	1.89	0.53
13:1M:307:TRP:HA	13:1M:310:MET:HG3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:215:SER:HA	15:1O:220:VAL:HG23	1.90	0.53
22:1W:52:LEU:HD21	22:1W:103:ILE:HG21	1.90	0.53
24:1Y:4:LEU:O	24:1Y:7:LYS:HG2	2.09	0.53
28:1c:32:ILE:HD12	28:1c:32:ILE:H	1.74	0.53
34:1i:30:ARG:HD3	34:1i:33:VAL:HG13	1.91	0.53
35:1j:33:TRP:HZ2	36:1k:67:LEU:HA	1.72	0.53
5:1E:55:GLN:HE22	5:1E:91:ASN:HB2	1.74	0.53
9:1I:7:MET:SD	43:1r:111:TYR:HD2	2.32	0.53
13:1M:51:ASN:HA	13:1M:57:PHE:HB2	1.90	0.53
13:1M:400:MET:H	13:1M:400:MET:HE2	1.74	0.53
24:1Y:126:MET:N	24:1Y:126:MET:SD	2.81	0.53
26:1a:37:ARG:NH2	26:1a:51:ASP:OD2	2.42	0.53
30:1e:50:ARG:HG3	30:1e:54:GLU:OE1	2.09	0.53
7:1G:115:ASP:O	7:1G:119:GLN:HG3	2.08	0.53
10:1J:127:ILE:HA	25:1Z:120:MET:CE	2.39	0.53
12:1L:198:LEU:HD13	12:1L:262:ARG:HD2	1.91	0.53
13:1M:234:VAL:HG13	13:1M:235:LEU:HD12	1.91	0.53
13:1M:389:SER:O	13:1M:392:THR:OG1	2.23	0.53
13:1M:438:ALA:HB3	32:1g:66:PHE:HE2	1.74	0.53
37:1l:55:GLN:HA	37:1l:58:ARG:HD2	1.90	0.53
4:1D:32:PRO:HG2	4:1D:37:ASP:HA	1.90	0.53
8:1H:24:GLU:OE2	8:1H:195:ARG:NH1	2.38	0.53
10:1J:159:TRP:O	10:1J:163:ILE:HD12	2.09	0.53
11:1K:79:VAL:HG22	11:1K:83:ASN:OD1	2.09	0.53
12:1L:177:ILE:HA	13:1M:401:MET:HE1	1.91	0.53
12:1L:465:GLY:O	12:1L:469:SER:N	2.41	0.53
12:1L:487:LYS:C	12:1L:488:MET:HE2	2.34	0.53
20:1U:49:GLU:HA	20:1U:52:MET:HE3	1.90	0.53
41:1p:53:GLN:OE1	41:1p:53:GLN:N	2.40	0.53
4:1D:338:MET:HE1	4:1D:348:HIS:ND1	2.23	0.52
7:1G:234:VAL:HG23	7:1G:388:ALA:HB1	1.89	0.52
7:1G:517:ASN:OD1	7:1G:517:ASN:O	2.27	0.52
10:1J:138:GLU:N	10:1J:138:GLU:OE2	2.41	0.52
12:1L:301:ILE:H	12:1L:301:ILE:HD12	1.74	0.52
15:1O:288:GLN:HE22	32:1g:27:GLN:C	2.16	0.52
37:1l:158:ILE:HD12	40:1o:103:ARG:HD3	1.91	0.52
40:1o:110:ARG:HG2	40:1o:114:ARG:HG2	1.92	0.52
41:1p:27:ASN:HB3	41:1p:30:THR:HG23	1.90	0.52
1:1A:32:GLU:OE1	1:1A:32:GLU:N	2.38	0.52
1:1A:59:ALA:HA	8:1H:140:ILE:HD11	1.91	0.52
3:1C:168:LEU:HD11	4:1D:90:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:162:PHE:CZ	7:1G:198:ASN:HB2	2.44	0.52
9:1I:52:PHE:CE2	42:1q:30:ALA:HA	2.44	0.52
12:1L:194:ASN:HB3	38:1m:124:PHE:HD1	1.74	0.52
13:1M:338:HIS:NE2	32:1g:34:ASP:OD2	2.35	0.52
15:1O:260:ARG:O	15:1O:264:GLN:HB2	2.09	0.52
20:1U:66:ASP:HA	20:1U:69:LYS:HB3	1.91	0.52
40:1o:67:LYS:HZ2	40:1o:70:ARG:HH12	1.57	0.52
3:1C:89:ARG:NH1	3:1C:163:ARG:HD2	2.24	0.52
12:1L:90:ILE:HB	12:1L:91:PRO:HD3	1.91	0.52
12:1L:385:TYR:HB3	35:1j:39:ARG:HH21	1.74	0.52
23:1X:6:LEU:HB2	25:1Z:88:ARG:NH2	2.16	0.52
30:1e:67:LEU:HB3	30:1e:69:GLN:HG2	1.90	0.52
34:1i:48:LYS:HA	34:1i:51:GLN:HG2	1.91	0.52
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.74	0.52
12:1L:280:LEU:O	12:1L:284:THR:HG23	2.09	0.52
13:1M:230:VAL:HG12	13:1M:235:LEU:CD1	2.39	0.52
21:1V:49:GLN:O	21:1V:53:GLU:HG2	2.09	0.52
31:1f:37:PHE:CE1	33:1h:91:MET:HB3	2.45	0.52
34:1i:11:LEU:O	34:1i:15:ARG:N	2.42	0.52
39:1n:108:PRO:HA	39:1n:111:LYS:HB2	1.92	0.52
2:1B:67:TYR:CZ	2:1B:154:GLU:HB2	2.45	0.52
4:1D:62:LEU:HD23	4:1D:425:PHE:HE2	1.73	0.52
12:1L:7:LEU:HD13	12:1L:49:VAL:HG12	1.92	0.52
12:1L:129:MET:HE2	12:1L:129:MET:C	2.34	0.52
12:1L:202:PHE:HB3	12:1L:265:PRO:HB2	1.92	0.52
12:1L:309:GLN:HA	12:1L:312:LEU:HG	1.91	0.52
13:1M:453:MET:HE3	13:1M:453:MET:H	1.74	0.52
14:1N:298:TYR:HA	14:1N:302:LEU:HD23	1.91	0.52
15:1O:126:ARG:HB3	15:1O:130:SER:OG	2.09	0.52
15:1O:163:TYR:OH	15:1O:269:VAL:HG23	2.10	0.52
16:1P:145:TYR:HE1	16:1P:149:LYS:HE2	1.75	0.52
25:1Z:93:GLU:OE1	25:1Z:97:ILE:HD11	2.10	0.52
25:1Z:97:ILE:HG23	30:1e:82:ARG:NH1	2.25	0.52
1:1A:55:PHE:HB2	1:1A:58:VAL:HG22	1.92	0.52
6:1F:242:PHE:O	6:1F:251:SER:OG	2.28	0.52
7:1G:258:ILE:HD11	7:1G:579:ARG:HE	1.73	0.52
12:1L:203:MET:HE1	41:1p:109:LEU:HD12	1.91	0.52
13:1M:274:SER:HA	13:1M:402:ILE:HG21	1.92	0.52
23:1X:122:GLY:HA3	27:1b:77:LEU:HD11	1.91	0.52
24:1Y:89:TYR:CE2	24:1Y:125:LYS:HE3	2.45	0.52
34:1i:10:ARG:NH1	39:1n:163:PRO:HB2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:93:PRO:HB3	38:1m:14:PRO:HG3	1.90	0.52
3:1C:125:LYS:HD2	4:1D:253:TYR:CZ	2.45	0.52
4:1D:222:ILE:HD13	4:1D:304:MET:HB3	1.92	0.52
5:1E:184:PRO:HD2	44:1s:44:HIS:HD2	1.74	0.52
6:1F:257:ASN:HB2	6:1F:333:ALA:HA	1.91	0.52
14:1N:100:MET:HE3	14:1N:100:MET:HA	1.91	0.52
14:1N:317:PHE:HE2	15:1O:270:LEU:HD21	1.74	0.52
15:1O:133:VAL:HG13	15:1O:205:ALA:HB3	1.91	0.52
15:1O:291:ARG:O	15:1O:295:LYS:HG2	2.10	0.52
16:1P:248:VAL:HG13	16:1P:322:ARG:HH21	1.74	0.52
31:1f:34:LEU:HD12	33:1h:92:ALA:HB3	1.92	0.52
36:1k:26:THR:OG1	36:1k:28:LEU:HD12	2.10	0.52
37:1l:30:ARG:NH1	38:1m:31:ALA:HB1	2.25	0.52
2:1B:122:GLY:O	2:1B:127:HIS:ND1	2.42	0.52
6:1F:189:GLU:HB2	6:1F:222:VAL:HG11	1.91	0.52
7:1G:704:CYS:SG	9:1I:104:ARG:HD2	2.50	0.52
9:1I:84:GLU:HA	9:1I:92:ILE:HB	1.91	0.52
9:1I:108:ARG:HH22	17:1Q:71:GLY:HA3	1.75	0.52
10:1J:111:GLU:HB2	30:1e:80:ARG:NH2	2.25	0.52
10:1J:171:ILE:HD11	11:1K:76:SER:HB2	1.92	0.52
12:1L:292:ALA:HB2	12:1L:304:PHE:HB2	1.92	0.52
13:1M:303:ILE:O	13:1M:304:GLN:NE2	2.43	0.52
13:1M:388:TRP:NE1	38:1m:108:ARG:HE	2.08	0.52
14:1N:237:MET:HA	14:1N:237:MET:HE3	1.91	0.52
22:1W:78:VAL:O	22:1W:82:LEU:HD12	2.10	0.52
27:1b:31:LEU:N	27:1b:32:PRO:HD2	2.25	0.52
30:1e:44:HIS:CG	33:1h:130:LYS:HD2	2.44	0.52
38:1m:49:GLN:OE1	38:1m:49:GLN:N	2.34	0.52
39:1n:33:ARG:HH22	39:1n:36:TYR:HE2	1.58	0.52
5:1E:104:THR:HG23	6:1F:349:ARG:NE	2.18	0.52
7:1G:8:LEU:HB3	7:1G:19:MET:HE2	1.91	0.52
7:1G:189:LYS:HG2	7:1G:190:MET:H	1.74	0.52
14:1N:248:LEU:O	14:1N:251:MET:HB2	2.10	0.52
16:1P:179:LEU:HD22	16:1P:245:ILE:HD11	1.90	0.52
20:1U:63:PRO:HD3	20:1U:79:TYR:OH	2.10	0.52
34:1i:30:ARG:HD2	34:1i:30:ARG:C	2.34	0.52
37:1l:27:TYR:O	37:1l:29:MET:HG3	2.09	0.52
5:1E:153:MET:HB2	5:1E:161:TYR:O	2.10	0.52
8:1H:30:TYR:CE2	26:1a:2:TRP:HA	2.44	0.52
11:1K:22:TYR:CE2	11:1K:90:VAL:HG11	2.45	0.52
13:1M:87:GLU:OE1	13:1M:91:ARG:HB2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:201:MET:HA	13:1M:201:MET:HE3	1.92	0.52
13:1M:375:LEU:O	13:1M:379:LEU:N	2.36	0.52
14:1N:147:GLN:HB2	33:1h:125:TYR:CE1	2.45	0.52
17:1Q:42:ARG:HG3	17:1Q:49:VAL:HG12	1.92	0.52
23:1X:15:GLN:NE2	23:1X:67:LEU:HD21	2.24	0.52
24:1Y:28:GLY:O	24:1Y:62:SER:HB2	2.09	0.52
38:1m:22:TYR:HB3	39:1n:64:ARG:CZ	2.40	0.52
2:1B:121:ASN:O	9:1I:144:HIS:NE2	2.43	0.51
4:1D:337:GLU:O	4:1D:341:SER:OG	2.26	0.51
6:1F:241:TRP:HE1	6:1F:245:PHE:HE2	1.57	0.51
6:1F:280:ILE:HD12	6:1F:286:GLY:HA2	1.92	0.51
7:1G:157:THR:O	7:1G:161:ARG:HG3	2.09	0.51
12:1L:144:TRP:O	12:1L:223:LYS:NZ	2.35	0.51
12:1L:154:LEU:HD13	12:1L:247:LEU:HD21	1.93	0.51
19:1S:63:LYS:HZ1	19:1S:75:ASN:CA	2.23	0.51
21:1V:48:GLU:O	21:1V:52:ASN:ND2	2.39	0.51
21:1V:97:LYS:HD2	21:1V:99:TRP:CZ3	2.45	0.51
24:1Y:87:LEU:HA	24:1Y:90:PHE:HB2	1.93	0.51
33:1h:68:LYS:HE2	41:1p:62:TYR:CE2	2.45	0.51
36:1k:48:GLU:HB2	36:1k:51:ARG:HD2	1.91	0.51
8:1H:196:ALA:CB	8:1H:197:PRO:HD3	2.39	0.51
10:1J:33:LEU:O	10:1J:36:SER:OG	2.23	0.51
10:1J:173:ARG:NH1	15:1O:254:ARG:HE	2.08	0.51
13:1M:47:GLU:HG3	41:1p:92:ARG:HG2	1.92	0.51
16:1P:206:TYR:HB3	16:1P:209:ASP:OD2	2.09	0.51
18:1R:95:HIS:O	18:1R:96:HIS:ND1	2.43	0.51
41:1p:54:GLN:HA	41:1p:57:LYS:HD3	1.92	0.51
2:1B:38:ASN:HD22	2:1B:170:GLU:CD	2.18	0.51
6:1F:257:ASN:O	6:1F:334:VAL:N	2.43	0.51
7:1G:335:LEU:HG	7:1G:340:SER:OG	2.11	0.51
9:1I:62:ARG:HB3	9:1I:133:GLU:OE2	2.09	0.51
10:1J:8:ILE:O	10:1J:11:THR:OG1	2.25	0.51
12:1L:302:VAL:O	12:1L:306:THR:HG23	2.10	0.51
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	1.92	0.51
14:1N:103:ALA:O	14:1N:107:GLY:N	2.44	0.51
18:1R:80:LYS:C	18:1R:80:LYS:HD3	2.35	0.51
24:1Y:68:ILE:HA	24:1Y:71:LEU:HG	1.93	0.51
33:1h:11:ILE:HD12	33:1h:12:LYS:H	1.75	0.51
39:1n:129:ARG:HH21	39:1n:130:GLU:HB3	1.75	0.51
41:1p:109:LEU:HD13	41:1p:127:GLU:HG3	1.91	0.51
5:1E:10:ARG:HE	18:1R:77:LYS:HD3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:313:ASN:ND2	7:1G:517:ASN:HD22	2.08	0.51
7:1G:644:GLN:HA	7:1G:647:GLU:OE2	2.10	0.51
12:1L:108:MET:HE3	12:1L:114:ILE:HA	1.91	0.51
12:1L:176:ARG:NH1	13:1M:401:MET:O	2.44	0.51
12:1L:401:MET:HA	37:1L:126:GLN:HG2	1.92	0.51
13:1M:226:ALA:O	13:1M:230:VAL:HG23	2.10	0.51
33:1h:83:PRO:HD2	33:1h:84:GLU:H	1.76	0.51
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.92	0.51
13:1M:406:TYR:HA	13:1M:409:TYR:HB3	1.93	0.51
16:1P:144:ARG:HB2	16:1P:144:ARG:HH11	1.76	0.51
29:1d:30:ARG:HH21	29:1d:76:LEU:HD12	1.76	0.51
39:1n:97:LYS:HG2	39:1n:177:PRO:HG2	1.93	0.51
42:1q:38:LEU:HD13	42:1q:49:TYR:CE1	2.45	0.51
1:1A:104:TYR:HE1	1:1A:108:GLN:HG2	1.74	0.51
3:1C:89:ARG:HH22	3:1C:163:ARG:HG3	1.74	0.51
3:1C:158:GLU:OE2	3:1C:158:GLU:N	2.41	0.51
4:1D:410:MET:N	4:1D:413:ASP:OD2	2.42	0.51
6:1F:302:SER:HB3	6:1F:350:LEU:HD21	1.91	0.51
7:1G:207:ALA:HB3	45:1G:802:SF4:S2	2.50	0.51
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.46	0.51
10:1J:51:PHE:H	10:1J:139:GLU:CD	2.19	0.51
12:1L:427:ILE:HG23	12:1L:431:PHE:CE2	2.46	0.51
12:1L:596:MET:SD	12:1L:596:MET:N	2.83	0.51
14:1N:308:THR:OG1	15:1O:282:ILE:HG13	2.10	0.51
15:1O:180:GLN:O	15:1O:183:ILE:HG13	2.10	0.51
16:1P:26:ALA:HA	16:1P:31:GLY:HA3	1.92	0.51
20:1U:50:ILE:HG13	20:1U:51:ILE:N	2.26	0.51
25:1Z:78:GLU:O	25:1Z:82:ARG:HG2	2.10	0.51
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.44	0.51
32:1g:88:TRP:CD1	32:1g:91:ARG:HH22	2.29	0.51
3:1C:152:LEU:HB3	4:1D:84:HIS:CD2	2.46	0.51
7:1G:449:PRO:HD2	7:1G:483:VAL:HG12	1.91	0.51
7:1G:620:ARG:NE	7:1G:633:TYR:OH	2.42	0.51
12:1L:55:MET:N	12:1L:55:MET:SD	2.83	0.51
14:1N:40:MET:HA	14:1N:40:MET:HE3	1.92	0.51
14:1N:164:ILE:H	14:1N:164:ILE:HD12	1.74	0.51
14:1N:234:TRP:HA	14:1N:241:THR:HG21	1.92	0.51
15:1O:279:LEU:HB2	15:1O:282:ILE:HG22	1.93	0.51
17:1Q:90:GLU:OE1	17:1Q:90:GLU:N	2.23	0.51
32:1g:73:GLY:O	32:1g:77:VAL:HG12	2.11	0.51
4:1D:137:ILE:HD11	4:1D:199:VAL:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:150:GLN:HB2	6:1F:177:VAL:HG21	1.92	0.51
7:1G:47:SER:OG	7:1G:48:VAL:N	2.43	0.51
12:1L:115:ASN:O	12:1L:119:LYS:HG2	2.11	0.51
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.25	0.51
12:1L:310:LEU:HD13	12:1L:313:MET:HE1	1.93	0.51
13:1M:285:LEU:O	13:1M:289:SER:OG	2.26	0.51
28:1c:23:THR:HG22	28:1c:27:LEU:HD23	1.92	0.51
37:1l:40:ASP:O	38:1m:84:LYS:NZ	2.44	0.51
3:1C:162:PHE:CE2	4:1D:88:GLU:HB2	2.46	0.51
7:1G:243:ARG:HG3	7:1G:244:THR:HG23	1.91	0.51
8:1H:30:TYR:CE1	8:1H:35:LYS:HA	2.46	0.51
8:1H:273:ILE:HG23	8:1H:277:TYR:CD1	2.46	0.51
12:1L:587:TYR:CD2	14:1N:113:PHE:HB3	2.46	0.51
13:1M:61:LEU:HD22	13:1M:241:TYR:HD1	1.76	0.51
13:1M:410:MET:O	13:1M:414:THR:OG1	2.24	0.51
14:1N:8:THR:O	14:1N:12:THR:HG23	2.11	0.51
14:1N:89:MET:HE2	14:1N:98:MET:HE2	1.92	0.51
15:1O:288:GLN:HG3	32:1g:29:ASP:OD2	2.11	0.51
18:1R:13:HIS:HD1	18:1R:13:HIS:H	1.59	0.51
24:1Y:49:LEU:H	24:1Y:49:LEU:HD12	1.76	0.51
29:1d:12:GLN:N	46:1d:201:PC1:O22	2.44	0.51
32:1g:64:PHE:HA	32:1g:68:ILE:HG13	1.92	0.51
2:1B:44:SER:O	8:1H:54:LYS:NZ	2.44	0.51
4:1D:256:SER:HG	4:1D:373:GLU:H	1.58	0.51
6:1F:294:LEU:HD13	6:1F:336:VAL:HG13	1.94	0.51
6:1F:307:ILE:HD12	6:1F:308:PRO:HD2	1.93	0.51
7:1G:218:ARG:HG2	7:1G:219:PRO:HD2	1.91	0.51
7:1G:465:ALA:HB1	7:1G:656:LEU:HD22	1.93	0.51
9:1I:25:LEU:HD23	27:1b:16:PRO:HB2	1.93	0.51
12:1L:250:SER:HB2	12:1L:333:ALA:HA	1.92	0.51
12:1L:435:PRO:HB3	12:1L:437:PHE:CE1	2.46	0.51
14:1N:106:LEU:HD11	14:1N:139:LEU:HD22	1.94	0.51
14:1N:339:MET:HE1	29:1d:30:ARG:HB3	1.93	0.51
15:1O:242:LYS:HD2	15:1O:243:CYS:N	2.25	0.51
19:1S:15:LEU:HD21	19:1S:97:LYS:HG3	1.93	0.51
34:1i:105:PRO:HA	34:1i:116:ILE:HG23	1.93	0.51
36:1k:29:GLU:N	36:1k:29:GLU:OE2	2.44	0.51
40:1o:83:GLN:NE2	40:1o:87:ASP:OD2	2.44	0.51
2:1B:95:LYS:HG3	3:1C:154:GLY:HA2	1.93	0.50
7:1G:114:CYS:O	7:1G:117:GLN:N	2.43	0.50
8:1H:124:ASN:O	8:1H:124:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:8:ILE:O	10:1J:12:ILE:HD12	2.11	0.50
12:1L:593:ILE:HD12	12:1L:593:ILE:H	1.76	0.50
13:1M:8:THR:HG22	13:1M:104:LEU:HD23	1.92	0.50
14:1N:186:HIS:O	14:1N:190:MET:HE2	2.11	0.50
15:1O:303:LYS:O	29:1d:50:ARG:NH1	2.45	0.50
39:1n:13:GLN:H	39:1n:13:GLN:CD	2.18	0.50
40:1o:75:ASN:ND2	40:1o:75:ASN:O	2.44	0.50
44:1s:63:MET:HE3	44:1s:63:MET:HA	1.92	0.50
4:1D:22:THR:OG1	4:1D:24:GLU:OE1	2.29	0.50
4:1D:396:PHE:HD1	4:1D:428:VAL:HG23	1.76	0.50
9:1I:83:CYS:HB3	45:1I:202:SF4:S4	2.51	0.50
9:1I:110:ASP:HA	9:1I:150:ASN:HA	1.93	0.50
12:1L:583:LEU:HB2	12:1L:586:LEU:CD1	2.41	0.50
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	1.93	0.50
15:1O:31:ILE:HD12	15:1O:202:ILE:HG21	1.93	0.50
15:1O:115:LEU:HD13	15:1O:121:GLY:HA2	1.93	0.50
15:1O:239:GLU:OE2	15:1O:239:GLU:N	2.35	0.50
19:1S:61:GLN:HE22	19:1S:63:LYS:HG3	1.75	0.50
20:1U:72:CYS:O	20:1U:76:ILE:HD12	2.10	0.50
22:1W:50:PHE:HB3	22:1W:52:LEU:HD13	1.94	0.50
24:1Y:31:THR:HA	24:1Y:34:ILE:HD12	1.93	0.50
25:1Z:4:SER:OG	25:1Z:5:LYS:N	2.42	0.50
31:1f:37:PHE:CD1	33:1h:91:MET:HB3	2.46	0.50
32:1g:120:LEU:HD12	32:1g:121:PRO:HD2	1.93	0.50
38:1m:126:ILE:HG22	41:1p:139:GLN:HG3	1.93	0.50
5:1E:111:ARG:HH11	5:1E:111:ARG:HG3	1.75	0.50
5:1E:143:GLU:HB3	6:1F:353:PHE:CD1	2.46	0.50
6:1F:134:ALA:HB3	6:1F:175:VAL:HA	1.93	0.50
8:1H:148:ILE:HG21	8:1H:297:THR:HB	1.92	0.50
9:1I:54:LYS:HD3	42:1q:91:HIS:CE1	2.46	0.50
10:1J:56:VAL:O	10:1J:60:TYR:HB2	2.11	0.50
11:1K:5:TYR:CD1	11:1K:43:MET:HE1	2.44	0.50
12:1L:245:ALA:HB2	12:1L:340:PHE:HB3	1.93	0.50
12:1L:358:LYS:HG3	39:1n:79:TYR:CZ	2.46	0.50
13:1M:201:MET:HE3	13:1M:204:MET:HB2	1.92	0.50
13:1M:232:ALA:O	13:1M:237:LYS:NZ	2.43	0.50
15:1O:110:ASP:HA	15:1O:113:GLU:HG3	1.91	0.50
20:1U:15:VAL:HA	20:1U:18:VAL:HG23	1.93	0.50
24:1Y:75:ILE:HG13	24:1Y:76:SER:N	2.26	0.50
29:1d:45:ASP:O	29:1d:49:ARG:HG2	2.11	0.50
34:1i:44:GLN:HA	34:1i:47:ASN:HD21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:48:LEU:HA	39:1n:132:TRP:HH2	1.76	0.50
38:1m:55:ARG:HD3	38:1m:59:ILE:HG23	1.93	0.50
5:1E:171:GLU:OE2	5:1E:171:GLU:N	2.41	0.50
7:1G:9:ILE:HG12	7:1G:22:PRO:HG3	1.93	0.50
10:1J:31:LEU:O	10:1J:35:VAL:HG12	2.12	0.50
12:1L:68:TRP:HZ3	12:1L:138:PHE:HE2	1.59	0.50
12:1L:88:MET:O	12:1L:91:PRO:HD2	2.11	0.50
13:1M:249:ILE:HD12	13:1M:250:LEU:HG	1.94	0.50
13:1M:437:MET:HA	13:1M:437:MET:HE3	1.94	0.50
14:1N:243:LEU:O	14:1N:247:THR:HG22	2.11	0.50
14:1N:322:GLN:OE1	29:1d:49:ARG:NH2	2.27	0.50
14:1N:331:VAL:HG13	29:1d:37:LEU:HD22	1.92	0.50
23:1X:58:GLU:OE1	23:1X:58:GLU:N	2.37	0.50
40:1o:41:THR:OG1	40:1o:42:GLN:N	2.43	0.50
8:1H:286:MET:HE1	8:1H:290:TRP:CD2	2.46	0.50
10:1J:173:ARG:HH22	14:1N:2:ASN:HB2	1.76	0.50
12:1L:306:THR:O	12:1L:309:GLN:N	2.45	0.50
12:1L:366:MET:HE1	12:1L:445:GLU:HB3	1.93	0.50
13:1M:168:GLN:HE22	13:1M:173:SER:HA	1.77	0.50
15:1O:48:LEU:HD11	15:1O:121:GLY:HA3	1.92	0.50
20:1T:79:TYR:O	20:1T:83:LYS:HG2	2.12	0.50
23:1X:3:ILE:HA	25:1Z:105:LYS:HZ1	1.77	0.50
30:1e:79:LYS:HD2	30:1e:82:ARG:HG3	1.93	0.50
34:1i:100:LYS:NZ	41:1p:116:GLU:O	2.45	0.50
7:1G:49:ALA:HB2	7:1G:161:ARG:HE	1.77	0.50
8:1H:102:VAL:HA	8:1H:105:MET:HG2	1.94	0.50
9:1I:12:MET:O	27:1b:9:LYS:NZ	2.34	0.50
13:1M:106:LEU:CD1	13:1M:238:LEU:HD11	2.42	0.50
15:1O:315:LYS:HD2	15:1O:316:TRP:HB2	1.92	0.50
34:1i:123:PRO:HB2	34:1i:125:GLN:HE22	1.76	0.50
6:1F:294:LEU:HD11	6:1F:297:VAL:HG23	1.94	0.50
8:1H:69:SER:O	8:1H:73:ILE:HG12	2.11	0.50
13:1M:12:LEU:HB2	13:1M:13:PRO:HD3	1.94	0.50
37:1l:30:ARG:HH21	38:1m:35:ARG:HB3	1.75	0.50
37:1l:70:ARG:HE	37:1l:86:ARG:HH11	1.59	0.50
2:1B:55:CYS:O	2:1B:116:MET:HE1	2.12	0.50
4:1D:259:MET:HG2	4:1D:398:HIS:CE1	2.45	0.50
8:1H:196:ALA:HB1	8:1H:273:ILE:HG22	1.94	0.50
9:1I:4:PHE:HB3	9:1I:7:MET:CE	2.42	0.50
10:1J:8:ILE:HG22	10:1J:12:ILE:HD11	1.92	0.50
12:1L:366:MET:SD	12:1L:443:ILE:HG22	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:444:ASN:CG	35:1j:7:ILE:HG21	2.37	0.50
13:1M:4:ILE:HG13	13:1M:37:ILE:HG22	1.94	0.50
13:1M:32:LEU:HD13	13:1M:74:PRO:HG2	1.93	0.50
13:1M:71:TRP:O	13:1M:74:PRO:HD2	2.12	0.50
13:1M:391:ILE:O	13:1M:394:ILE:HG22	2.11	0.50
15:1O:92:ASN:OD1	15:1O:95:ARG:NH2	2.45	0.50
20:1T:55:GLU:O	20:1T:59:GLY:N	2.36	0.50
20:1U:9:GLU:OE1	20:1U:9:GLU:N	2.31	0.50
24:1Y:128:GLN:NE2	52:1Y:202:3PE:H11	2.26	0.50
25:1Z:88:ARG:HG3	25:1Z:92:GLU:HG2	1.93	0.50
27:1b:39:ASN:N	27:1b:39:ASN:OD1	2.45	0.50
46:1d:201:PC1:O14	46:1d:201:PC1:H252	2.12	0.50
2:1B:126:TYR:O	2:1B:132:VAL:HG11	2.11	0.50
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.94	0.50
4:1D:121:ALA:HA	4:1D:365:THR:HG21	1.93	0.50
5:1E:181:ILE:HD12	5:1E:181:ILE:O	2.11	0.50
9:1I:43:ARG:NH2	43:1r:24:GLN:HE21	2.10	0.50
12:1L:352:ASP:O	39:1n:82:PRO:HG2	2.12	0.50
15:1O:141:GLN:HG3	15:1O:198:TYR:HB2	1.92	0.50
28:1c:40:LEU:HD13	28:1c:44:ARG:HH22	1.76	0.50
31:1f:55:THR:HG23	31:1f:56:TRP:CD1	2.47	0.50
37:1l:50:LEU:HG	37:1l:78:HIS:HA	1.93	0.50
41:1p:120:TYR:HA	41:1p:123:ASN:HB2	1.93	0.50
12:1L:21:MET:HA	12:1L:21:MET:HE3	1.92	0.49
12:1L:414:ILE:O	12:1L:418:LEU:HG	2.11	0.49
12:1L:432:LEU:HD11	36:1k:62:PHE:HA	1.94	0.49
15:1O:54:ALA:HB3	15:1O:104:ARG:HH11	1.77	0.49
20:1U:51:ILE:O	20:1U:54:MET:HG3	2.12	0.49
25:1Z:111:PHE:CD2	25:1Z:117:VAL:HG11	2.47	0.49
30:1e:85:LEU:HA	30:1e:88:GLU:HB3	1.94	0.49
32:1g:45:HIS:N	32:1g:54:ASP:OD2	2.45	0.49
37:1l:81:LEU:O	37:1l:85:ILE:HG23	2.12	0.49
39:1n:43:MET:HA	39:1n:46:ARG:HB3	1.94	0.49
39:1n:103:LEU:HB3	39:1n:121:ARG:HD2	1.93	0.49
40:1o:58:CYS:HA	40:1o:60:HIS:CE1	2.47	0.49
42:1q:32:ASP:CG	42:1q:34:ARG:HE	2.20	0.49
1:1A:104:TYR:CE2	10:1J:166:VAL:HG22	2.48	0.49
7:1G:49:ALA:HB3	7:1G:161:ARG:HH21	1.77	0.49
7:1G:328:LEU:O	7:1G:507:TYR:OH	2.30	0.49
8:1H:26:LYS:HZ2	26:1a:4:GLU:HB3	1.75	0.49
8:1H:314:ILE:HD12	8:1H:314:ILE:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:6:ALA:HB2	10:1J:46:ASN:ND2	2.27	0.49
10:1J:26:PRO:HB3	11:1K:27:MET:HG2	1.94	0.49
12:1L:176:ARG:CZ	13:1M:404:ALA:HB3	2.42	0.49
12:1L:232:TRP:HH2	12:1L:252:MET:HE1	1.77	0.49
12:1L:422:TYR:HA	12:1L:425:ARG:HB3	1.95	0.49
13:1M:5:ILE:O	13:1M:9:THR:HG23	2.12	0.49
14:1N:69:MET:HB2	14:1N:101:ALA:HB2	1.93	0.49
14:1N:128:LEU:HD11	14:1N:213:LEU:HD23	1.94	0.49
16:1P:16:VAL:HG22	17:1Q:68:PRO:HG3	1.94	0.49
21:1V:78:GLU:OE2	21:1V:78:GLU:N	2.29	0.49
24:1Y:116:TYR:O	24:1Y:120:THR:HG23	2.12	0.49
25:1Z:101:VAL:HG11	25:1Z:104:TRP:HB3	1.93	0.49
37:1l:156:TYR:CD1	40:1o:33:ARG:HG3	2.47	0.49
38:1m:108:ARG:O	38:1m:112:GLU:HG2	2.12	0.49
39:1n:153:LEU:HD21	39:1n:165:LEU:HB2	1.94	0.49
4:1D:62:LEU:CD1	4:1D:64:LEU:HB2	2.43	0.49
9:1I:68:ARG:HD3	9:1I:165:ILE:HG21	1.92	0.49
10:1J:23:LYS:HE2	11:1K:29:SER:HA	1.94	0.49
12:1L:149:ILE:HD12	12:1L:150:MET:N	2.27	0.49
12:1L:400:ASN:HB3	12:1L:486:MET:HG2	1.93	0.49
14:1N:234:TRP:NE1	14:1N:305:PHE:H	2.10	0.49
18:1R:18:TYR:CE2	18:1R:24:ARG:HB3	2.47	0.49
25:1Z:104:TRP:CZ3	25:1Z:106:VAL:HA	2.47	0.49
26:1a:31:ASN:HA	26:1a:61:HIS:CD2	2.47	0.49
28:1c:28:TRP:O	28:1c:31:LEU:N	2.43	0.49
31:1f:9:ASP:OD1	31:1f:10:HIS:N	2.45	0.49
31:1f:14:ILE:HG12	31:1f:15:LEU:HD23	1.93	0.49
36:1k:32:GLN:HG2	36:1k:42:ASP:H	1.77	0.49
37:1l:135:TYR:CD1	40:1o:42:GLN:HB3	2.47	0.49
39:1n:127:LEU:O	39:1n:131:SER:OG	2.21	0.49
1:1A:44:MET:HE3	1:1A:44:MET:C	2.38	0.49
3:1C:127:ALA:O	3:1C:131:GLU:N	2.43	0.49
4:1D:20:TYR:CE2	12:1L:575:ILE:HD11	2.46	0.49
4:1D:301:VAL:O	4:1D:304:MET:HB2	2.12	0.49
6:1F:90:PRO:HB2	6:1F:92:TYR:HE2	1.76	0.49
6:1F:99:GLU:OE2	6:1F:108:ARG:N	2.40	0.49
6:1F:254:LYS:HZ2	6:1F:332:ALA:HB3	1.77	0.49
9:1I:3:LYS:NZ	43:1r:109:GLN:HE21	2.10	0.49
12:1L:7:LEU:HB2	12:1L:50:PRO:HG3	1.94	0.49
13:1M:291:VAL:O	13:1M:295:ALA:N	2.35	0.49
13:1M:453:MET:HA	32:1g:83:TYR:OH	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:92:LYS:HA	21:1V:95:ARG:NH1	2.27	0.49
22:1W:126:HIS:CD2	22:1W:126:HIS:H	2.30	0.49
23:1X:125:SER:N	25:1Z:66:GLU:OE2	2.45	0.49
25:1Z:131:GLU:OE1	25:1Z:131:GLU:N	2.45	0.49
31:1f:48:LEU:HD11	31:1f:54:VAL:HA	1.93	0.49
32:1g:68:ILE:HA	32:1g:72:LEU:HB2	1.94	0.49
33:1h:122:TRP:HD1	33:1h:123:TYR:HB2	1.77	0.49
38:1m:109:ASP:O	38:1m:113:LYS:HG2	2.13	0.49
38:1m:112:GLU:HB2	38:1m:113:LYS:NZ	2.26	0.49
39:1n:25:HIS:CE1	39:1n:74:GLN:HG2	2.47	0.49
39:1n:43:MET:O	39:1n:47:PHE:N	2.46	0.49
5:1E:205:PRO:HG3	44:1s:33:PHE:CG	2.47	0.49
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.94	0.49
7:1G:343:LEU:H	7:1G:343:LEU:HD22	1.77	0.49
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.12	0.49
13:1M:293:HIS:HB3	13:1M:315:LEU:HD21	1.94	0.49
14:1N:213:LEU:HD21	51:1O:403:CDL:H581	1.93	0.49
52:1N:401:3PE:O14	52:1N:401:3PE:N	2.28	0.49
20:1U:37:MET:HE1	20:1U:71:MET:SD	2.52	0.49
52:1Y:202:3PE:O12	52:1Y:202:3PE:N	2.44	0.49
25:1Z:48:TRP:CZ2	25:1Z:52:LYS:HD2	2.48	0.49
25:1Z:111:PHE:CE1	30:1e:64:GLU:HB3	2.47	0.49
28:1c:17:VAL:O	28:1c:21:LEU:HD12	2.12	0.49
32:1g:120:LEU:HD11	41:1p:162:MET:HB3	1.94	0.49
33:1h:87:TYR:HE1	41:1p:89:MET:HG3	1.78	0.49
39:1n:47:PHE:HD1	39:1n:47:PHE:O	1.96	0.49
40:1o:114:ARG:O	40:1o:117:ARG:HG3	2.13	0.49
2:1B:90:GLY:HA2	45:1B:201:SF4:S4	2.53	0.49
6:1F:24:ASN:O	6:1F:113:HIS:HB3	2.13	0.49
13:1M:24:TRP:HE1	13:1M:92:LYS:CG	2.25	0.49
25:1Z:113:THR:HG22	25:1Z:115:ARG:H	1.77	0.49
28:1c:43:LYS:O	28:1c:48:LEU:N	2.45	0.49
30:1e:82:ARG:NH2	30:1e:85:LEU:HD21	2.27	0.49
37:1l:6:LYS:O	37:1l:6:LYS:HD2	2.12	0.49
37:1l:156:TYR:CE1	37:1l:158:ILE:HG22	2.47	0.49
39:1n:25:HIS:HB3	39:1n:75:HIS:HB2	1.95	0.49
3:1C:137:MET:HE1	3:1C:153:THR:HG23	1.95	0.49
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.95	0.49
6:1F:300:GLY:O	6:1F:304:THR:OG1	2.21	0.49
11:1K:20:LEU:HB2	12:1L:592:LEU:CD2	2.42	0.49
12:1L:343:SER:O	12:1L:347:ILE:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:400:ASN:HA	12:1L:409:LEU:HD11	1.93	0.49
12:1L:491:LEU:H	12:1L:491:LEU:HD12	1.78	0.49
15:1O:33:SER:HB2	15:1O:174:VAL:HG11	1.95	0.49
21:1V:72:GLN:N	21:1V:72:GLN:OE1	2.46	0.49
28:1c:32:ILE:HG22	28:1c:36:LYS:HD3	1.94	0.49
29:1d:-1:MET:HG3	29:1d:2:MET:HE3	1.94	0.49
34:1i:65:ARG:NH2	34:1i:68:ILE:HG12	2.28	0.49
37:1l:127:PRO:HD3	40:1o:3:HIS:CE1	2.47	0.49
38:1m:122:GLN:HB3	41:1p:139:GLN:HE22	1.78	0.49
6:1F:388:GLU:HA	43:1r:48:LEU:HD11	1.94	0.49
7:1G:6:SER:OG	7:1G:7:ASN:N	2.45	0.49
7:1G:144:PRO:HD2	7:1G:192:MET:HE1	1.95	0.49
10:1J:57:PHE:HE1	10:1J:61:LEU:HD11	1.78	0.49
12:1L:93:ALA:O	12:1L:97:THR:HG23	2.12	0.49
12:1L:508:THR:O	39:1n:32:HIS:HD2	1.96	0.49
13:1M:206:LYS:HZ1	13:1M:239:GLY:HA3	1.78	0.49
13:1M:395:LEU:HD21	38:1m:100:TRP:CZ3	2.48	0.49
14:1N:239:VAL:HA	52:1N:401:3PE:H221	1.94	0.49
15:1O:210:PHE:O	15:1O:214:MET:HB3	2.12	0.49
31:1f:10:HIS:NE2	52:1g:201:3PE:H241	2.28	0.49
34:1i:93:PRO:HB3	41:1p:4:TRP:CG	2.48	0.49
34:1i:122:PHE:CD2	40:1o:61:TYR:HE1	2.30	0.49
37:1l:61:TRP:CH2	39:1n:85:PRO:HD2	2.47	0.49
38:1m:27:GLU:HG2	38:1m:28:THR:N	2.28	0.49
2:1B:144:ILE:HA	9:1I:142:GLU:HA	1.95	0.49
5:1E:145:LEU:N	47:1E:301:FES:S1	2.82	0.49
6:1F:65:LEU:HD13	6:1F:242:PHE:HE1	1.77	0.49
6:1F:248:GLU:OE1	6:1F:249:ARG:HG2	2.12	0.49
6:1F:403:THR:HB	45:1F:502:SF4:S3	2.52	0.49
12:1L:387:THR:HG22	12:1L:464:ALA:HB2	1.95	0.49
12:1L:407:TRP:HA	12:1L:410:LEU:HB3	1.94	0.49
12:1L:568:PHE:HE2	46:1m:201:PC1:H322	1.77	0.49
13:1M:22:MET:O	13:1M:25:ILE:N	2.42	0.49
16:1P:57:MET:SD	16:1P:60:ARG:NH1	2.86	0.49
23:1X:142:HIS:HB2	25:1Z:115:ARG:HB2	1.94	0.49
24:1Y:28:GLY:HA3	24:1Y:66:GLY:HA3	1.94	0.49
28:1c:25:VAL:O	28:1c:29:ILE:HG13	2.12	0.49
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.36	0.49
34:1i:125:GLN:HB2	40:1o:61:TYR:HE2	1.78	0.49
40:1o:38:MET:SD	40:1o:39:VAL:N	2.86	0.49
40:1o:105:ARG:HG2	40:1o:109:GLN:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:167:LYS:HE3	41:1p:167:LYS:HB3	1.64	0.49
3:1C:74:SER:OG	3:1C:97:LEU:O	2.31	0.49
5:1E:214:GLN:NE2	6:1F:236:ARG:O	2.45	0.49
10:1J:83:TRP:HB3	10:1J:93:PHE:CD1	2.48	0.49
12:1L:117:PHE:HB2	12:1L:157:TRP:CZ2	2.48	0.49
12:1L:176:ARG:NH2	13:1M:404:ALA:H	2.11	0.49
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.13	0.49
15:1O:112:LEU:HD13	15:1O:259:LEU:HD11	1.94	0.49
19:1S:29:SER:O	19:1S:33:ARG:HG3	2.13	0.49
34:1i:16:GLU:HA	34:1i:19:ARG:HB2	1.95	0.49
39:1n:11:HIS:O	39:1n:15:VAL:HG13	2.11	0.49
2:1B:55:CYS:SG	2:1B:117:GLY:HA3	2.52	0.48
5:1E:107:PRO:HB3	6:1F:335:ILE:HD12	1.94	0.48
7:1G:236:SER:HB3	7:1G:259:ASN:HD22	1.78	0.48
8:1H:85:MET:O	8:1H:105:MET:HE1	2.12	0.48
8:1H:110:SER:O	8:1H:113:VAL:HG12	2.12	0.48
8:1H:114:TYR:HE1	10:1J:34:ILE:HD12	1.77	0.48
12:1L:37:LYS:HD3	12:1L:102:GLU:HG2	1.94	0.48
12:1L:139:GLN:HA	12:1L:142:ILE:HD12	1.94	0.48
12:1L:493:VAL:HA	12:1L:496:MET:HE1	1.94	0.48
15:1O:5:PRO:HB3	51:1O:403:CDL:HA4	1.94	0.48
33:1h:129:ASP:OD1	33:1h:130:LYS:N	2.45	0.48
37:1l:13:TYR:HD2	37:1l:15:LYS:HZ2	1.59	0.48
44:1s:54:LEU:O	44:1s:57:GLU:HG3	2.13	0.48
4:1D:212:TYR:CZ	4:1D:216:LYS:HD2	2.47	0.48
12:1L:152:PHE:HD1	12:1L:168:ALA:HB1	1.78	0.48
15:1O:285:GLY:HA3	32:1g:26:LEU:HD11	1.95	0.48
16:1P:52:GLU:HG3	16:1P:54:TYR:H	1.78	0.48
19:1S:72:GLN:OE1	19:1S:72:GLN:HA	2.12	0.48
20:1U:35:HIS:ND1	20:1U:38:LYS:HG2	2.28	0.48
29:1d:107:LYS:HD3	29:1d:108:THR:H	1.78	0.48
31:1f:1:MET:N	31:1f:1:MET:HE3	2.28	0.48
2:1B:118:SER:OG	2:1B:124:GLY:HA2	2.13	0.48
4:1D:199:VAL:HG23	4:1D:323:ILE:HB	1.94	0.48
5:1E:111:ARG:HB2	5:1E:152:PRO:CD	2.42	0.48
7:1G:565:ALA:N	7:1G:568:GLU:OE1	2.47	0.48
51:1H:402:CDL:HA62	51:1H:402:CDL:H1	1.96	0.48
12:1L:137:LEU:N	12:1L:196:TRP:O	2.28	0.48
13:1M:299:VAL:O	13:1M:303:ILE:HD12	2.13	0.48
17:1Q:55:TRP:O	17:1Q:86:PHE:N	2.45	0.48
23:1X:29:HIS:NE2	25:1Z:63:GLU:OE1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:91:ILE:HD12	24:1Y:92:GLY:N	2.28	0.48
38:1m:62:PRO:O	38:1m:66:ARG:HG3	2.12	0.48
41:1p:104:ILE:HG22	41:1p:105:ILE:HD12	1.95	0.48
1:1A:87:MET:HE3	1:1A:88:LEU:N	2.28	0.48
4:1D:110:SER:HA	4:1D:145:THR:HG22	1.95	0.48
4:1D:193:TYR:HE1	4:1D:201:GLN:H	1.61	0.48
7:1G:424:ASP:OD1	7:1G:424:ASP:N	2.45	0.48
8:1H:86:TRP:NE1	8:1H:233:MET:HB2	2.28	0.48
12:1L:199:GLN:HB2	41:1p:113:GLN:OE1	2.14	0.48
12:1L:592:LEU:HD12	12:1L:596:MET:HE1	1.93	0.48
13:1M:11:LEU:HB3	13:1M:100:ILE:HD13	1.95	0.48
13:1M:95:TYR:HD2	13:1M:136:TRP:CE2	2.32	0.48
20:1T:49:GLU:HA	20:1T:52:MET:HG2	1.95	0.48
22:1W:68:MET:H	22:1W:68:MET:CE	2.26	0.48
32:1g:97:VAL:HG13	41:1p:8:VAL:HG12	1.95	0.48
34:1i:94:TYR:HE2	41:1p:108:ARG:HA	1.77	0.48
1:1A:106:TRP:CH2	27:1b:18:LEU:HD21	2.49	0.48
4:1D:166:PRO:HG2	4:1D:229:LEU:HD21	1.94	0.48
4:1D:290:ARG:HB2	4:1D:290:ARG:HH11	1.79	0.48
5:1E:183:LYS:O	5:1E:187:ARG:NH1	2.47	0.48
6:1F:78:LYS:HG2	6:1F:79:TRP:CD1	2.47	0.48
9:1I:43:ARG:HB3	9:1I:43:ARG:NH1	2.28	0.48
12:1L:97:THR:HG22	12:1L:246:LEU:HD11	1.95	0.48
13:1M:50:LEU:HB3	13:1M:52:PHE:CE1	2.48	0.48
14:1N:34:GLU:OE1	14:1N:34:GLU:N	2.36	0.48
15:1O:41:GLU:HB3	15:1O:231:ALA:HB1	1.96	0.48
15:1O:278:TYR:HA	15:1O:283:THR:HG21	1.94	0.48
22:1W:24:ASP:OD2	22:1W:26:ASN:N	2.42	0.48
24:1Y:14:GLY:HA2	24:1Y:74:CYS:HA	1.96	0.48
32:1g:36:ASN:O	32:1g:39:GLU:HG3	2.13	0.48
37:1l:97:SER:O	37:1l:100:THR:OG1	2.16	0.48
38:1m:109:ASP:O	38:1m:113:LYS:NZ	2.29	0.48
40:1o:38:MET:HE1	40:1o:40:ALA:O	2.14	0.48
40:1o:62:LEU:HG	40:1o:86:TRP:NE1	2.28	0.48
3:1C:88:ASN:HB2	21:1V:110:GLN:NE2	2.28	0.48
4:1D:85:ARG:HD3	4:1D:85:ARG:H	1.77	0.48
4:1D:153:ALA:O	4:1D:157:HIS:HB2	2.13	0.48
5:1E:34:ILE:HD11	44:1s:52:LEU:HD12	1.96	0.48
6:1F:359:CYS:SG	6:1F:361:GLN:HB2	2.54	0.48
7:1G:137:VAL:HB	7:1G:151:THR:HA	1.94	0.48
9:1I:32:ARG:NH2	25:1Z:26:PRO:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:48:ILE:HD12	11:1K:49:LEU:N	2.28	0.48
12:1L:18:PRO:HB3	12:1L:36:VAL:HG12	1.94	0.48
12:1L:176:ARG:NH2	13:1M:403:THR:OG1	2.47	0.48
12:1L:194:ASN:HB3	38:1m:124:PHE:CD1	2.47	0.48
12:1L:342:CYS:O	12:1L:346:ILE:HD12	2.14	0.48
13:1M:14:MET:CE	13:1M:26:ASN:HB3	2.44	0.48
13:1M:80:SER:OG	13:1M:226:ALA:HB2	2.14	0.48
13:1M:373:ILE:HG21	13:1M:454:ILE:HD11	1.95	0.48
28:1c:21:LEU:O	28:1c:25:VAL:HG12	2.14	0.48
31:1f:25:TYR:O	31:1f:29:ARG:N	2.33	0.48
31:1f:44:PHE:CD2	33:1h:84:GLU:HA	2.49	0.48
38:1m:32:GLN:O	38:1m:32:GLN:NE2	2.40	0.48
40:1o:67:LYS:HE3	40:1o:67:LYS:HB3	1.49	0.48
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	1.95	0.48
41:1p:75:GLU:OE1	41:1p:75:GLU:N	2.45	0.48
7:1G:52:CYS:SG	7:1G:54:MET:HB3	2.53	0.48
7:1G:180:ASP:OD1	7:1G:180:ASP:N	2.38	0.48
12:1L:193:SER:HB2	12:1L:204:LEU:HD12	1.96	0.48
13:1M:18:SER:HB3	13:1M:26:ASN:ND2	2.28	0.48
13:1M:23:ILE:HG23	13:1M:24:TRP:HD1	1.78	0.48
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.14	0.48
14:1N:149:ILE:HG21	14:1N:154:MET:HG2	1.95	0.48
16:1P:315:ILE:HD13	16:1P:319:ARG:HE	1.79	0.48
18:1R:59:CYS:HB2	18:1R:91:PHE:HE2	1.78	0.48
19:1S:15:LEU:O	19:1S:50:LEU:HD23	2.14	0.48
23:1X:10:GLU:HA	23:1X:13:LYS:HG3	1.95	0.48
28:1c:43:LYS:N	28:1c:43:LYS:HD2	2.29	0.48
31:1f:2:ASN:HB3	31:1f:5:GLN:NE2	2.29	0.48
31:1f:7:VAL:HG12	31:1f:8:ARG:HD2	1.96	0.48
37:1l:47:TYR:OH	37:1l:77:ILE:O	2.25	0.48
40:1o:23:THR:N	40:1o:104:GLU:OE1	2.46	0.48
42:1q:71:ARG:HD2	42:1q:115:PHE:CZ	2.48	0.48
7:1G:143:GLY:HA2	7:1G:190:MET:SD	2.54	0.48
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	1.95	0.48
10:1J:17:PHE:CD1	10:1J:20:PHE:HE1	2.32	0.48
10:1J:45:LEU:HD13	10:1J:50:SER:HA	1.96	0.48
12:1L:443:ILE:H	12:1L:443:ILE:HD12	1.79	0.48
13:1M:123:GLU:O	13:1M:126:LEU:HG	2.14	0.48
13:1M:355:MET:HE2	13:1M:358:TRP:HD1	1.77	0.48
14:1N:95:MET:HG2	14:1N:148:SER:O	2.13	0.48
14:1N:159:MET:O	14:1N:162:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:239:GLU:H	15:1O:239:GLU:CD	2.20	0.48
19:1S:63:LYS:HD3	19:1S:64:LEU:N	2.29	0.48
20:1T:35:HIS:CE1	20:1T:71:MET:HE2	2.49	0.48
20:1T:54:MET:SD	20:1T:76:ILE:HG12	2.53	0.48
20:1U:37:MET:SD	20:1U:71:MET:HE2	2.54	0.48
21:1V:64:VAL:O	21:1V:68:GLU:HG2	2.13	0.48
2:1B:52:LEU:HB2	2:1B:89:ALA:O	2.14	0.48
2:1B:116:MET:HG3	2:1B:156:LEU:HD13	1.95	0.48
3:1C:181:LYS:HD2	16:1P:174:ARG:HD2	1.95	0.48
4:1D:233:ARG:HH22	9:1I:24:THR:HA	1.79	0.48
4:1D:425:PHE:HA	4:1D:428:VAL:HG12	1.95	0.48
5:1E:127:LYS:N	5:1E:130:GLU:OE2	2.38	0.48
6:1F:190:THR:HB	6:1F:204:ARG:HG2	1.96	0.48
7:1G:41:CYS:SG	7:1G:52:CYS:N	2.85	0.48
7:1G:104:ASP:O	7:1G:107:ILE:N	2.40	0.48
7:1G:158:ARG:HH11	7:1G:204:PRO:HD3	1.79	0.48
8:1H:92:PRO:HD3	8:1H:255:TYR:CD1	2.48	0.48
9:1I:120:GLY:O	9:1I:123:GLN:HG2	2.14	0.48
11:1K:84:THR:C	11:1K:85:TYR:HD2	2.21	0.48
12:1L:237:MET:O	12:1L:299:LYS:NZ	2.46	0.48
12:1L:363:TYR:CE2	36:1k:65:ALA:HA	2.49	0.48
15:1O:232:GLU:HA	15:1O:235:VAL:HG22	1.95	0.48
19:1S:19:ARG:NH2	19:1S:73:GLU:OE2	2.27	0.48
21:1V:103:VAL:HG23	21:1V:104:GLU:OE2	2.13	0.48
39:1n:15:VAL:HA	39:1n:18:LEU:HB2	1.96	0.48
2:1B:42:ARG:NH1	46:1q:201:PC1:O12	2.39	0.48
6:1F:99:GLU:O	6:1F:139:ARG:NH2	2.45	0.48
6:1F:110:ILE:HD12	6:1F:111:ILE:HD12	1.95	0.48
6:1F:394:GLU:HB2	7:1G:129:ARG:HH22	1.79	0.48
8:1H:248:ASP:OD2	8:1H:251:THR:N	2.47	0.48
9:1I:68:ARG:HD3	9:1I:132:VAL:HG11	1.96	0.48
12:1L:76:LEU:HD22	12:1L:196:TRP:CZ3	2.49	0.48
12:1L:293:ILE:HD11	12:1L:418:LEU:HD22	1.96	0.48
12:1L:313:MET:HG2	12:1L:329:ILE:HG23	1.96	0.48
12:1L:500:LEU:HD23	12:1L:504:LEU:HD23	1.96	0.48
13:1M:206:LYS:HA	13:1M:215:TRP:CZ2	2.49	0.48
13:1M:244:MET:HE1	13:1M:316:MET:HE1	1.96	0.48
14:1N:237:MET:HE3	14:1N:238:PRO:HD2	1.96	0.48
16:1P:136:ASN:HD21	16:1P:291:ASP:HA	1.79	0.48
20:1T:49:GLU:HB2	22:1W:40:TYR:HE1	1.79	0.48
24:1Y:55:THR:O	24:1Y:59:THR:OG1	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1c:15:LEU:HD23	28:1c:16:LYS:H	1.78	0.48
34:1i:85:LEU:HG	34:1i:86:LYS:HG3	1.94	0.48
37:1l:74:GLY:HA3	38:1m:42:LEU:HD22	1.96	0.48
37:1l:133:TYR:CD2	37:1l:134:PRO:HD2	2.49	0.48
39:1n:20:LYS:O	39:1n:24:ARG:HG2	2.14	0.48
40:1o:44:GLU:O	40:1o:48:ALA:N	2.47	0.48
41:1p:69:ARG:HA	41:1p:69:ARG:HD2	1.67	0.48
41:1p:145:LEU:HB3	41:1p:149:TYR:HB3	1.95	0.48
1:1A:7:LEU:O	1:1A:11:VAL:HG23	2.14	0.47
3:1C:51:PHE:CE1	3:1C:108:LYS:HE2	2.49	0.47
3:1C:192:GLN:HE22	9:1I:93:THR:HG21	1.78	0.47
3:1C:207:PRO:HB3	3:1C:210:ARG:HH22	1.80	0.47
7:1G:278:ARG:HA	7:1G:278:ARG:HD2	1.71	0.47
9:1I:54:LYS:HG3	42:1q:90:LEU:HD21	1.96	0.47
12:1L:439:PRO:HD2	20:1U:57:GLU:HB2	1.96	0.47
20:1U:9:GLU:H	20:1U:9:GLU:CD	2.20	0.47
34:1i:82:HIS:HE1	34:1i:86:LYS:HD2	1.79	0.47
34:1i:83:TYR:HE1	41:1p:48:ARG:HD3	1.79	0.47
36:1k:41:ARG:HD3	36:1k:41:ARG:N	2.29	0.47
1:1A:102:LEU:O	1:1A:106:TRP:N	2.45	0.47
4:1D:20:TYR:CZ	12:1L:571:MET:HG3	2.49	0.47
6:1F:237:ARG:HB2	6:1F:241:TRP:HE3	1.77	0.47
6:1F:374:LYS:O	6:1F:378:ARG:HG3	2.14	0.47
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.47	0.47
14:1N:4:ILE:O	14:1N:7:THR:OG1	2.28	0.47
14:1N:106:LEU:HG	14:1N:138:PRO:HB2	1.96	0.47
15:1O:50:HIS:NE2	15:1O:125:GLU:OE2	2.47	0.47
15:1O:104:ARG:NH2	15:1O:126:ARG:HD2	2.29	0.47
15:1O:236:GLU:CD	21:1V:29:LYS:HZ1	2.22	0.47
20:1U:17:TYR:O	20:1U:21:LEU:HB3	2.15	0.47
32:1g:97:VAL:O	32:1g:101:GLU:HB2	2.13	0.47
36:1k:28:LEU:HD11	36:1k:52:TYR:CE2	2.49	0.47
37:1l:82:ASP:OD1	37:1l:82:ASP:N	2.43	0.47
39:1n:60:THR:HB	39:1n:64:ARG:NH1	2.30	0.47
39:1n:82:PRO:O	39:1n:90:TYR:N	2.47	0.47
40:1o:41:THR:OG1	40:1o:42:GLN:OE1	2.29	0.47
4:1D:255:PHE:HB3	4:1D:259:MET:HB2	1.95	0.47
8:1H:113:VAL:O	8:1H:116:ILE:HG13	2.14	0.47
9:1I:99:ARG:NH2	9:1I:101:ASP:OD2	2.44	0.47
9:1I:120:GLY:O	9:1I:124:GLU:HG3	2.15	0.47
12:1L:68:TRP:HB3	12:1L:69:MET:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:83:HIS:ND1	13:1M:84:LEU:HB2	2.28	0.47
13:1M:361:MET:HE2	13:1M:441:ILE:HG21	1.96	0.47
20:1U:24:LYS:HE2	36:1k:41:ARG:NE	2.29	0.47
24:1Y:109:ILE:HG22	46:1m:201:PC1:H321	1.95	0.47
34:1i:13:GLN:OE1	34:1i:13:GLN:HA	2.14	0.47
36:1k:33:GLU:HA	36:1k:36:ALA:HB3	1.95	0.47
39:1n:138:GLN:NE2	39:1n:142:GLU:OE2	2.44	0.47
40:1o:18:PRO:HA	40:1o:21:MET:HE2	1.97	0.47
2:1B:171:LYS:HE2	2:1B:171:LYS:HA	1.95	0.47
9:1I:49:ASN:O	9:1I:53:GLU:HG2	2.15	0.47
13:1M:47:GLU:HG2	41:1p:89:MET:HE1	1.95	0.47
13:1M:349:GLN:OE1	13:1M:349:GLN:N	2.48	0.47
14:1N:95:MET:HE2	14:1N:95:MET:HA	1.96	0.47
16:1P:192:PRO:HB3	16:1P:256:TYR:CZ	2.48	0.47
20:1U:71:MET:HE3	20:1U:71:MET:HB3	1.46	0.47
21:1V:98:PRO:HD2	21:1V:99:TRP:CE2	2.50	0.47
27:1b:15:GLU:OE1	27:1b:19:VAL:N	2.47	0.47
35:1j:37:LEU:HG	36:1k:77:PHE:HE2	1.80	0.47
39:1n:117:TYR:O	39:1n:120:LYS:HG3	2.14	0.47
5:1E:145:LEU:HD13	5:1E:160:TYR:CZ	2.49	0.47
5:1E:193:CYS:SG	6:1F:109:GLU:HG2	2.55	0.47
11:1K:79:VAL:O	11:1K:83:ASN:N	2.41	0.47
12:1L:107:TYR:HD2	12:1L:348:HIS:HB2	1.78	0.47
12:1L:162:THR:OG1	37:1l:86:ARG:NH2	2.48	0.47
12:1L:176:ARG:HH12	13:1M:405:LEU:H	1.63	0.47
12:1L:521:LYS:HB2	12:1L:528:TYR:OH	2.15	0.47
13:1M:325:MET:SD	13:1M:440:HIS:HB3	2.55	0.47
13:1M:442:LEU:HD12	32:1g:70:LEU:HD13	1.96	0.47
13:1M:455:LEU:HD22	13:1M:459:TYR:HB2	1.95	0.47
13:1M:457:PRO:HA	32:1g:84:ARG:HH12	1.80	0.47
14:1N:251:MET:HB3	14:1N:293:TYR:CZ	2.50	0.47
15:1O:94:TYR:HE1	15:1O:152:TYR:HB2	1.80	0.47
20:1T:19:LEU:HD12	20:1T:30:LEU:HD21	1.96	0.47
36:1k:68:LYS:HD3	36:1k:69:GLY:N	2.28	0.47
37:1l:82:ASP:OD2	38:1m:71:ARG:NH1	2.48	0.47
41:1p:30:THR:O	41:1p:34:LYS:HG2	2.15	0.47
41:1p:70:VAL:HG11	41:1p:86:GLU:HB3	1.96	0.47
1:1A:27:LEU:HA	8:1H:59:GLU:OE2	2.14	0.47
1:1A:73:LEU:HA	1:1A:73:LEU:HD23	1.71	0.47
2:1B:129:SER:OG	2:1B:132:VAL:HG12	2.14	0.47
4:1D:270:ARG:NH2	4:1D:303:GLU:OE2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:205:LEU:HD12	17:1Q:118:TYR:CE2	2.50	0.47
7:1G:113:GLU:OE1	7:1G:219:PRO:HG3	2.14	0.47
7:1G:248:MET:N	7:1G:248:MET:SD	2.88	0.47
12:1L:101:MET:HA	12:1L:104:SER:OG	2.14	0.47
12:1L:260:LEU:HD23	12:1L:267:MET:SD	2.55	0.47
15:1O:63:THR:OG1	15:1O:302:ARG:NH1	2.47	0.47
20:1U:51:ILE:HG21	20:1U:67:ALA:HB1	1.97	0.47
34:1i:6:ASP:OD1	39:1n:155:PRO:HD3	2.14	0.47
1:1A:1:FME:O1	1:1A:2:ASN:N	2.48	0.47
1:1A:63:LEU:HD13	10:1J:63:GLY:HA2	1.97	0.47
2:1B:158:TYR:O	2:1B:158:TYR:HD1	1.97	0.47
4:1D:94:LYS:HE3	9:1I:88:PRO:O	2.15	0.47
6:1F:33:LEU:HD23	6:1F:116:HIS:ND1	2.30	0.47
6:1F:197:GLU:OE1	17:1Q:129:ARG:NH1	2.48	0.47
6:1F:366:ARG:NH1	6:1F:367:GLU:HG2	2.29	0.47
7:1G:556:MET:HE2	7:1G:556:MET:HB3	1.82	0.47
7:1G:613:TYR:CE1	7:1G:622:ARG:HG2	2.50	0.47
9:1I:145:GLU:OE2	16:1P:66:GLY:N	2.38	0.47
10:1J:51:PHE:HD2	10:1J:143:ILE:HD13	1.79	0.47
12:1L:134:ALA:HB3	12:1L:140:LEU:HG	1.97	0.47
12:1L:492:ILE:O	12:1L:495:ILE:HG13	2.14	0.47
12:1L:542:LEU:CB	37:1l:83:MET:HE1	2.40	0.47
13:1M:22:MET:N	13:1M:22:MET:SD	2.88	0.47
13:1M:139:GLN:HB2	13:1M:340:ARG:NH2	2.30	0.47
14:1N:153:LEU:O	14:1N:157:MET:HG3	2.15	0.47
16:1P:322:ARG:HD3	16:1P:326:TRP:O	2.15	0.47
19:1S:78:LEU:HD22	19:1S:86:VAL:HG23	1.95	0.47
23:1X:44:LEU:HD13	23:1X:134:ARG:HH22	1.80	0.47
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.15	0.47
29:1d:10:PRO:HD2	30:1e:7:LYS:HE2	1.95	0.47
46:1d:201:PC1:H3D2	46:1d:201:PC1:H392	1.97	0.47
30:1e:79:LYS:HD2	30:1e:79:LYS:HA	1.62	0.47
33:1h:61:PRO:HB2	33:1h:66:TYR:CE1	2.50	0.47
33:1h:63:HIS:CE1	33:1h:64:TRP:HD1	2.33	0.47
33:1h:68:LYS:HA	33:1h:68:LYS:HE3	1.96	0.47
34:1i:21:TRP:O	34:1i:25:GLN:N	2.47	0.47
38:1m:51:ASN:HD21	39:1n:168:HIS:CD2	2.33	0.47
39:1n:133:GLU:O	39:1n:137:LYS:HG2	2.15	0.47
40:1o:62:LEU:HG	40:1o:86:TRP:CE2	2.50	0.47
42:1q:78:ASP:OD2	42:1q:78:ASP:C	2.58	0.47
43:1r:105:LEU:HD21	43:1r:111:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:135:TRP:HE1	22:1W:88:MET:HE1	1.79	0.47
4:1D:233:ARG:NE	9:1I:29:GLU:OE2	2.38	0.47
8:1H:130:ILE:HG22	8:1H:207:LEU:HD21	1.97	0.47
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	1.97	0.47
13:1M:187:SER:OG	13:1M:188:ASN:N	2.48	0.47
14:1N:72:MET:HG3	14:1N:76:ILE:HG12	1.97	0.47
15:1O:128:ILE:HG22	15:1O:156:LYS:HE3	1.96	0.47
22:1W:81:LEU:HD23	22:1W:81:LEU:HA	1.75	0.47
23:1X:53:ARG:HH22	25:1Z:116:TRP:CD1	2.31	0.47
34:1i:85:LEU:HA	34:1i:89:VAL:HG23	1.97	0.47
39:1n:111:LYS:HA	39:1n:118:PHE:CE2	2.50	0.47
2:1B:96:MET:HB2	4:1D:82:LEU:HD12	1.97	0.47
4:1D:338:MET:HE1	4:1D:348:HIS:CG	2.50	0.47
6:1F:363:THR:HA	6:1F:366:ARG:NH2	2.30	0.47
7:1G:150:MET:HE2	7:1G:150:MET:HA	1.96	0.47
8:1H:15:LEU:HB2	26:1a:15:CYS:SG	2.55	0.47
8:1H:35:LYS:HE3	9:1I:47:THR:OG1	2.15	0.47
8:1H:134:ARG:HH12	8:1H:206:GLU:CD	2.20	0.47
11:1K:82:SER:O	11:1K:86:GLY:N	2.45	0.47
12:1L:127:THR:O	12:1L:131:LEU:HD12	2.15	0.47
13:1M:63:ALA:HA	13:1M:66:LEU:HG	1.97	0.47
13:1M:123:GLU:OE2	14:1N:255:PRO:HG2	2.15	0.47
13:1M:325:MET:HG3	13:1M:440:HIS:HB3	1.97	0.47
17:1Q:19:ILE:O	17:1Q:23:THR:HG23	2.14	0.47
21:1V:77:GLU:O	21:1V:80:ILE:HG13	2.15	0.47
23:1X:74:LYS:HE3	26:1a:66:LEU:HB3	1.95	0.47
46:1d:201:PC1:H2	46:1d:201:PC1:H222	1.44	0.47
1:1A:22:PHE:HZ	8:1H:62:ARG:NH2	2.13	0.47
6:1F:15:LEU:HD23	6:1F:20:ARG:HE	1.79	0.47
7:1G:366:THR:HB	7:1G:491:ASN:HD21	1.80	0.47
8:1H:81:LEU:HA	8:1H:84:THR:HG22	1.97	0.47
12:1L:54:PHE:CE1	12:1L:84:TYR:HB2	2.50	0.47
13:1M:90:THR:OG1	52:1N:401:3PE:H31	2.15	0.47
14:1N:25:HIS:NE2	30:1e:17:MET:SD	2.87	0.47
14:1N:147:GLN:HB2	33:1h:125:TYR:CD1	2.50	0.47
14:1N:170:LEU:HD23	14:1N:292:PHE:HB3	1.96	0.47
14:1N:267:ILE:O	14:1N:271:THR:OG1	2.26	0.47
20:1T:24:LYS:NZ	20:1T:40:LEU:O	2.48	0.47
21:1V:66:LYS:HD2	21:1V:66:LYS:HA	1.69	0.47
36:1k:17:ASP:OD1	36:1k:20:GLN:HB2	2.15	0.47
37:1l:34:TYR:CE1	37:1l:48:PRO:HB3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:27:LEU:HD12	1:1A:27:LEU:H	1.79	0.46
2:1B:69:MET:HG3	2:1B:74:VAL:CG2	2.36	0.46
2:1B:175:ILE:HG21	16:1P:51:CYS:HA	1.97	0.46
4:1D:52:GLY:HA2	4:1D:54:GLN:H	1.81	0.46
5:1E:110:LEU:O	6:1F:261:HIS:NE2	2.48	0.46
8:1H:236:ALA:HA	8:1H:263:THR:HG22	1.97	0.46
11:1K:59:MET:HE3	11:1K:60:PRO:CD	2.45	0.46
12:1L:310:LEU:HA	12:1L:313:MET:HE1	1.97	0.46
13:1M:32:LEU:O	13:1M:36:LEU:HD23	2.14	0.46
14:1N:59:TYR:HE2	14:1N:63:GLN:NE2	2.12	0.46
16:1P:113:ILE:O	16:1P:116:ALA:N	2.48	0.46
16:1P:167:LYS:HB2	16:1P:229:ALA:HA	1.97	0.46
17:1Q:11:ILE:HB	22:1W:23:ARG:NH2	2.29	0.46
21:1V:24:LYS:HZ3	21:1V:59:LYS:HG2	1.80	0.46
26:1a:1:MET:HE2	26:1a:4:GLU:OE2	2.15	0.46
36:1k:48:GLU:OE2	39:1n:37:ARG:HG3	2.14	0.46
39:1n:60:THR:HB	39:1n:64:ARG:HH12	1.80	0.46
41:1p:124:CYS:O	41:1p:128:LEU:N	2.35	0.46
43:1r:12:ASN:ND2	43:1r:19:LEU:H	2.13	0.46
6:1F:418:LEU:HD11	6:1F:426:LEU:HD21	1.97	0.46
7:1G:111:GLY:O	7:1G:218:ARG:NH1	2.48	0.46
7:1G:367:THR:HG22	7:1G:636:VAL:HG21	1.96	0.46
9:1I:82:LEU:O	9:1I:86:VAL:HG12	2.16	0.46
12:1L:364:LYS:NZ	36:1k:57:ALA:O	2.48	0.46
13:1M:122:PHE:C	13:1M:122:PHE:CD1	2.91	0.46
13:1M:135:ARG:O	13:1M:142:ARG:NH1	2.48	0.46
14:1N:218:LEU:HD23	14:1N:326:LEU:HD21	1.97	0.46
15:1O:308:TYR:CE2	29:1d:51:ARG:HD2	2.50	0.46
16:1P:118:ALA:HA	16:1P:129:LEU:HD11	1.97	0.46
23:1X:112:ASP:OD1	23:1X:113:LYS:N	2.48	0.46
51:1a:101:CDL:H712	42:1q:3:LEU:HD21	1.97	0.46
32:1g:56:TRP:O	32:1g:60:VAL:HG23	2.15	0.46
35:1j:14:PHE:CD1	36:1k:55:GLY:HA3	2.51	0.46
36:1k:31:VAL:HB	39:1n:38:TYR:HB2	1.98	0.46
37:1l:75:GLU:HB3	38:1m:39:ARG:NH1	2.30	0.46
38:1m:37:ALA:HB1	38:1m:41:ARG:HH21	1.80	0.46
40:1o:60:HIS:NE2	40:1o:89:CYS:SG	2.85	0.46
1:1A:51:PHE:HD2	8:1H:133:LEU:HD12	1.80	0.46
6:1F:43:TYR:HD1	6:1F:44:LYS:N	2.13	0.46
6:1F:383:ASP:HA	6:1F:433:PHE:CD2	2.50	0.46
7:1G:669:LYS:HE3	7:1G:669:LYS:HB3	1.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:55:LEU:HD21	30:1e:24:GLN:HA	1.98	0.46
12:1L:192:HIS:O	38:1m:124:PHE:HB3	2.15	0.46
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.96	0.46
14:1N:290:LEU:HA	14:1N:293:TYR:CD2	2.50	0.46
14:1N:290:LEU:HA	14:1N:293:TYR:HD2	1.80	0.46
14:1N:323:MET:HB2	51:1O:403:CDL:H712	1.97	0.46
23:1X:79:GLU:O	23:1X:82:THR:OG1	2.25	0.46
24:1Y:126:MET:CE	24:1Y:126:MET:H	2.27	0.46
28:1c:26:PHE:HA	28:1c:29:ILE:HD11	1.96	0.46
29:1d:108:THR:OG1	41:1p:74:THR:O	2.19	0.46
41:1p:139:GLN:O	41:1p:157:LYS:NZ	2.49	0.46
42:1q:75:TRP:HB3	46:1q:201:PC1:H153	1.96	0.46
1:1A:106:TRP:CH2	8:1H:291:LYS:HG2	2.50	0.46
4:1D:169:TRP:CZ3	8:1H:33:LEU:HD13	2.49	0.46
7:1G:407:ALA:HB1	7:1G:422:LEU:HD21	1.96	0.46
7:1G:462:ASP:OD1	7:1G:462:ASP:N	2.47	0.46
9:1I:8:ARG:CZ	9:1I:8:ARG:HA	2.46	0.46
10:1J:67:VAL:O	10:1J:71:THR:HG23	2.14	0.46
10:1J:119:PHE:CD1	11:1K:6:MET:HG3	2.51	0.46
11:1K:66:PHE:CE2	14:1N:31:ILE:HG12	2.50	0.46
12:1L:35:TYR:O	12:1L:38:THR:OG1	2.34	0.46
12:1L:302:VAL:O	12:1L:336:LYS:NZ	2.49	0.46
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.50	0.46
13:1M:365:THR:HG21	13:1M:444:LEU:HD13	1.97	0.46
14:1N:339:MET:HB2	46:1d:201:PC1:H3E2	1.96	0.46
16:1P:271:GLU:OE1	16:1P:281:ARG:NH1	2.40	0.46
19:1S:20:ILE:HG13	19:1S:64:LEU:HD23	1.97	0.46
20:1U:64:ASP:O	39:1n:17:ARG:NH2	2.47	0.46
33:1h:16:PHE:HD2	39:1n:107:HIS:CD2	2.34	0.46
34:1i:101:PRO:HD2	41:1p:14:ARG:NH2	2.30	0.46
34:1i:107:ASP:HB3	41:1p:18:ALA:H	1.80	0.46
41:1p:5:ASP:OD1	41:1p:5:ASP:N	2.46	0.46
1:1A:63:LEU:HD21	11:1K:68:ALA:HB1	1.97	0.46
4:1D:337:GLU:OE2	4:1D:337:GLU:N	2.32	0.46
6:1F:137:TYR:HB3	6:1F:192:LEU:HD11	1.98	0.46
6:1F:391:SER:HB3	43:1r:48:LEU:HD12	1.97	0.46
7:1G:91:GLU:OE2	7:1G:125:SER:N	2.49	0.46
9:1I:44:GLU:HG2	43:1r:0:ACE:H1	1.97	0.46
13:1M:1:FME:C	13:1M:3:LYS:H	2.28	0.46
15:1O:73:LEU:HD21	15:1O:295:LYS:HB2	1.97	0.46
22:1W:27:GLU:O	22:1W:31:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:45:ASN:OD1	22:1W:46:THR:N	2.49	0.46
32:1g:40:LYS:NZ	32:1g:41:ASN:HB3	2.30	0.46
34:1i:85:LEU:HA	34:1i:89:VAL:CG2	2.45	0.46
39:1n:42:LEU:HG	39:1n:43:MET:HE2	1.97	0.46
39:1n:117:TYR:CE1	39:1n:120:LYS:HE2	2.50	0.46
41:1p:29:VAL:O	41:1p:33:THR:HG23	2.16	0.46
4:1D:342:MET:HE1	7:1G:103:LEU:HA	1.96	0.46
6:1F:123:LEU:HA	6:1F:173:PHE:CD1	2.51	0.46
6:1F:250:ASN:HB3	6:1F:318:ASP:HB2	1.97	0.46
7:1G:673:MET:HG2	7:1G:688:VAL:HG21	1.96	0.46
10:1J:7:PHE:CZ	10:1J:123:GLY:HA2	2.51	0.46
10:1J:33:LEU:HD22	10:1J:64:MET:SD	2.56	0.46
12:1L:345:SER:O	12:1L:349:SER:OG	2.22	0.46
12:1L:482:MET:HE1	12:1L:487:LYS:HE3	1.97	0.46
13:1M:163:ALA:O	13:1M:167:ILE:HG12	2.16	0.46
13:1M:300:ALA:HA	13:1M:308:SER:HB2	1.97	0.46
20:1T:29:LYS:HZ3	20:1T:40:LEU:HA	1.81	0.46
22:1W:19:PRO:HG3	22:1W:23:ARG:NH1	2.30	0.46
24:1Y:52:VAL:O	24:1Y:56:GLY:N	2.49	0.46
30:1e:64:GLU:OE2	30:1e:70:LYS:N	2.48	0.46
35:1j:27:PHE:C	35:1j:27:PHE:CD2	2.93	0.46
39:1n:58:LYS:O	39:1n:58:LYS:HD3	2.16	0.46
1:1A:24:LEU:N	1:1A:25:PRO:HD3	2.31	0.46
5:1E:120:ILE:HG12	5:1E:173:ILE:HD11	1.98	0.46
6:1F:15:LEU:H	6:1F:270:GLU:CD	2.24	0.46
6:1F:54:ASP:OD2	6:1F:55:TRP:N	2.49	0.46
7:1G:533:THR:OG1	7:1G:534:ARG:N	2.49	0.46
10:1J:115:ILE:O	10:1J:117:PHE:N	2.48	0.46
11:1K:95:LEU:O	14:1N:51:ARG:NH2	2.49	0.46
12:1L:69:MET:HE3	12:1L:69:MET:N	2.31	0.46
12:1L:480:THR:OG1	12:1L:481:THR:N	2.49	0.46
13:1M:132:ILE:HA	13:1M:136:TRP:HD1	1.80	0.46
13:1M:139:GLN:HB2	13:1M:340:ARG:HH22	1.79	0.46
13:1M:152:TYR:O	13:1M:205:VAL:HG11	2.15	0.46
15:1O:183:ILE:O	15:1O:192:MET:HE1	2.15	0.46
20:1T:65:ILE:HA	22:1W:30:ARG:HH12	1.79	0.46
23:1X:5:GLU:O	23:1X:53:ARG:NE	2.49	0.46
23:1X:12:LEU:HD23	23:1X:12:LEU:H	1.81	0.46
23:1X:25:LYS:HD3	23:1X:94:GLN:HB3	1.98	0.46
23:1X:75:ARG:HG2	23:1X:76:HIS:CE1	2.51	0.46
46:1Y:201:PC1:H371	46:1Y:201:PC1:H332	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:48:TRP:CE2	25:1Z:52:LYS:HD2	2.50	0.46
36:1k:33:GLU:O	36:1k:37:ALA:N	2.48	0.46
39:1n:89:SER:HA	39:1n:92:ARG:HG3	1.96	0.46
4:1D:154:VAL:HG11	4:1D:225:LEU:HD21	1.97	0.46
5:1E:161:TYR:CE2	5:1E:182:PRO:HB2	2.50	0.46
6:1F:137:TYR:HE2	6:1F:186:CYS:SG	2.38	0.46
7:1G:56:LEU:HD12	7:1G:65:VAL:HB	1.98	0.46
7:1G:268:ARG:HD2	7:1G:269:PHE:CZ	2.51	0.46
7:1G:309:SER:OG	7:1G:310:PHE:N	2.49	0.46
7:1G:451:VAL:HG22	7:1G:489:VAL:HG12	1.96	0.46
7:1G:453:LEU:O	7:1G:493:LEU:N	2.37	0.46
13:1M:211:GLY:H	13:1M:213:HIS:CE1	2.34	0.46
13:1M:271:MET:O	13:1M:271:MET:HE3	2.15	0.46
14:1N:217:MET:CB	14:1N:326:LEU:HD13	2.45	0.46
22:1W:51:GLN:O	22:1W:100:ARG:NH1	2.49	0.46
23:1X:40:LYS:HD3	23:1X:40:LYS:HA	1.65	0.46
27:1b:40:TYR:CE2	27:1b:83:LEU:HG	2.50	0.46
33:1h:83:PRO:O	33:1h:87:TYR:HB2	2.16	0.46
37:1l:47:TYR:CG	37:1l:79:TRP:HE3	2.34	0.46
1:1A:59:ALA:HA	8:1H:140:ILE:CD1	2.46	0.46
4:1D:61:VAL:HG11	4:1D:83:LEU:HD12	1.98	0.46
5:1E:86:PHE:O	7:1G:177:ARG:NE	2.49	0.46
5:1E:116:ILE:HG13	5:1E:166:PRO:HD3	1.98	0.46
8:1H:30:TYR:HE1	8:1H:35:LYS:HA	1.81	0.46
12:1L:197:ASP:HB2	12:1L:200:GLN:HB2	1.98	0.46
12:1L:568:PHE:CE2	46:1m:201:PC1:H322	2.51	0.46
13:1M:127:VAL:O	13:1M:131:ILE:HG12	2.16	0.46
13:1M:288:TYR:O	13:1M:292:SER:OG	2.33	0.46
15:1O:94:TYR:CE1	15:1O:152:TYR:HB2	2.51	0.46
22:1W:80:ASP:O	22:1W:83:VAL:HG12	2.15	0.46
36:1k:24:GLU:OE1	36:1k:24:GLU:N	2.47	0.46
37:1l:133:TYR:OH	40:1o:55:ARG:N	2.49	0.46
43:1r:101:LYS:HA	43:1r:101:LYS:HE2	1.98	0.46
2:1B:39:TRP:HH2	8:1H:49:ILE:HG22	1.81	0.46
4:1D:137:ILE:HA	4:1D:140:LEU:HB3	1.97	0.46
8:1H:264:LEU:O	8:1H:268:ILE:HG12	2.16	0.46
12:1L:15:LEU:C	12:1L:18:PRO:HD2	2.41	0.46
12:1L:236:ALA:HB1	12:1L:248:HIS:CE1	2.51	0.46
13:1M:43:ASN:HB3	33:1h:80:TYR:CZ	2.51	0.46
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.15	0.46
13:1M:324:SER:HG	13:1M:440:HIS:CE1	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:378:GLU:OE2	13:1M:382:ILE:HD11	2.16	0.46
13:1M:420:THR:OG1	13:1M:422:HIS:ND1	2.49	0.46
15:1O:266:LYS:HD3	15:1O:269:VAL:HG11	1.98	0.46
16:1P:50:ARG:NH2	55:1P:501:NDP:O3X	2.48	0.46
16:1P:83:LYS:HB3	16:1P:83:LYS:HE2	1.67	0.46
16:1P:203:GLN:HG2	16:1P:231:VAL:HG22	1.98	0.46
19:1S:38:LYS:HB2	19:1S:38:LYS:HE2	1.77	0.46
20:1T:36:PHE:O	20:1T:42:LEU:N	2.41	0.46
30:1e:57:ILE:HD12	30:1e:58:GLU:N	2.31	0.46
33:1h:15:GLY:O	33:1h:19:ARG:HG2	2.16	0.46
34:1i:42:MET:H	34:1i:42:MET:CE	2.24	0.46
34:1i:93:PRO:HB2	41:1p:9:TYR:CD2	2.50	0.46
39:1n:136:VAL:C	39:1n:140:GLN:HE21	2.24	0.46
42:1q:135:GLN:OE1	42:1q:135:GLN:N	2.46	0.46
46:1B:202:PC1:H322	46:1B:202:PC1:H31	1.65	0.45
4:1D:233:ARG:NH2	9:1I:24:THR:HA	2.31	0.45
5:1E:161:TYR:HE2	5:1E:182:PRO:HB2	1.80	0.45
7:1G:60:GLU:OE1	7:1G:61:LYS:N	2.46	0.45
7:1G:215:PHE:HD2	9:1I:104:ARG:HD3	1.80	0.45
12:1L:411:MET:N	12:1L:411:MET:SD	2.89	0.45
12:1L:432:LEU:HD21	36:1k:62:PHE:N	2.31	0.45
13:1M:215:TRP:O	13:1M:219:ALA:N	2.48	0.45
13:1M:238:LEU:H	13:1M:238:LEU:HD22	1.81	0.45
13:1M:305:THR:HG22	13:1M:307:TRP:H	1.81	0.45
14:1N:124:LEU:HD13	14:1N:220:ILE:HD12	1.97	0.45
22:1W:31:ARG:HA	22:1W:34:GLU:OE1	2.16	0.45
24:1Y:27:ILE:HD12	24:1Y:27:ILE:H	1.81	0.45
28:1c:32:ILE:O	28:1c:36:LYS:HG2	2.16	0.45
46:1d:201:PC1:H32	46:1d:201:PC1:H321	1.74	0.45
36:1k:26:THR:HG22	36:1k:52:TYR:HB2	1.98	0.45
37:1l:99:ASN:O	37:1l:103:LYS:HG2	2.15	0.45
5:1E:27:ASN:O	5:1E:31:ILE:HD12	2.15	0.45
6:1F:319:PHE:O	6:1F:323:VAL:HG23	2.16	0.45
9:1I:51:PRO:HB2	42:1q:64:TYR:CE2	2.52	0.45
9:1I:83:CYS:SG	9:1I:109:TYR:OH	2.73	0.45
10:1J:117:PHE:HB2	10:1J:119:PHE:CZ	2.52	0.45
12:1L:281:GLY:O	12:1L:285:THR:HG23	2.16	0.45
12:1L:452:ASN:O	12:1L:456:ARG:HG2	2.15	0.45
13:1M:183:SER:OG	13:1M:248:THR:O	2.33	0.45
14:1N:6:TYR:CZ	14:1N:10:ILE:HD11	2.51	0.45
14:1N:213:LEU:HD23	14:1N:213:LEU:HA	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:72:GLN:HE21	23:1X:116:TRP:HZ2	1.63	0.45
36:1k:48:GLU:HG3	36:1k:52:TYR:HE2	1.81	0.45
36:1k:49:ALA:O	36:1k:53:SER:OG	2.32	0.45
42:1q:1:MET:HE2	42:1q:1:MET:O	2.16	0.45
4:1D:72:MET:HA	4:1D:410:MET:HA	1.98	0.45
4:1D:203:LEU:H	4:1D:203:LEU:HD12	1.80	0.45
6:1F:30:ASP:HB3	6:1F:35:GLY:HA3	1.96	0.45
7:1G:199:ILE:HA	7:1G:202:ILE:HG12	1.99	0.45
7:1G:306:MET:HB2	7:1G:306:MET:HE3	1.70	0.45
9:1I:70:TYR:HE1	9:1I:76:ARG:HA	1.81	0.45
9:1I:83:CYS:SG	9:1I:92:ILE:HG21	2.56	0.45
10:1J:4:TYR:HB2	10:1J:7:PHE:HB2	1.97	0.45
12:1L:407:TRP:HB3	37:1L:115:MET:HE1	1.98	0.45
12:1L:462:ILE:HG21	35:1j:32:MET:HB2	1.98	0.45
13:1M:186:LEU:O	13:1M:252:PRO:HD2	2.16	0.45
13:1M:203:PHE:CE2	13:1M:246:ILE:HG12	2.51	0.45
14:1N:2:ASN:HB3	14:1N:5:ILE:CG1	2.46	0.45
14:1N:5:ILE:O	14:1N:9:LEU:HD23	2.15	0.45
14:1N:213:LEU:O	14:1N:217:MET:HG3	2.15	0.45
20:1T:71:MET:SD	20:1T:71:MET:C	3.00	0.45
20:1U:35:HIS:NE2	20:1U:37:MET:SD	2.89	0.45
21:1V:13:LEU:HD22	21:1V:77:GLU:HB3	1.97	0.45
25:1Z:88:ARG:CZ	25:1Z:88:ARG:HB2	2.45	0.45
32:1g:67:SER:O	32:1g:71:VAL:HB	2.17	0.45
32:1g:95:ARG:NH2	32:1g:96:LEU:HA	2.31	0.45
34:1i:127:HIS:HB2	40:1o:88:TYR:CE2	2.51	0.45
38:1m:9:ARG:HG2	38:1m:10:LEU:N	2.31	0.45
39:1n:25:HIS:NE2	39:1n:74:GLN:HG2	2.31	0.45
44:1s:74:ARG:CZ	44:1s:74:ARG:HB2	2.46	0.45
1:1A:41:PHE:CE2	4:1D:63:ARG:HD2	2.50	0.45
2:1B:62:MET:SD	2:1B:69:MET:HG2	2.56	0.45
2:1B:67:TYR:CE1	2:1B:154:GLU:HB2	2.51	0.45
4:1D:86:GLY:O	4:1D:90:LEU:HG	2.17	0.45
6:1F:20:ARG:NH2	6:1F:270:GLU:OE1	2.49	0.45
10:1J:57:PHE:O	10:1J:61:LEU:HG	2.16	0.45
12:1L:231:PRO:HA	12:1L:234:PRO:HG2	1.98	0.45
12:1L:384:PRO:HA	12:1L:389:PHE:HB2	1.97	0.45
15:1O:167:HIS:CD2	15:1O:248:TRP:CD2	3.04	0.45
15:1O:242:LYS:CD	15:1O:244:ASP:H	2.27	0.45
20:1T:69:LYS:H	20:1T:69:LYS:HD2	1.81	0.45
24:1Y:64:ALA:O	24:1Y:68:ILE:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:33:TRP:CZ2	36:1k:67:LEU:HA	2.50	0.45
2:1B:125:TYR:CE1	4:1D:102:TYR:CZ	3.01	0.45
4:1D:51:PHE:HZ	4:1D:57:ALA:HB3	1.81	0.45
4:1D:138:ARG:HD2	4:1D:194:ILE:HG12	1.98	0.45
5:1E:11:ASP:OD1	5:1E:17:PRO:HD3	2.16	0.45
6:1F:273:SER:HB3	6:1F:318:ASP:HB3	1.98	0.45
6:1F:426:LEU:H	6:1F:426:LEU:HD12	1.80	0.45
7:1G:146:VAL:HG12	7:1G:200:ILE:HD11	1.98	0.45
7:1G:147:LYS:NZ	7:1G:704:CYS:SG	2.70	0.45
7:1G:214:ALA:O	9:1I:104:ARG:NH2	2.48	0.45
7:1G:276:ARG:NH2	42:1q:135:GLN:HE21	2.15	0.45
8:1H:172:ILE:HD11	25:1Z:50:MET:HE2	1.98	0.45
12:1L:289:ALA:O	12:1L:293:ILE:HG12	2.17	0.45
12:1L:316:THR:OG1	12:1L:325:ALA:HB2	2.16	0.45
13:1M:312:ALA:O	13:1M:316:MET:HB2	2.16	0.45
14:1N:255:PRO:HG3	14:1N:260:PHE:CD1	2.51	0.45
15:1O:37:ARG:O	15:1O:41:GLU:HG2	2.17	0.45
15:1O:278:TYR:O	32:1g:25:ARG:NH1	2.45	0.45
15:1O:293:PHE:C	15:1O:293:PHE:CD2	2.95	0.45
19:1S:13:LEU:HA	19:1S:69:ALA:HB2	1.98	0.45
19:1S:63:LYS:HZ1	19:1S:75:ASN:HB2	1.81	0.45
20:1T:42:LEU:HD12	20:1T:46:ASP:HB3	1.98	0.45
21:1V:32:ASP:C	21:1V:32:ASP:OD2	2.59	0.45
35:1j:29:SER:O	35:1j:32:MET:HE3	2.16	0.45
37:1l:85:ILE:HD11	37:1l:88:ARG:HG2	1.97	0.45
38:1m:108:ARG:HD2	38:1m:108:ARG:HA	1.65	0.45
39:1n:30:CYS:O	39:1n:35:LYS:NZ	2.44	0.45
4:1D:19:MET:CE	4:1D:20:TYR:HB3	2.47	0.45
6:1F:253:THR:OG1	6:1F:269:GLU:OE2	2.31	0.45
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.15	0.45
7:1G:624:GLU:HB2	7:1G:631:VAL:HG21	1.98	0.45
7:1G:690:ALA:HB2	7:1G:698:VAL:HG11	1.98	0.45
8:1H:16:ALA:HB2	26:1a:15:CYS:HB3	1.98	0.45
12:1L:38:THR:OG1	34:1i:69:PHE:HE2	2.00	0.45
12:1L:101:MET:C	12:1L:101:MET:HE2	2.41	0.45
12:1L:332:HIS:CE1	12:1L:336:LYS:HG3	2.52	0.45
12:1L:451:ILE:O	12:1L:455:LYS:HG2	2.17	0.45
13:1M:398:MET:HA	13:1M:401:MET:HG3	1.98	0.45
14:1N:198:THR:O	14:1N:201:THR:HG22	2.16	0.45
15:1O:144:ILE:HG13	15:1O:145:ARG:N	2.32	0.45
20:1U:17:TYR:OH	35:1j:12:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:30:ILE:O	21:1V:34:LEU:HG	2.17	0.45
24:1Y:71:LEU:HA	24:1Y:74:CYS:HB2	1.98	0.45
51:1a:101:CDL:HA61	42:1q:6:VAL:HG22	1.99	0.45
34:1i:65:ARG:HH11	34:1i:65:ARG:HG2	1.81	0.45
34:1i:109:ILE:HG13	34:1i:111:GLU:HG2	1.98	0.45
37:1l:68:ASP:O	37:1l:69:LEU:HD13	2.16	0.45
1:1A:80:GLN:NE2	8:1H:315:PRO:O	2.49	0.45
5:1E:102:VAL:HG11	5:1E:117:LEU:HD12	1.98	0.45
6:1F:256:PHE:CE2	6:1F:270:GLU:HB3	2.52	0.45
7:1G:211:LYS:HE3	7:1G:700:GLU:HB2	1.98	0.45
7:1G:242:THR:HA	7:1G:248:MET:HE1	1.98	0.45
7:1G:257:ASP:OD1	7:1G:257:ASP:N	2.47	0.45
7:1G:462:ASP:HB2	7:1G:465:ALA:HB3	1.99	0.45
7:1G:628:PRO:HD3	19:1S:21:HIS:CD2	2.52	0.45
12:1L:127:THR:O	12:1L:130:ILE:HG13	2.17	0.45
12:1L:407:TRP:HE1	37:1l:119:GLY:H	1.63	0.45
13:1M:139:GLN:OE1	13:1M:141:GLU:N	2.29	0.45
13:1M:352:LEU:HB3	13:1M:355:MET:HB2	1.98	0.45
14:1N:289:ASN:HA	14:1N:292:PHE:CE1	2.52	0.45
15:1O:24:VAL:HG11	15:1O:108:TYR:HE1	1.81	0.45
19:1S:50:LEU:HD22	19:1S:51:PRO:HD2	1.99	0.45
23:1X:3:ILE:HD12	25:1Z:105:LYS:HZ1	1.80	0.45
23:1X:101:LYS:HE2	23:1X:101:LYS:HB2	1.73	0.45
27:1b:27:LEU:O	27:1b:31:LEU:HD12	2.17	0.45
33:1h:64:TRP:H	33:1h:64:TRP:CD1	2.34	0.45
33:1h:87:TYR:CE1	41:1p:89:MET:HG3	2.51	0.45
37:1l:58:ARG:NE	37:1l:70:ARG:O	2.48	0.45
37:1l:66:HIS:HB2	37:1l:71:LEU:HB2	1.97	0.45
37:1l:68:ASP:OD1	37:1l:69:LEU:N	2.45	0.45
39:1n:23:LEU:HD12	39:1n:27:GLU:OE1	2.17	0.45
40:1o:64:GLN:HA	40:1o:67:LYS:HG3	1.98	0.45
40:1o:81:HIS:HA	40:1o:84:HIS:CE1	2.52	0.45
2:1B:81:ARG:HG3	8:1H:61:LEU:HD13	1.98	0.45
4:1D:396:PHE:CD1	4:1D:428:VAL:HG23	2.52	0.45
4:1D:410:MET:HE1	8:1H:282:TYR:HE1	1.82	0.45
6:1F:276:LEU:HD12	6:1F:312:CYS:HB3	1.99	0.45
6:1F:331:THR:O	6:1F:331:THR:OG1	2.34	0.45
10:1J:163:ILE:HD12	10:1J:163:ILE:H	1.82	0.45
10:1J:168:ILE:HA	10:1J:168:ILE:HD12	1.77	0.45
12:1L:237:MET:HE3	12:1L:300:LYS:HZ2	1.82	0.45
12:1L:295:GLN:H	12:1L:425:ARG:NH2	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:179:ILE:HD11	13:1M:249:ILE:HG12	1.99	0.45
13:1M:459:TYR:HD2	32:1g:84:ARG:HD3	1.80	0.45
14:1N:93:VAL:O	14:1N:97:MET:HB2	2.17	0.45
14:1N:128:LEU:HD21	51:1O:403:CDL:H722	1.99	0.45
15:1O:24:VAL:HG12	15:1O:166:PRO:HB3	1.98	0.45
15:1O:242:LYS:HD2	15:1O:244:ASP:N	2.29	0.45
16:1P:127:GLU:N	16:1P:127:GLU:OE1	2.50	0.45
16:1P:145:TYR:CD2	16:1P:286:ARG:HD3	2.52	0.45
20:1T:18:VAL:HA	20:1T:21:LEU:HD23	1.98	0.45
21:1V:107:PRO:HD2	21:1V:110:GLN:HG3	1.99	0.45
23:1X:84:TYR:CZ	23:1X:103:GLN:HB2	2.52	0.45
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.41	0.45
39:1n:82:PRO:HB3	39:1n:89:SER:H	1.81	0.45
41:1p:62:TYR:CD1	41:1p:62:TYR:C	2.94	0.45
1:1A:63:LEU:O	1:1A:67:LEU:HG	2.16	0.45
3:1C:141:PHE:HE1	22:1W:84:ILE:HG21	1.82	0.45
3:1C:175:ARG:HE	3:1C:186:GLU:CD	2.24	0.45
6:1F:203:PRO:HG2	6:1F:405:CYS:SG	2.57	0.45
6:1F:430:MET:HB2	6:1F:430:MET:HE2	1.63	0.45
7:1G:54:MET:HE3	7:1G:93:VAL:HG23	1.99	0.45
11:1K:48:ILE:HD12	11:1K:49:LEU:H	1.81	0.45
12:1L:114:ILE:H	12:1L:114:ILE:CD1	2.26	0.45
12:1L:499:MET:C	12:1L:499:MET:HE2	2.42	0.45
14:1N:109:SER:HB3	14:1N:110:PRO:HD2	1.99	0.45
20:1T:23:ASP:OD2	20:1T:24:LYS:N	2.50	0.45
20:1U:36:PHE:HA	20:1U:40:LEU:HD23	1.99	0.45
21:1V:92:LYS:HA	21:1V:95:ARG:HH12	1.81	0.45
23:1X:141:TYR:HA	25:1Z:115:ARG:HD3	1.99	0.45
24:1Y:119:LEU:HD23	24:1Y:119:LEU:HA	1.80	0.45
31:1f:42:LEU:HD12	31:1f:45:LYS:HE2	1.98	0.45
32:1g:96:LEU:HD11	41:1p:101:ILE:CG2	2.46	0.45
33:1h:20:ARG:HA	33:1h:23:LYS:NZ	2.32	0.45
36:1k:42:ASP:CG	39:1n:37:ARG:HE	2.25	0.45
37:1l:126:GLN:O	37:1l:128:VAL:N	2.46	0.45
38:1m:101:TYR:CE1	38:1m:105:LYS:HE3	2.52	0.45
2:1B:91:THR:HA	2:1B:119:CYS:HB3	1.99	0.45
4:1D:19:MET:HB3	14:1N:173:THR:HB	1.99	0.45
4:1D:371:LYS:HD3	4:1D:422:ASP:O	2.17	0.45
7:1G:63:PRO:O	7:1G:85:LYS:NZ	2.50	0.45
8:1H:53:LEU:O	8:1H:57:THR:HG23	2.16	0.45
8:1H:99:ASN:ND2	26:1a:40:HIS:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:80:CYS:SG	9:1I:82:LEU:HG	2.57	0.45
12:1L:62:ILE:HG13	12:1L:81:LYS:HA	1.98	0.45
12:1L:375:ILE:HA	12:1L:378:LEU:HB3	1.99	0.45
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.81	0.45
13:1M:147:LEU:HD13	14:1N:291:TYR:HE1	1.81	0.45
14:1N:214:ALA:HB2	14:1N:329:MET:CB	2.47	0.45
14:1N:317:PHE:CE2	15:1O:270:LEU:HD21	2.52	0.45
14:1N:322:GLN:HB3	29:1d:49:ARG:HH12	1.81	0.45
20:1T:77:VAL:HA	20:1T:80:ILE:HD11	1.99	0.45
23:1X:9:LEU:CD2	25:1Z:88:ARG:HG2	2.47	0.45
23:1X:70:PHE:O	23:1X:73:ILE:HG22	2.16	0.45
30:1e:82:ARG:HH11	30:1e:82:ARG:HG2	1.81	0.45
31:1f:10:HIS:CD2	52:1g:201:3PE:H3C2	2.52	0.45
33:1h:14:SER:HB3	39:1n:107:HIS:CE1	2.52	0.45
33:1h:62:GLU:CD	33:1h:65:GLU:HB2	2.42	0.45
34:1i:65:ARG:CZ	34:1i:65:ARG:HA	2.47	0.45
35:1j:12:ARG:NH2	36:1k:47:ASN:O	2.50	0.45
39:1n:36:TYR:CE1	39:1n:40:ALA:HB2	2.52	0.45
39:1n:56:MET:HE3	39:1n:56:MET:N	2.32	0.45
1:1A:54:LYS:HB3	1:1A:114:ALA:HB3	1.97	0.44
1:1A:73:LEU:O	1:1A:76:PRO:HD2	2.17	0.44
4:1D:334:LYS:HB2	4:1D:337:GLU:OE2	2.17	0.44
4:1D:342:MET:HE2	4:1D:342:MET:HA	1.99	0.44
5:1E:191:PHE:CG	44:1s:38:TYR:HB2	2.52	0.44
7:1G:358:LEU:HD11	19:1S:40:TYR:CE2	2.52	0.44
11:1K:16:LEU:O	11:1K:20:LEU:HD12	2.16	0.44
12:1L:123:LEU:HA	12:1L:126:ILE:HG12	2.00	0.44
12:1L:274:GLN:O	12:1L:278:LEU:HD22	2.17	0.44
13:1M:278:ARG:HA	13:1M:278:ARG:HD2	1.59	0.44
14:1N:7:THR:O	14:1N:11:MET:HG2	2.17	0.44
16:1P:201:VAL:N	16:1P:290:SER:OG	2.43	0.44
18:1R:30:ASP:O	18:1R:31:ARG:HD3	2.17	0.44
21:1V:39:LYS:HA	21:1V:44:ARG:HE	1.81	0.44
33:1h:55:ILE:HG22	33:1h:57:GLU:H	1.82	0.44
5:1E:6:LEU:O	5:1E:92:ARG:NH2	2.50	0.44
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.52	0.44
5:1E:134:ASP:C	5:1E:134:ASP:OD2	2.59	0.44
5:1E:209:PRO:HA	6:1F:40:GLY:HA2	1.99	0.44
6:1F:337:MET:HG3	6:1F:341:THR:HG21	1.99	0.44
6:1F:383:ASP:HA	6:1F:433:PHE:CE2	2.52	0.44
8:1H:136:VAL:O	8:1H:140:ILE:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:15:LYS:HD2	25:1Z:33:TYR:CE2	2.52	0.44
10:1J:18:VAL:HG11	10:1J:96:GLY:HA3	1.98	0.44
12:1L:227:PHE:N	12:1L:284:THR:HG22	2.33	0.44
12:1L:272:LEU:HD13	12:1L:276:MET:HE1	1.99	0.44
13:1M:102:LEU:O	13:1M:106:LEU:HD23	2.18	0.44
14:1N:2:ASN:HA	15:1O:254:ARG:CZ	2.48	0.44
19:1S:32:VAL:O	19:1S:36:ILE:HG13	2.16	0.44
28:1c:2:PHE:C	28:1c:2:PHE:CD2	2.95	0.44
31:1f:37:PHE:HB3	31:1f:40:LYS:HG2	1.98	0.44
33:1h:16:PHE:H	39:1n:107:HIS:CE1	2.35	0.44
37:1l:69:LEU:HD12	37:1l:86:ARG:HG3	2.00	0.44
40:1o:61:TYR:O	40:1o:65:LEU:HB2	2.17	0.44
40:1o:69:LYS:HE3	40:1o:69:LYS:HB3	1.79	0.44
40:1o:70:ARG:NE	40:1o:71:ASP:OD1	2.45	0.44
1:1A:12:THR:O	1:1A:16:LEU:HG	2.17	0.44
1:1A:53:MET:HB2	1:1A:55:PHE:CE2	2.51	0.44
4:1D:40:LYS:HE2	4:1D:40:LYS:HB3	1.76	0.44
6:1F:27:GLY:HA3	44:1s:38:TYR:HE1	1.82	0.44
6:1F:44:LYS:HD2	6:1F:44:LYS:HA	1.90	0.44
6:1F:206:LYS:HD2	6:1F:206:LYS:HA	1.76	0.44
7:1G:276:ARG:HH21	42:1q:135:GLN:HE21	1.64	0.44
8:1H:142:TYR:CE2	8:1H:191:ALA:HB1	2.52	0.44
8:1H:301:CYS:O	8:1H:305:ILE:HG22	2.18	0.44
9:1I:70:TYR:CE1	9:1I:76:ARG:HA	2.53	0.44
10:1J:14:VAL:HA	10:1J:17:PHE:HB2	1.97	0.44
12:1L:143:GLY:O	12:1L:147:VAL:HG22	2.17	0.44
12:1L:383:MET:HA	12:1L:384:PRO:HD2	1.87	0.44
13:1M:294:MET:O	13:1M:297:VAL:HG22	2.18	0.44
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.50	0.44
14:1N:211:MET:HE3	14:1N:211:MET:C	2.41	0.44
15:1O:48:LEU:HA	15:1O:120:GLN:HE22	1.82	0.44
15:1O:145:ARG:HH22	15:1O:280:PRO:HD2	1.82	0.44
16:1P:23:VAL:O	16:1P:48:PRO:HD2	2.18	0.44
16:1P:108:ASP:O	16:1P:113:ILE:HD12	2.17	0.44
29:1d:91:PHE:HA	29:1d:94:VAL:HG12	1.99	0.44
32:1g:90:ARG:NH2	41:1p:100:GLU:O	2.39	0.44
33:1h:74:TRP:HE3	33:1h:77:ARG:HH21	1.66	0.44
34:1i:108:THR:HB	34:1i:113:GLY:HA2	2.00	0.44
35:1j:12:ARG:O	36:1k:21:TRP:NE1	2.51	0.44
36:1k:44:TRP:HB2	39:1n:37:ARG:NE	2.32	0.44
37:1l:135:TYR:CE1	40:1o:42:GLN:HB3	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:95:VAL:HA	40:1o:98:MET:HB3	1.99	0.44
40:1o:104:GLU:O	40:1o:108:LEU:N	2.49	0.44
2:1B:175:ILE:O	2:1B:179:ARG:N	2.50	0.44
4:1D:31:PRO:O	4:1D:33:TRP:HD1	1.99	0.44
5:1E:98:TYR:N	5:1E:136:LEU:O	2.45	0.44
5:1E:105:THR:O	5:1E:109:MET:N	2.45	0.44
6:1F:249:ARG:N	6:1F:249:ARG:NE	2.65	0.44
7:1G:145:LEU:HD12	7:1G:269:PHE:CE2	2.52	0.44
7:1G:218:ARG:HD3	7:1G:220:TRP:CH2	2.52	0.44
7:1G:659:ASP:OD1	7:1G:659:ASP:N	2.49	0.44
12:1L:202:PHE:CE1	12:1L:263:PHE:HA	2.52	0.44
12:1L:384:PRO:O	12:1L:386:LEU:HD12	2.18	0.44
13:1M:90:THR:HG1	52:1N:401:3PE:H31	1.82	0.44
13:1M:203:PHE:CD1	13:1M:239:GLY:HA2	2.52	0.44
13:1M:368:ALA:HB1	13:1M:375:LEU:HA	1.99	0.44
15:1O:293:PHE:HD2	15:1O:293:PHE:C	2.25	0.44
16:1P:64:ASP:HB3	16:1P:67:GLN:HG3	1.98	0.44
24:1Y:61:THR:HG22	24:1Y:103:ARG:HB3	1.99	0.44
33:1h:18:ASP:OD1	33:1h:18:ASP:N	2.49	0.44
44:1s:41:LEU:HD23	44:1s:42:GLN:HE21	1.83	0.44
1:1A:41:PHE:CE1	2:1B:99:ALA:HB2	2.53	0.44
2:1B:25:ARG:HG2	2:1B:27:GLU:H	1.81	0.44
6:1F:151:VAL:HG23	6:1F:154:ARG:HH21	1.82	0.44
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.58	0.44
7:1G:126:ASP:OD1	7:1G:126:ASP:N	2.49	0.44
7:1G:136:ALA:HB3	18:1R:56:VAL:HG22	1.99	0.44
9:1I:95:GLU:N	9:1I:95:GLU:OE1	2.50	0.44
10:1J:163:ILE:HA	10:1J:166:VAL:HB	1.99	0.44
10:1J:169:MET:HA	10:1J:172:THR:HG22	1.99	0.44
12:1L:145:GLU:O	12:1L:149:ILE:HG13	2.18	0.44
12:1L:383:MET:HE3	12:1L:383:MET:HB2	1.74	0.44
12:1L:574:SER:C	12:1L:578:SER:HG	2.24	0.44
13:1M:360:LEU:HD12	13:1M:361:MET:N	2.33	0.44
15:1O:46:LEU:HD21	15:1O:235:VAL:HB	2.00	0.44
15:1O:91:GLY:HA3	15:1O:281:GLU:HG2	1.99	0.44
15:1O:135:LEU:O	15:1O:138:MET:HE3	2.17	0.44
15:1O:173:ASP:O	15:1O:226:ARG:NH1	2.48	0.44
15:1O:290:ASP:O	15:1O:294:GLN:HG2	2.18	0.44
16:1P:172:PHE:HB2	16:1P:179:LEU:HG	1.99	0.44
23:1X:73:ILE:HD12	23:1X:73:ILE:HA	1.80	0.44
31:1f:31:ASP:OD1	33:1h:89:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:53:GLU:CD	31:1f:54:VAL:H	2.25	0.44
37:1l:11:GLY:O	38:1m:78:ASN:ND2	2.46	0.44
37:1l:73:TRP:CZ3	38:1m:59:ILE:HB	2.53	0.44
38:1m:44:ARG:CZ	39:1n:139:LEU:HD11	2.48	0.44
38:1m:101:TYR:HE1	38:1m:105:LYS:HE3	1.83	0.44
52:1n:202:3PE:H231	52:1n:202:3PE:H321	1.98	0.44
1:1A:73:LEU:N	1:1A:74:PRO:HD2	2.33	0.44
7:1G:201:ASP:OD1	7:1G:201:ASP:N	2.32	0.44
8:1H:145:THR:O	8:1H:149:ILE:HD12	2.18	0.44
8:1H:227:GLU:O	8:1H:231:ILE:HG13	2.18	0.44
12:1L:310:LEU:HA	12:1L:313:MET:CE	2.48	0.44
13:1M:150:LEU:HD13	14:1N:290:LEU:HD21	2.00	0.44
14:1N:190:MET:HB3	14:1N:201:THR:OG1	2.18	0.44
14:1N:292:PHE:HA	14:1N:295:ARG:HH11	1.81	0.44
15:1O:275:ILE:O	15:1O:277:VAL:N	2.47	0.44
20:1U:14:ARG:NH2	20:1U:57:GLU:HG2	2.32	0.44
24:1Y:61:THR:O	24:1Y:64:ALA:N	2.51	0.44
24:1Y:94:CYS:HB3	24:1Y:118:GLY:CA	2.48	0.44
29:1d:120:ARG:NH2	41:1p:144:ASP:OD2	2.50	0.44
33:1h:74:TRP:O	33:1h:78:THR:HG22	2.17	0.44
41:1p:7:ASP:OD1	41:1p:7:ASP:N	2.48	0.44
2:1B:101:ARG:HD2	2:1B:101:ARG:HA	1.62	0.44
3:1C:135:TRP:NE1	22:1W:88:MET:HE1	2.32	0.44
4:1D:33:TRP:CE3	15:1O:275:ILE:HG23	2.52	0.44
7:1G:258:ILE:HD11	7:1G:579:ARG:NE	2.31	0.44
9:1I:63:GLY:O	9:1I:133:GLU:HB3	2.17	0.44
10:1J:133:SER:HB2	10:1J:138:GLU:OE2	2.18	0.44
10:1J:147:TYR:N	10:1J:147:TYR:CD2	2.86	0.44
12:1L:66:TRP:HB3	12:1L:78:LEU:HB2	2.00	0.44
12:1L:237:MET:HE3	12:1L:300:LYS:NZ	2.32	0.44
12:1L:584:ILE:HG23	12:1L:588:PHE:CE2	2.49	0.44
12:1L:605:HIS:CD2	14:1N:92:PRO:HB2	2.53	0.44
14:1N:128:LEU:O	14:1N:132:THR:OG1	2.23	0.44
15:1O:260:ARG:HA	15:1O:263:VAL:HG22	1.98	0.44
16:1P:237:LEU:HB3	16:1P:240:ASP:OD2	2.18	0.44
20:1T:40:LEU:HB3	20:1T:42:LEU:HD22	1.99	0.44
20:1U:52:MET:SD	39:1n:23:LEU:HD21	2.57	0.44
25:1Z:71:LEU:HD21	25:1Z:75:PHE:CZ	2.53	0.44
30:1e:46:ILE:HG23	30:1e:50:ARG:NH1	2.32	0.44
33:1h:69:HIS:O	33:1h:73:ARG:HG3	2.17	0.44
34:1i:104:PHE:CZ	40:1o:63:ILE:HG13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:49:GLN:H	38:1m:49:GLN:CD	2.23	0.44
38:1m:76:TYR:HA	38:1m:79:PHE:HB3	1.99	0.44
39:1n:127:LEU:HA	39:1n:130:GLU:HG3	1.99	0.44
39:1n:134:ARG:HA	39:1n:137:LYS:HG2	2.00	0.44
42:1q:72:ASP:C	42:1q:72:ASP:OD2	2.61	0.44
5:1E:98:TYR:CE2	5:1E:176:LEU:HD12	2.52	0.44
7:1G:74:MET:HE1	7:1G:77:TRP:CH2	2.52	0.44
7:1G:205:VAL:HB	45:1G:802:SF4:S3	2.58	0.44
7:1G:637:GLU:OE2	19:1S:58:SER:N	2.51	0.44
8:1H:102:VAL:O	8:1H:105:MET:HB2	2.17	0.44
8:1H:181:LEU:HG	8:1H:300:LEU:HD13	1.99	0.44
12:1L:32:TYR:HB3	12:1L:115:ASN:HD22	1.82	0.44
12:1L:366:MET:HA	12:1L:366:MET:HE3	2.00	0.44
12:1L:581:LYS:NZ	12:1L:581:LYS:HB3	2.33	0.44
13:1M:114:GLU:HG2	23:1X:168:PHE:HB3	1.99	0.44
13:1M:267:TRP:HB2	38:1m:100:TRP:CD1	2.53	0.44
15:1O:107:GLN:NE2	15:1O:124:LEU:HD23	2.32	0.44
16:1P:203:GLN:CD	16:1P:235:ARG:HG2	2.43	0.44
16:1P:258:LEU:HD13	16:1P:263:TYR:CD1	2.53	0.44
16:1P:311:GLU:HG2	16:1P:336:PRO:HB3	1.98	0.44
17:1Q:97:GLU:OE2	17:1Q:97:GLU:N	2.50	0.44
22:1W:65:GLU:OE1	22:1W:66:MET:HE2	2.18	0.44
22:1W:68:MET:HE3	22:1W:68:MET:N	2.32	0.44
22:1W:114:ARG:HD3	22:1W:115:PRO:HD2	2.00	0.44
23:1X:88:ILE:HG12	23:1X:99:CYS:SG	2.58	0.44
32:1g:41:ASN:OD1	32:1g:41:ASN:N	2.50	0.44
39:1n:30:CYS:HB3	39:1n:35:LYS:HE3	1.99	0.44
40:1o:80:LYS:HD2	40:1o:80:LYS:N	2.33	0.44
4:1D:144:ILE:HA	4:1D:147:LEU:HD13	1.99	0.44
4:1D:390:LYS:NZ	4:1D:430:ARG:HH22	2.16	0.44
4:1D:413:ASP:OD1	8:1H:281:ARG:NH1	2.50	0.44
5:1E:22:ASP:OD1	5:1E:22:ASP:C	2.61	0.44
5:1E:37:ASN:O	44:1s:65:GLN:NE2	2.51	0.44
8:1H:141:SER:HA	8:1H:290:TRP:HE1	1.82	0.44
9:1I:161:TRP:O	9:1I:165:ILE:HG12	2.17	0.44
11:1K:80:MET:H	11:1K:80:MET:HG2	1.58	0.44
12:1L:97:THR:HA	12:1L:100:ILE:HG22	1.99	0.44
12:1L:200:GLN:O	12:1L:204:LEU:HG	2.18	0.44
12:1L:462:ILE:HG12	35:1j:32:MET:HB2	1.99	0.44
12:1L:556:ILE:O	12:1L:560:THR:N	2.51	0.44
12:1L:605:HIS:ND1	12:1L:606:GLU:HG3	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:76:MET:O	13:1M:80:SER:OG	2.28	0.44
13:1M:357:THR:O	13:1M:361:MET:HG2	2.17	0.44
16:1P:1:LEU:HD23	16:1P:1:LEU:HA	1.84	0.44
17:1Q:65:TRP:HH2	17:1Q:76:ALA:HB2	1.83	0.44
24:1Y:56:GLY:O	24:1Y:60:PHE:HB2	2.17	0.44
24:1Y:65:ILE:HA	24:1Y:68:ILE:HG22	1.99	0.44
25:1Z:108:GLU:H	30:1e:74:ARG:NH2	2.03	0.44
32:1g:33:GLU:OE2	32:1g:33:GLU:HA	2.18	0.44
35:1j:37:LEU:HG	36:1k:77:PHE:CE2	2.53	0.44
37:1l:136:ASN:ND2	37:1l:150:PRO:HB2	2.33	0.44
38:1m:117:GLU:CD	38:1m:119:LYS:HZ1	2.26	0.44
2:1B:143:ASP:OD1	2:1B:144:ILE:N	2.47	0.43
6:1F:101:GLU:OE1	6:1F:302:SER:N	2.38	0.43
10:1J:147:TYR:N	10:1J:147:TYR:HD2	2.16	0.43
11:1K:5:TYR:HA	11:1K:43:MET:HE1	2.00	0.43
11:1K:43:MET:HG3	14:1N:75:ILE:HG21	2.00	0.43
12:1L:363:TYR:CD2	12:1L:370:THR:HG21	2.53	0.43
12:1L:550:SER:OG	12:1L:551:SER:N	2.51	0.43
13:1M:396:MET:O	13:1M:400:MET:HE2	2.18	0.43
14:1N:211:MET:HB2	14:1N:333:SER:OG	2.17	0.43
17:1Q:126:LYS:HB2	17:1Q:126:LYS:HE2	1.83	0.43
21:1V:23:LEU:HB2	21:1V:58:VAL:HG21	2.01	0.43
23:1X:9:LEU:HD12	23:1X:13:LYS:HZ1	1.83	0.43
28:1c:2:PHE:C	28:1c:2:PHE:HD2	2.26	0.43
29:1d:40:CYS:HA	29:1d:43:LEU:HD23	2.00	0.43
30:1e:94:PRO:HD2	30:1e:97:HIS:ND1	2.33	0.43
32:1g:68:ILE:HD12	32:1g:69:VAL:N	2.33	0.43
33:1h:62:GLU:HG3	33:1h:64:TRP:CE2	2.53	0.43
34:1i:74:VAL:O	34:1i:78:VAL:HG12	2.17	0.43
37:1l:15:LYS:HD3	37:1l:15:LYS:HA	1.85	0.43
38:1m:75:ILE:H	38:1m:75:ILE:HG12	1.54	0.43
39:1n:58:LYS:HD3	39:1n:62:LEU:HD23	2.00	0.43
3:1C:35:LYS:HA	21:1V:102:LEU:HA	2.00	0.43
4:1D:335:ARG:H	4:1D:335:ARG:HG2	1.66	0.43
4:1D:423:ILE:O	4:1D:423:ILE:HD12	2.19	0.43
7:1G:138:GLU:CD	7:1G:138:GLU:H	2.26	0.43
7:1G:257:ASP:C	7:1G:394:ARG:HH22	2.27	0.43
7:1G:296:TRP:CZ3	7:1G:561:LEU:HD22	2.53	0.43
8:1H:173:TRP:HB2	8:1H:176:PHE:HD1	1.83	0.43
12:1L:483:PRO:HG3	35:1j:53:TYR:CE2	2.52	0.43
14:1N:5:ILE:HA	14:1N:8:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:183:ILE:HD13	15:1O:191:GLU:O	2.18	0.43
24:1Y:31:THR:O	24:1Y:35:VAL:HG12	2.18	0.43
25:1Z:86:MET:HE3	25:1Z:86:MET:HB2	1.75	0.43
32:1g:90:ARG:NH2	41:1p:100:GLU:HB3	2.34	0.43
34:1i:123:PRO:HG2	34:1i:125:GLN:OE1	2.18	0.43
38:1m:51:ASN:HD21	39:1n:168:HIS:HB3	1.83	0.43
38:1m:82:THR:O	38:1m:85:THR:OG1	2.31	0.43
1:1A:21:ALA:CB	8:1H:218:GLY:HA3	2.48	0.43
2:1B:102:LYS:O	2:1B:102:LYS:HD3	2.18	0.43
4:1D:71:GLU:O	4:1D:411:LEU:HD23	2.18	0.43
5:1E:98:TYR:CZ	5:1E:176:LEU:HD12	2.53	0.43
5:1E:126:ILE:HD13	5:1E:126:ILE:HA	1.84	0.43
12:1L:2:ASN:HA	34:1i:86:LYS:HE3	2.00	0.43
12:1L:121:LEU:O	12:1L:125:LEU:HD12	2.18	0.43
12:1L:455:LYS:HA	12:1L:458:LEU:HB2	1.99	0.43
12:1L:556:ILE:O	12:1L:560:THR:OG1	2.18	0.43
12:1L:574:SER:O	12:1L:578:SER:OG	2.36	0.43
13:1M:141:GLU:OE2	13:1M:218:LYS:HG2	2.18	0.43
13:1M:269:MET:HE1	13:1M:296:LEU:HD13	2.00	0.43
13:1M:290:SER:HB2	13:1M:319:HIS:NE2	2.33	0.43
13:1M:298:ILE:O	13:1M:302:MET:HG2	2.18	0.43
13:1M:346:ARG:HH22	13:1M:420:THR:HB	1.83	0.43
13:1M:442:LEU:N	13:1M:443:PRO:HD2	2.33	0.43
14:1N:65:THR:O	14:1N:69:MET:HG3	2.18	0.43
14:1N:105:LYS:HB3	14:1N:105:LYS:HE2	1.76	0.43
14:1N:227:THR:O	14:1N:231:SER:N	2.46	0.43
15:1O:108:TYR:CD2	15:1O:128:ILE:HD12	2.46	0.43
15:1O:126:ARG:HH21	53:1O:401:GTP:PA	2.41	0.43
21:1V:13:LEU:HD21	21:1V:81:LEU:HD23	1.99	0.43
23:1X:52:PRO:HD2	25:1Z:116:TRP:CE3	2.53	0.43
30:1e:81:GLN:OE1	30:1e:82:ARG:NH1	2.47	0.43
33:1h:45:VAL:HA	41:1p:54:GLN:HE22	1.84	0.43
37:1l:4:VAL:HG13	37:1l:8:MET:CG	2.49	0.43
40:1o:77:LEU:HD12	40:1o:77:LEU:HA	1.87	0.43
41:1p:89:MET:O	41:1p:93:ARG:HG3	2.18	0.43
43:1r:60:ARG:H	43:1r:60:ARG:HG2	1.65	0.43
2:1B:138:ARG:NE	3:1C:173:GLU:OE2	2.51	0.43
3:1C:76:ALA:O	4:1D:392:LYS:HD3	2.18	0.43
3:1C:148:LEU:HD12	3:1C:148:LEU:HA	1.88	0.43
4:1D:335:ARG:O	4:1D:338:MET:HB3	2.18	0.43
9:1I:15:LYS:HD2	25:1Z:33:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:97:THR:O	12:1L:101:MET:HG3	2.18	0.43
12:1L:252:MET:C	12:1L:252:MET:HE2	2.44	0.43
12:1L:358:LYS:HD2	12:1L:358:LYS:HA	1.74	0.43
12:1L:557:TRP:O	12:1L:561:ILE:HG12	2.18	0.43
14:1N:8:THR:HA	14:1N:11:MET:HB2	1.99	0.43
14:1N:130:LEU:O	14:1N:134:GLN:HB2	2.19	0.43
15:1O:97:GLN:OE1	53:1O:401:GTP:N2	2.37	0.43
15:1O:173:ASP:HB3	15:1O:224:SER:HA	2.00	0.43
16:1P:211:SER:O	16:1P:215:ILE:HG12	2.18	0.43
23:1X:48:GLU:OE1	27:1b:57:ARG:NH2	2.52	0.43
25:1Z:100:ASP:OD1	25:1Z:100:ASP:N	2.35	0.43
29:1d:72:GLY:O	29:1d:76:LEU:HD23	2.17	0.43
31:1f:26:LEU:H	31:1f:26:LEU:HD12	1.84	0.43
32:1g:56:TRP:O	32:1g:59:ARG:HG2	2.18	0.43
33:1h:41:THR:O	33:1h:45:VAL:HG22	2.18	0.43
37:1l:79:TRP:CZ3	38:1m:70:ALA:HB1	2.53	0.43
40:1o:20:ARG:HH12	40:1o:108:LEU:HD21	1.82	0.43
40:1o:51:MET:N	40:1o:51:MET:HE3	2.33	0.43
40:1o:110:ARG:HE	40:1o:114:ARG:HG3	1.83	0.43
1:1A:30:TYR:CZ	1:1A:33:LYS:HB2	2.54	0.43
5:1E:81:TYR:HE2	7:1G:187:ILE:HG12	1.83	0.43
7:1G:380:VAL:HB	7:1G:453:LEU:HD13	2.01	0.43
8:1H:228:TYR:OH	50:1H:401:U10:H28	2.17	0.43
10:1J:173:ARG:HH12	15:1O:254:ARG:HE	1.66	0.43
12:1L:60:GLU:HB3	12:1L:83:ASP:HA	2.00	0.43
12:1L:88:MET:SD	12:1L:88:MET:C	3.02	0.43
12:1L:124:PHE:O	12:1L:128:MET:HG2	2.19	0.43
12:1L:602:PHE:CD1	12:1L:602:PHE:C	2.97	0.43
12:1L:605:HIS:CE1	12:1L:606:GLU:HG3	2.53	0.43
13:1M:24:TRP:HZ2	13:1M:84:LEU:HD12	1.83	0.43
13:1M:206:LYS:HA	13:1M:215:TRP:HZ2	1.83	0.43
13:1M:215:TRP:CD1	13:1M:215:TRP:H	2.35	0.43
15:1O:25:ILE:HA	15:1O:168:VAL:O	2.18	0.43
15:1O:238:ILE:O	15:1O:241:LEU:HB2	2.19	0.43
16:1P:319:ARG:NH1	16:1P:327:LEU:O	2.51	0.43
20:1T:11:ILE:CG2	20:1T:77:VAL:HG13	2.48	0.43
20:1U:26:ASP:HB2	20:1U:29:LYS:HB2	2.01	0.43
20:1U:45:LEU:HG	39:1n:44:ARG:NH1	2.34	0.43
20:1U:54:MET:HA	20:1U:57:GLU:HG3	2.00	0.43
23:1X:3:ILE:HD12	25:1Z:105:LYS:NZ	2.33	0.43
23:1X:44:LEU:HB2	27:1b:55:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:69:PHE:C	24:1Y:69:PHE:CD2	2.96	0.43
24:1Y:139:LYS:HD3	33:1h:112:ARG:HG3	2.00	0.43
28:1c:45:ARG:NH1	29:1d:20:SER:OG	2.48	0.43
35:1j:67:LEU:HD22	35:1j:71:GLU:CD	2.44	0.43
37:1l:128:VAL:O	40:1o:21:MET:HE1	2.19	0.43
40:1o:27:ASP:OD2	40:1o:33:ARG:HB2	2.18	0.43
40:1o:88:TYR:O	40:1o:92:LEU:N	2.43	0.43
41:1p:105:ILE:HG22	41:1p:131:PHE:HD1	1.83	0.43
1:1A:49:LEU:HD21	4:1D:47:LEU:HD22	2.01	0.43
2:1B:79:SER:OG	8:1H:208:VAL:HG12	2.18	0.43
4:1D:83:LEU:O	4:1D:85:ARG:HD3	2.19	0.43
4:1D:164:MET:O	4:1D:167:PHE:HB3	2.18	0.43
5:1E:26:GLU:O	5:1E:29:LYS:HG2	2.18	0.43
7:1G:156:CYS:C	7:1G:158:ARG:N	2.75	0.43
7:1G:366:THR:O	7:1G:367:THR:OG1	2.29	0.43
8:1H:14:LEU:HA	8:1H:14:LEU:HD12	1.80	0.43
10:1J:20:PHE:HZ	11:1K:35:GLY:HA3	1.83	0.43
12:1L:263:PHE:O	12:1L:267:MET:N	2.51	0.43
12:1L:295:GLN:HB2	12:1L:301:ILE:HG13	2.00	0.43
12:1L:559:GLU:O	12:1L:563:PRO:HG2	2.19	0.43
12:1L:591:PHE:O	12:1L:595:ILE:HG12	2.18	0.43
13:1M:101:LEU:HD12	13:1M:101:LEU:HA	1.81	0.43
16:1P:35:VAL:HG21	16:1P:59:LEU:CD1	2.49	0.43
21:1V:53:GLU:O	21:1V:57:MET:HG3	2.19	0.43
22:1W:62:LYS:NZ	22:1W:106:PHE:O	2.41	0.43
24:1Y:121:ALA:O	24:1Y:124:VAL:HG22	2.18	0.43
34:1i:9:LEU:O	34:1i:13:GLN:HB2	2.19	0.43
34:1i:125:GLN:HB2	40:1o:61:TYR:CE2	2.53	0.43
38:1m:121:ASP:OD2	38:1m:121:ASP:C	2.60	0.43
2:1B:145:TYR:N	9:1I:141:THR:O	2.41	0.43
3:1C:79:THR:HG21	4:1D:377:TYR:HD2	1.84	0.43
4:1D:269:LEU:HD21	4:1D:373:GLU:HG3	2.00	0.43
4:1D:421:GLN:HE21	4:1D:421:GLN:HB2	1.48	0.43
6:1F:366:ARG:NE	7:1G:155:GLN:HG2	2.33	0.43
10:1J:3:MET:HE3	10:1J:4:TYR:N	2.34	0.43
11:1K:1:FME:HCN	30:1e:72:MET:HE1	2.01	0.43
12:1L:188:TRP:CD1	12:1L:211:MET:HB2	2.53	0.43
12:1L:488:MET:C	12:1L:492:ILE:HD12	2.43	0.43
13:1M:102:LEU:HD23	13:1M:128:PRO:HG2	2.00	0.43
14:1N:176:ARG:NH1	14:1N:225:THR:OG1	2.51	0.43
15:1O:47:GLY:O	15:1O:120:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:287:HIS:HB2	32:1g:28:GLU:OE2	2.19	0.43
16:1P:133:SER:O	16:1P:167:LYS:HA	2.18	0.43
17:1Q:17:LEU:HD12	17:1Q:17:LEU:HA	1.82	0.43
18:1R:49:VAL:HG12	18:1R:90:GLN:HB2	1.99	0.43
28:1c:29:ILE:HD12	28:1c:30:TYR:N	2.33	0.43
34:1i:21:TRP:CZ3	39:1n:171:THR:HA	2.54	0.43
39:1n:25:HIS:HB3	39:1n:75:HIS:H	1.84	0.43
4:1D:410:MET:HE1	8:1H:282:TYR:CE1	2.53	0.43
5:1E:152:PRO:O	5:1E:164:LEU:HB2	2.19	0.43
6:1F:84:LYS:HB2	6:1F:84:LYS:HE3	1.80	0.43
6:1F:163:GLY:O	6:1F:172:ASP:HA	2.19	0.43
6:1F:300:GLY:HA2	6:1F:333:ALA:N	2.33	0.43
6:1F:351:ILE:HD12	6:1F:373:ASN:OD1	2.19	0.43
8:1H:129:LEU:HD23	8:1H:129:LEU:HA	1.75	0.43
12:1L:321:GLN:HE22	12:1L:476:THR:HB	1.84	0.43
12:1L:363:TYR:OH	36:1k:68:LYS:HE3	2.18	0.43
13:1M:104:LEU:CD1	13:1M:108:MET:HE2	2.49	0.43
13:1M:216:LEU:HB2	13:1M:217:PRO:HD3	2.00	0.43
14:1N:117:GLU:OE2	14:1N:117:GLU:HA	2.18	0.43
14:1N:200:MET:HE2	14:1N:269:GLU:HB2	2.00	0.43
14:1N:318:GLU:CD	29:1d:50:ARG:HD2	2.44	0.43
14:1N:324:LYS:HG3	14:1N:325:LEU:HD23	2.00	0.43
15:1O:46:LEU:HD13	15:1O:238:ILE:HG21	2.01	0.43
19:1S:63:LYS:HD2	19:1S:65:TRP:NE1	2.33	0.43
20:1T:52:MET:HG3	22:1W:40:TYR:CD1	2.53	0.43
25:1Z:137:THR:OG1	25:1Z:138:TYR:N	2.52	0.43
33:1h:45:VAL:HG23	33:1h:46:PHE:HD1	1.83	0.43
40:1o:73:PHE:CG	40:1o:74:PRO:HA	2.54	0.43
41:1p:45:THR:O	41:1p:49:GLU:N	2.43	0.43
41:1p:91:TRP:NE1	41:1p:154:CYS:SG	2.91	0.43
42:1q:4:VAL:HA	42:1q:7:LEU:HB2	2.01	0.43
3:1C:195:ARG:NH2	9:1I:90:GLN:O	2.43	0.43
3:1C:199:LEU:HD11	4:1D:385:ARG:HD3	2.00	0.43
5:1E:43:LYS:NZ	5:1E:74:GLN:OE1	2.49	0.43
10:1J:156:VAL:HG13	14:1N:35:MET:HE1	2.01	0.43
11:1K:35:GLY:O	11:1K:38:LEU:HB2	2.18	0.43
11:1K:96:LEU:HD12	11:1K:96:LEU:HA	1.88	0.43
13:1M:207:MET:O	13:1M:236:LEU:HD11	2.19	0.43
13:1M:349:GLN:NE2	13:1M:416:ARG:HA	2.33	0.43
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	2.01	0.43
17:1Q:54:LYS:HB3	17:1Q:85:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:83:ALA:O	19:1S:87:THR:HG23	2.19	0.43
20:1T:14:ARG:NH1	20:1T:58:PHE:CD1	2.87	0.43
25:1Z:79:LYS:O	25:1Z:83:VAL:HG12	2.18	0.43
33:1h:122:TRP:C	33:1h:122:TRP:CD1	2.97	0.43
34:1i:80:ILE:HD12	34:1i:81:ILE:N	2.34	0.43
42:1q:5:GLN:OE1	42:1q:9:ARG:NH2	2.51	0.43
1:1A:57:LEU:HD21	10:1J:169:MET:HG2	2.01	0.43
3:1C:8:ARG:HG2	3:1C:11:ILE:HD13	2.01	0.43
3:1C:189:GLU:OE2	16:1P:15:SER:OG	2.37	0.43
4:1D:143:GLU:HG3	4:1D:310:ILE:HG21	2.00	0.43
4:1D:291:GLY:O	4:1D:296:ARG:NH1	2.51	0.43
5:1E:56:ARG:NH1	5:1E:56:ARG:HG3	2.34	0.43
7:1G:154:ILE:HG13	7:1G:205:VAL:HG21	2.00	0.43
7:1G:341:ASP:OD2	19:1S:67:ARG:NH2	2.49	0.43
8:1H:218:GLY:HA2	8:1H:221:ALA:HB3	2.01	0.43
8:1H:224:PHE:CE1	50:1H:401:U10:H352	2.51	0.43
9:1I:152:GLU:HG2	18:1R:35:VAL:HA	2.01	0.43
12:1L:61:MET:HB2	34:1i:97:VAL:O	2.18	0.43
13:1M:225:ILE:HG22	13:1M:229:MET:HE3	1.99	0.43
13:1M:307:TRP:CH2	38:1m:127:SER:HB2	2.53	0.43
14:1N:124:LEU:HB3	14:1N:220:ILE:HD11	2.01	0.43
14:1N:337:LEU:O	14:1N:340:THR:HG23	2.19	0.43
16:1P:318:LEU:O	16:1P:322:ARG:HG3	2.18	0.43
19:1S:30:GLN:NE2	19:1S:34:ASP:OD1	2.52	0.43
19:1S:40:TYR:CZ	19:1S:54:ILE:HD11	2.53	0.43
20:1T:12:LYS:CE	20:1T:77:VAL:HG11	2.46	0.43
20:1U:54:MET:HB2	20:1U:58:PHE:CE2	2.54	0.43
33:1h:8:LEU:HD12	33:1h:8:LEU:HA	1.83	0.43
35:1j:7:ILE:N	35:1j:7:ILE:HD12	2.34	0.43
38:1m:94:ILE:HA	38:1m:97:LEU:HD12	2.01	0.43
42:1q:6:VAL:HG23	42:1q:9:ARG:HH21	1.83	0.43
3:1C:79:THR:HG21	4:1D:377:TYR:CD2	2.54	0.42
5:1E:56:ARG:HG3	5:1E:56:ARG:HH11	1.84	0.42
6:1F:185:ILE:HG21	6:1F:359:CYS:HB2	2.01	0.42
6:1F:241:TRP:C	6:1F:241:TRP:CD1	2.97	0.42
6:1F:288:ILE:O	6:1F:288:ILE:HD12	2.19	0.42
7:1G:344:CYS:HB2	7:1G:514:ILE:HD11	2.01	0.42
7:1G:477:ILE:C	7:1G:477:ILE:HD12	2.44	0.42
7:1G:505:LEU:HD23	7:1G:505:LEU:HA	1.81	0.42
7:1G:570:SER:HA	7:1G:583:THR:O	2.19	0.42
8:1H:9:LEU:O	8:1H:13:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.54	0.42
12:1L:202:PHE:HA	12:1L:266:LEU:HD11	2.01	0.42
12:1L:415:ALA:O	12:1L:419:THR:HG23	2.19	0.42
13:1M:75:LEU:HD13	13:1M:75:LEU:HA	1.84	0.42
13:1M:423:ILE:HG23	38:1m:58:VAL:HG22	2.01	0.42
15:1O:308:TYR:HA	15:1O:317:ILE:HD11	2.00	0.42
20:1T:29:LYS:NZ	20:1T:40:LEU:HA	2.34	0.42
21:1V:8:THR:O	21:1V:75:GLN:NE2	2.52	0.42
24:1Y:101:GLY:O	24:1Y:106:SER:N	2.52	0.42
31:1f:6:ILE:HA	31:1f:9:ASP:OD1	2.20	0.42
33:1h:42:LEU:O	33:1h:46:PHE:N	2.52	0.42
33:1h:67:PHE:N	33:1h:67:PHE:CD1	2.87	0.42
34:1i:109:ILE:HD12	34:1i:110:LEU:H	1.83	0.42
36:1k:34:LYS:HB3	39:1n:38:TYR:CE1	2.54	0.42
39:1n:126:ARG:HA	39:1n:129:ARG:HH12	1.84	0.42
41:1p:121:ARG:HH11	41:1p:121:ARG:HA	1.83	0.42
2:1B:140:VAL:HG12	2:1B:142:VAL:HG23	2.02	0.42
5:1E:30:ARG:O	5:1E:34:ILE:HG12	2.19	0.42
5:1E:81:TYR:O	5:1E:85:THR:HG22	2.19	0.42
6:1F:43:TYR:CE1	6:1F:44:LYS:HG2	2.54	0.42
7:1G:549:HIS:ND1	7:1G:677:ILE:HG12	2.34	0.42
10:1J:13:PHE:O	10:1J:17:PHE:HB2	2.18	0.42
12:1L:199:GLN:HE22	41:1p:110:LYS:HG2	1.84	0.42
12:1L:323:HIS:NE2	12:1L:475:MET:HG3	2.34	0.42
13:1M:1:FME:C	13:1M:3:LYS:N	2.81	0.42
13:1M:189:SER:OG	24:1Y:130:GLU:OE2	2.34	0.42
17:1Q:34:LYS:HE3	17:1Q:34:LYS:HB2	1.83	0.42
18:1R:39:PHE:O	18:1R:43:LEU:HB2	2.19	0.42
20:1U:79:TYR:CD2	20:1U:79:TYR:C	2.98	0.42
28:1c:31:LEU:HD23	29:1d:70:PHE:CD1	2.54	0.42
30:1e:19:ILE:HG21	33:1h:128:ILE:HG21	2.01	0.42
37:1l:55:GLN:HG2	37:1l:85:ILE:HA	2.00	0.42
37:1l:158:ILE:HG13	40:1o:99:LYS:HG2	2.01	0.42
38:1m:80:ARG:HH21	38:1m:82:THR:HG22	1.84	0.42
4:1D:236:ARG:O	4:1D:240:VAL:N	2.48	0.42
4:1D:242:ILE:HD11	4:1D:413:ASP:CG	2.44	0.42
7:1G:30:CYS:SG	7:1G:79:ILE:HG21	2.59	0.42
7:1G:45:ARG:HH22	7:1G:256:GLU:CD	2.26	0.42
7:1G:48:VAL:HG13	17:1Q:118:TYR:HD2	1.84	0.42
7:1G:203:CYS:SG	7:1G:208:LEU:HB2	2.59	0.42
7:1G:404:LEU:HD23	7:1G:405:LYS:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:450:MET:HB2	7:1G:450:MET:HE3	1.58	0.42
9:1I:56:PRO:O	9:1I:57:LEU:HD23	2.20	0.42
10:1J:11:THR:O	10:1J:14:VAL:N	2.46	0.42
10:1J:51:PHE:O	10:1J:55:MET:HG2	2.18	0.42
12:1L:176:ARG:NH1	13:1M:404:ALA:HB3	2.34	0.42
12:1L:556:ILE:HG22	12:1L:557:TRP:N	2.34	0.42
13:1M:447:LEU:HD12	13:1M:454:ILE:HG21	2.02	0.42
14:1N:2:ASN:O	14:1N:6:TYR:N	2.44	0.42
16:1P:99:TRP:CD2	16:1P:277:PRO:HD2	2.55	0.42
16:1P:144:ARG:O	16:1P:148:SER:OG	2.34	0.42
16:1P:268:ARG:HB2	16:1P:281:ARG:HD2	2.00	0.42
17:1Q:50:ASN:O	17:1Q:50:ASN:ND2	2.48	0.42
20:1T:20:LYS:HZ2	20:1T:30:LEU:HD22	1.82	0.42
20:1U:47:GLN:O	20:1U:50:ILE:HG23	2.19	0.42
21:1V:97:LYS:N	21:1V:98:PRO:HD3	2.33	0.42
25:1Z:58:ARG:HA	25:1Z:58:ARG:HD2	1.80	0.42
26:1a:61:HIS:ND1	26:1a:61:HIS:O	2.52	0.42
32:1g:50:ASP:OD2	32:1g:52:ILE:HG13	2.19	0.42
35:1j:10:ARG:HG2	35:1j:11:TYR:N	2.34	0.42
39:1n:139:LEU:HD23	39:1n:140:GLN:HE22	1.85	0.42
4:1D:16:GLY:O	14:1N:173:THR:HG21	2.19	0.42
7:1G:378:LEU:HD13	7:1G:439:PHE:CE2	2.55	0.42
7:1G:501:ALA:HB2	7:1G:574:VAL:HG12	2.01	0.42
8:1H:232:ILE:HG21	26:1a:16:LEU:HD11	1.99	0.42
9:1I:1:THR:OG1	9:1I:2:TYR:N	2.53	0.42
11:1K:59:MET:HE3	11:1K:60:PRO:HD3	2.01	0.42
13:1M:172:GLY:O	33:1h:104:ARG:HD3	2.20	0.42
13:1M:200:ILE:HD11	13:1M:250:LEU:HD13	2.02	0.42
13:1M:321:LEU:O	13:1M:324:SER:N	2.49	0.42
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.02	0.42
15:1O:216:GLU:OE1	15:1O:216:GLU:N	2.51	0.42
20:1U:21:LEU:O	36:1k:46:ARG:HD3	2.18	0.42
21:1V:75:GLN:O	21:1V:79:VAL:HG23	2.20	0.42
25:1Z:98:MET:HE2	25:1Z:98:MET:HA	2.01	0.42
34:1i:119:MET:HE3	40:1o:67:LYS:CD	2.50	0.42
36:1k:44:TRP:HB2	39:1n:37:ARG:HD2	2.01	0.42
37:1l:29:MET:HG2	37:1l:76:PRO:HG3	2.00	0.42
37:1l:97:SER:HB2	38:1m:6:LYS:H	1.84	0.42
42:1q:53:LYS:HE2	42:1q:53:LYS:HA	2.01	0.42
1:1A:21:ALA:O	8:1H:60:PRO:HG3	2.20	0.42
1:1A:104:TYR:HE2	10:1J:166:VAL:HG22	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:283:PHE:HA	4:1D:309:ARG:NH1	2.35	0.42
4:1D:294:TYR:CE2	4:1D:298:LEU:HD21	2.55	0.42
4:1D:425:PHE:N	4:1D:425:PHE:CD1	2.87	0.42
7:1G:404:LEU:HD22	7:1G:406:VAL:HG23	2.02	0.42
7:1G:518:PRO:HB3	7:1G:538:PRO:HD3	2.02	0.42
12:1L:4:PHE:H	12:1L:7:LEU:CD1	2.33	0.42
12:1L:240:PRO:HB2	12:1L:243:VAL:HG12	2.00	0.42
13:1M:210:TYR:CD1	13:1M:213:HIS:HE1	2.38	0.42
13:1M:297:VAL:O	13:1M:301:ILE:HG12	2.20	0.42
13:1M:386:PHE:CZ	13:1M:390:ASN:HB3	2.54	0.42
13:1M:407:SER:C	13:1M:410:MET:HE1	2.44	0.42
15:1O:278:TYR:HD1	15:1O:283:THR:HG21	1.84	0.42
17:1Q:90:GLU:HA	17:1Q:93:VAL:HG12	2.00	0.42
24:1Y:132:TRP:HA	24:1Y:132:TRP:CE3	2.55	0.42
27:1b:15:GLU:OE2	27:1b:17:VAL:N	2.53	0.42
36:1k:44:TRP:HD1	39:1n:37:ARG:NH1	2.18	0.42
40:1o:61:TYR:HA	40:1o:64:GLN:HG3	2.01	0.42
41:1p:50:PHE:HD2	41:1p:50:PHE:O	2.02	0.42
41:1p:85:PHE:O	41:1p:89:MET:HG2	2.19	0.42
2:1B:47:PRO:CD	2:1B:74:VAL:HB	2.49	0.42
4:1D:167:PHE:HD2	4:1D:168:PHE:CD1	2.38	0.42
4:1D:209:ASP:OD1	4:1D:209:ASP:N	2.52	0.42
5:1E:135:LYS:HA	5:1E:135:LYS:HD3	1.90	0.42
6:1F:109:GLU:HA	6:1F:112:ARG:NE	2.34	0.42
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.84	0.42
8:1H:204:GLU:HB2	50:1H:401:U10:H203	2.01	0.42
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.20	0.42
12:1L:87:VAL:O	12:1L:91:PRO:HD3	2.20	0.42
13:1M:71:TRP:O	13:1M:71:TRP:CD1	2.73	0.42
13:1M:71:TRP:HH2	13:1M:443:PRO:HB3	1.84	0.42
13:1M:235:LEU:HA	13:1M:238:LEU:CD2	2.50	0.42
13:1M:363:SER:OG	13:1M:411:LEU:HD11	2.20	0.42
13:1M:444:LEU:O	13:1M:448:THR:OG1	2.32	0.42
15:1O:190:HIS:HA	15:1O:193:LYS:HD2	2.01	0.42
19:1S:55:ARG:HA	19:1S:55:ARG:HD3	1.82	0.42
20:1U:21:LEU:HD21	36:1k:47:ASN:HB2	2.01	0.42
22:1W:33:ARG:O	22:1W:37:ARG:N	2.45	0.42
36:1k:44:TRP:HB2	39:1n:37:ARG:CD	2.49	0.42
41:1p:79:LYS:HA	41:1p:79:LYS:HD2	1.77	0.42
43:1r:61:GLU:OE1	43:1r:61:GLU:N	2.53	0.42
4:1D:366:ALA:HB1	4:1D:373:GLU:HG2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:99:HIS:HD2	5:1E:138:THR:HB	1.85	0.42
7:1G:149:ILE:HD11	7:1G:704:CYS:HB2	2.02	0.42
7:1G:228:ILE:HG22	7:1G:583:THR:HB	2.00	0.42
7:1G:278:ARG:O	42:1q:136:GLU:HG2	2.19	0.42
7:1G:360:SER:HB3	7:1G:640:ASN:O	2.20	0.42
7:1G:538:PRO:HD2	7:1G:541:CYS:SG	2.60	0.42
8:1H:195:ARG:HE	8:1H:195:ARG:HB3	1.71	0.42
11:1K:38:LEU:O	11:1K:42:ILE:HG13	2.19	0.42
11:1K:85:TYR:HE1	11:1K:93:LEU:HA	1.84	0.42
12:1L:17:ILE:HA	12:1L:20:MET:SD	2.60	0.42
12:1L:107:TYR:HA	12:1L:348:HIS:ND1	2.35	0.42
12:1L:247:LEU:HD12	12:1L:248:HIS:CE1	2.55	0.42
12:1L:550:SER:HB3	13:1M:275:ILE:HD11	2.00	0.42
13:1M:1:FME:CN	13:1M:52:PHE:HB3	2.49	0.42
13:1M:328:CYS:O	13:1M:332:THR:HG23	2.19	0.42
15:1O:242:LYS:HD2	15:1O:242:LYS:C	2.44	0.42
20:1T:70:LEU:HB3	20:1T:76:ILE:HD12	2.02	0.42
20:1U:24:LYS:HE2	36:1k:41:ARG:CZ	2.50	0.42
22:1W:29:LYS:HE3	22:1W:29:LYS:HB3	1.57	0.42
24:1Y:99:THR:HA	24:1Y:102:ALA:HB3	2.00	0.42
24:1Y:100:LEU:O	24:1Y:104:THR:HG22	2.19	0.42
46:1Y:201:PC1:H322	46:1Y:201:PC1:H32	1.32	0.42
25:1Z:101:VAL:HG21	25:1Z:104:TRP:HB2	2.02	0.42
30:1e:79:LYS:HA	30:1e:82:ARG:HG3	2.02	0.42
32:1g:58:MET:HB3	32:1g:62:PHE:CD2	2.54	0.42
32:1g:61:VAL:HG22	32:1g:66:PHE:CE1	2.55	0.42
33:1h:114:MET:HE2	33:1h:120:GLY:HA3	2.02	0.42
34:1i:35:PRO:O	34:1i:37:ARG:HD2	2.20	0.42
34:1i:41:PRO:HD2	34:1i:42:MET:HE1	2.01	0.42
35:1j:64:LEU:HD12	40:1o:99:LYS:NZ	2.34	0.42
4:1D:62:LEU:HB2	4:1D:425:PHE:CE2	2.55	0.42
4:1D:338:MET:HB2	4:1D:338:MET:HE2	1.68	0.42
5:1E:40:GLU:OE2	44:1s:68:SER:N	2.53	0.42
7:1G:397:LYS:HE3	7:1G:397:LYS:HB2	1.80	0.42
8:1H:32:GLN:OE1	8:1H:34:ARG:NE	2.50	0.42
8:1H:70:MET:HE2	8:1H:70:MET:HB2	1.71	0.42
8:1H:91:MET:HE2	8:1H:91:MET:HB2	1.78	0.42
9:1I:69:ARG:HB3	9:1I:75:GLU:HA	2.02	0.42
12:1L:79:SER:HB2	12:1L:135:ASN:HD22	1.85	0.42
12:1L:125:LEU:HD12	12:1L:125:LEU:H	1.83	0.42
12:1L:203:MET:HB3	41:1p:113:GLN:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:335:PHE:CE1	12:1L:336:LYS:HG2	2.55	0.42
12:1L:439:PRO:HA	36:1k:50:TRP:CZ2	2.55	0.42
13:1M:116:ILE:HG21	23:1X:167:PHE:CD1	2.55	0.42
13:1M:310:MET:SD	13:1M:455:LEU:HD21	2.60	0.42
13:1M:403:THR:O	13:1M:407:SER:N	2.46	0.42
13:1M:409:TYR:O	13:1M:413:THR:HG22	2.20	0.42
13:1M:457:PRO:C	32:1g:84:ARG:HH12	2.28	0.42
14:1N:184:ILE:O	14:1N:187:MET:HB2	2.18	0.42
15:1O:56:ILE:HD13	15:1O:100:LEU:HG	2.01	0.42
15:1O:186:LYS:HB2	15:1O:191:GLU:OE2	2.20	0.42
15:1O:212:PRO:HB2	15:1O:213:GLU:OE1	2.20	0.42
16:1P:183:ALA:O	16:1P:186:ARG:HG2	2.20	0.42
28:1c:43:LYS:HD2	28:1c:43:LYS:H	1.85	0.42
30:1e:62:PHE:CE1	30:1e:66:LEU:HD21	2.55	0.42
34:1i:105:PRO:HB3	34:1i:117:PRO:O	2.19	0.42
36:1k:30:THR:O	36:1k:33:GLU:HG3	2.19	0.42
37:1l:73:TRP:NE1	38:1m:45:GLU:HG3	2.34	0.42
37:1l:136:ASN:OD1	37:1l:139:TYR:HB3	2.20	0.42
3:1C:88:ASN:HD22	21:1V:110:GLN:NE2	2.18	0.42
5:1E:36:LYS:NZ	44:1s:62:ARG:HG3	2.33	0.42
6:1F:150:GLN:HE22	44:1s:55:ASN:HB2	1.85	0.42
7:1G:208:LEU:HD13	45:1G:802:SF4:S2	2.59	0.42
7:1G:504:ASP:HB3	7:1G:630:LEU:HD11	2.01	0.42
8:1H:134:ARG:HD3	8:1H:200:LEU:HB3	2.02	0.42
50:1H:401:U10:H401	50:1H:401:U10:H43	2.01	0.42
12:1L:362:LEU:HG	12:1L:366:MET:HB2	2.00	0.42
12:1L:435:PRO:O	36:1k:51:ARG:HD3	2.20	0.42
13:1M:143:LEU:HD13	13:1M:143:LEU:HA	1.92	0.42
13:1M:427:LYS:HG2	13:1M:428:ALA:H	1.84	0.42
14:1N:66:ALA:HB2	14:1N:104:MET:HB3	2.02	0.42
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	2.02	0.42
19:1S:13:LEU:H	19:1S:13:LEU:HG	1.60	0.42
22:1W:70:ASN:ND2	22:1W:82:LEU:HD22	2.24	0.42
27:1b:56:LEU:HD13	27:1b:62:MET:HE1	2.01	0.42
29:1d:2:MET:HE2	29:1d:2:MET:HB3	1.92	0.42
32:1g:70:LEU:O	32:1g:74:SER:N	2.45	0.42
37:1l:83:MET:O	37:1l:89:VAL:HG22	2.20	0.42
39:1n:12:GLN:O	39:1n:16:LEU:HG	2.19	0.42
41:1p:140:ASP:O	41:1p:161:ARG:NH2	2.52	0.42
4:1D:266:GLN:HB2	43:1r:103:TRP:CE3	2.55	0.42
6:1F:126:GLY:HA2	6:1F:129:MET:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:293:ASN:HA	6:1F:339:ARG:HG2	2.02	0.42
7:1G:80:LEU:HD13	7:1G:80:LEU:HA	1.91	0.42
7:1G:138:GLU:HG2	18:1R:76:ASP:HB3	2.01	0.42
8:1H:26:LYS:NZ	26:1a:4:GLU:HB3	2.35	0.42
8:1H:150:LEU:HD23	8:1H:150:LEU:HA	1.80	0.42
8:1H:281:ARG:NH2	8:1H:283:ASP:OD2	2.31	0.42
10:1J:150:GLY:O	10:1J:154:VAL:HG23	2.20	0.42
10:1J:152:TRP:CD1	30:1e:13:LEU:HB3	2.54	0.42
13:1M:7:PRO:HB2	13:1M:34:ILE:HD11	2.01	0.42
13:1M:116:ILE:HD12	13:1M:116:ILE:HA	1.81	0.42
13:1M:136:TRP:C	13:1M:224:PRO:HG3	2.44	0.42
13:1M:286:ILE:O	13:1M:290:SER:HB3	2.20	0.42
13:1M:386:PHE:HD2	13:1M:393:ILE:HD13	1.84	0.42
15:1O:27:VAL:HG11	15:1O:38:LEU:HD12	2.02	0.42
15:1O:57:HIS:CG	15:1O:68:PRO:HB3	2.55	0.42
16:1P:44:GLN:OE1	16:1P:67:GLN:HA	2.20	0.42
16:1P:92:ILE:HD11	16:1P:218:ILE:HD11	2.02	0.42
16:1P:335:LYS:HD2	16:1P:335:LYS:O	2.19	0.42
20:1U:24:LYS:HD3	36:1k:43:PRO:HB3	2.02	0.42
20:1U:64:ASP:HB3	39:1n:17:ARG:NE	2.35	0.42
21:1V:87:LEU:HD11	21:1V:91:ARG:NH2	2.35	0.42
22:1W:68:MET:HA	22:1W:71:ALA:HB2	2.02	0.42
37:1l:138:LEU:HB2	37:1l:142:ARG:HB2	2.02	0.42
38:1m:8:SER:HB2	38:1m:11:ALA:H	1.85	0.42
43:1r:7:ILE:HA	43:1r:10:LEU:HB2	2.01	0.42
1:1A:72:LEU:HA	10:1J:147:TYR:OH	2.20	0.41
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.20	0.41
6:1F:307:ILE:HG23	6:1F:312:CYS:SG	2.60	0.41
7:1G:275:LYS:HA	42:1q:134:ILE:HD12	2.02	0.41
7:1G:644:GLN:H	7:1G:644:GLN:CD	2.27	0.41
9:1I:2:TYR:HE2	9:1I:4:PHE:HE2	1.68	0.41
9:1I:8:ARG:HG2	9:1I:8:ARG:HH11	1.85	0.41
10:1J:83:TRP:HB3	10:1J:93:PHE:HD1	1.85	0.41
11:1K:94:ASN:ND2	12:1L:583:LEU:HD13	2.35	0.41
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	2.01	0.41
13:1M:3:LYS:HB2	13:1M:4:ILE:HD12	2.02	0.41
13:1M:5:ILE:HA	13:1M:107:ILE:HD11	2.02	0.41
13:1M:114:GLU:OE1	13:1M:174:LEU:HB2	2.20	0.41
13:1M:129:THR:HG21	13:1M:235:LEU:CD2	2.50	0.41
13:1M:410:MET:HA	13:1M:413:THR:HG22	2.02	0.41
14:1N:39:ALA:O	14:1N:42:PRO:HD2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:71:MET:HE3	14:1N:71:MET:O	2.20	0.41
14:1N:308:THR:HG23	14:1N:311:MET:H	1.85	0.41
16:1P:14:SER:O	16:1P:14:SER:OG	2.36	0.41
17:1Q:109:LYS:HB2	17:1Q:109:LYS:HE2	1.71	0.41
20:1T:35:HIS:O	20:1T:40:LEU:N	2.35	0.41
20:1T:52:MET:HG3	22:1W:40:TYR:HD1	1.85	0.41
20:1U:36:PHE:HB2	20:1U:71:MET:HE1	2.02	0.41
26:1a:48:MET:HE3	26:1a:48:MET:HB2	1.85	0.41
33:1h:74:TRP:HE3	33:1h:77:ARG:NH2	2.17	0.41
34:1i:7:GLU:HA	34:1i:10:ARG:HB2	2.02	0.41
41:1p:25:LEU:HD12	41:1p:25:LEU:HA	1.95	0.41
41:1p:96:LYS:HA	41:1p:96:LYS:HD2	1.85	0.41
41:1p:130:GLN:O	41:1p:134:VAL:HG23	2.19	0.41
42:1q:65:THR:HG23	42:1q:73:THR:HG21	2.02	0.41
1:1A:68:GLU:CD	1:1A:98:LEU:HD22	2.46	0.41
4:1D:33:TRP:N	4:1D:33:TRP:CD1	2.84	0.41
4:1D:173:GLU:HA	4:1D:176:LYS:HD2	2.02	0.41
6:1F:91:LYS:O	6:1F:132:ARG:N	2.50	0.41
6:1F:258:ILE:HA	6:1F:334:VAL:HB	2.02	0.41
7:1G:64:LYS:HA	7:1G:64:LYS:HD3	1.78	0.41
7:1G:524:LEU:O	7:1G:545:TYR:HA	2.20	0.41
7:1G:615:THR:HG23	7:1G:618:GLN:H	1.85	0.41
8:1H:277:TYR:CE2	9:1I:30:LEU:HD12	2.55	0.41
9:1I:2:TYR:HE2	9:1I:4:PHE:CE2	2.38	0.41
11:1K:36:MET:SD	14:1N:68:MET:HG3	2.60	0.41
12:1L:65:ASN:HA	34:1i:89:VAL:CG1	2.48	0.41
12:1L:366:MET:HE1	12:1L:445:GLU:CG	2.50	0.41
12:1L:511:LEU:HD13	39:1n:35:LYS:HA	2.02	0.41
13:1M:276:CYS:O	13:1M:285:LEU:HD22	2.20	0.41
13:1M:313:THR:HA	13:1M:316:MET:HE3	2.02	0.41
16:1P:200:THR:O	16:1P:237:LEU:HD12	2.20	0.41
19:1S:82:SER:OG	19:1S:84:ASP:OD2	2.38	0.41
20:1T:52:MET:CE	22:1W:37:ARG:HA	2.50	0.41
24:1Y:126:MET:H	24:1Y:126:MET:HE3	1.85	0.41
30:1e:90:LYS:HD2	30:1e:90:LYS:O	2.20	0.41
32:1g:62:PHE:HA	32:1g:66:PHE:HD1	1.82	0.41
32:1g:63:PHE:O	32:1g:65:GLY:N	2.54	0.41
32:1g:83:TYR:CE2	32:1g:84:ARG:HG3	2.55	0.41
33:1h:84:GLU:H	33:1h:84:GLU:CD	2.28	0.41
36:1k:35:LEU:HD12	36:1k:38:ARG:HB2	2.02	0.41
36:1k:50:TRP:CE2	36:1k:51:ARG:HG3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:85:ASP:HA	40:1o:88:TYR:HB2	2.02	0.41
41:1p:113:GLN:HA	41:1p:120:TYR:HB2	2.01	0.41
3:1C:189:GLU:HG2	16:1P:14:SER:HB3	2.03	0.41
4:1D:67:GLU:O	4:1D:74:ARG:HG2	2.20	0.41
4:1D:342:MET:HE3	7:1G:101:HIS:O	2.20	0.41
5:1E:114:ASP:OD1	5:1E:114:ASP:N	2.52	0.41
6:1F:320:ASP:OD1	6:1F:320:ASP:N	2.53	0.41
7:1G:368:ILE:N	7:1G:577:GLU:OE1	2.44	0.41
7:1G:378:LEU:HD13	7:1G:439:PHE:HE2	1.85	0.41
7:1G:534:ARG:HH22	7:1G:556:MET:HA	1.86	0.41
8:1H:31:MET:HE3	8:1H:272:TRP:CD1	2.56	0.41
8:1H:114:TYR:CE1	10:1J:34:ILE:HD12	2.54	0.41
12:1L:324:LEU:HD12	12:1L:327:LEU:HD11	2.02	0.41
12:1L:375:ILE:HG21	35:1j:32:MET:HG2	2.02	0.41
13:1M:24:TRP:NE1	13:1M:92:LYS:HG2	2.31	0.41
14:1N:6:TYR:HA	14:1N:9:LEU:HB2	2.03	0.41
14:1N:187:MET:HE3	14:1N:190:MET:HE1	2.02	0.41
15:1O:3:TYR:CD2	15:1O:260:ARG:HD3	2.55	0.41
15:1O:271:ASN:OD1	15:1O:271:ASN:C	2.64	0.41
21:1V:6:LYS:CE	21:1V:6:LYS:H	2.33	0.41
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.52	0.41
32:1g:112:CYS:SG	32:1g:113:PHE:N	2.94	0.41
37:1l:114:PHE:O	37:1l:117:TRP:HB3	2.21	0.41
38:1m:56:LEU:O	38:1m:56:LEU:HD13	2.20	0.41
38:1m:111:LYS:HG2	38:1m:115:ILE:HD11	2.01	0.41
39:1n:46:ARG:O	39:1n:46:ARG:HG2	2.19	0.41
41:1p:81:ILE:HD12	41:1p:81:ILE:HA	1.85	0.41
43:1r:57:ASP:OD1	43:1r:59:ARG:N	2.52	0.41
2:1B:79:SER:O	2:1B:81:ARG:N	2.54	0.41
2:1B:93:THR:OG1	2:1B:94:ASN:N	2.54	0.41
4:1D:145:THR:H	4:1D:145:THR:HG1	1.56	0.41
4:1D:148:LEU:HG	4:1D:177:MET:HE3	2.03	0.41
4:1D:158:ALA:O	4:1D:163:ALA:N	2.53	0.41
5:1E:7:PHE:HB2	7:1G:182:GLN:HG3	2.01	0.41
6:1F:249:ARG:NE	6:1F:249:ARG:H	2.19	0.41
7:1G:41:CYS:SG	7:1G:52:CYS:HB3	2.58	0.41
12:1L:85:PHE:HA	12:1L:326:PHE:CZ	2.54	0.41
12:1L:176:ARG:HA	12:1L:179:ASP:OD2	2.20	0.41
12:1L:212:PRO:O	12:1L:216:LEU:HG	2.21	0.41
12:1L:324:LEU:HG	12:1L:395:ILE:HG22	2.00	0.41
13:1M:24:TRP:HE1	13:1M:92:LYS:CD	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:58:TYR:CE1	15:1O:106:LEU:HG	2.51	0.41
15:1O:182:ARG:NH2	15:1O:185:LYS:HG3	2.36	0.41
16:1P:192:PRO:HG2	16:1P:263:TYR:OH	2.20	0.41
25:1Z:93:GLU:O	25:1Z:97:ILE:HG13	2.21	0.41
26:1a:55:SER:O	26:1a:64:LYS:NZ	2.45	0.41
31:1f:41:SER:O	31:1f:45:LYS:HG2	2.21	0.41
35:1j:33:TRP:CE3	35:1j:33:TRP:HA	2.55	0.41
37:1l:155:HIS:HA	40:1o:33:ARG:NH2	2.36	0.41
40:1o:53:GLN:HG2	40:1o:54:GLN:HG3	2.02	0.41
41:1p:104:ILE:HD12	41:1p:104:ILE:HA	1.67	0.41
2:1B:61:HIS:HE1	4:1D:174:ARG:NH2	2.18	0.41
4:1D:249:ASP:N	4:1D:249:ASP:OD1	2.53	0.41
6:1F:256:PHE:HD1	6:1F:332:ALA:HB1	1.86	0.41
7:1G:546:GLN:HA	7:1G:561:LEU:O	2.19	0.41
8:1H:174:MET:HB2	8:1H:242:PHE:HA	2.01	0.41
10:1J:59:ILE:O	10:1J:63:GLY:N	2.44	0.41
11:1K:34:GLU:H	11:1K:34:GLU:HG2	1.62	0.41
12:1L:21:MET:O	12:1L:25:ASN:N	2.53	0.41
12:1L:213:LEU:CD1	12:1L:273:VAL:HG11	2.50	0.41
13:1M:16:TRP:O	13:1M:93:LYS:NZ	2.54	0.41
14:1N:91:ASN:OD1	14:1N:93:VAL:HG13	2.21	0.41
16:1P:147:ARG:O	16:1P:151:VAL:HG12	2.20	0.41
23:1X:129:LYS:HG2	27:1b:66:PRO:O	2.21	0.41
25:1Z:110:VAL:O	30:1e:70:LYS:NZ	2.54	0.41
29:1d:15:PRO:HB2	29:1d:17:GLU:OE2	2.19	0.41
38:1m:16:THR:HA	38:1m:22:TYR:OH	2.21	0.41
38:1m:49:GLN:N	38:1m:49:GLN:CD	2.78	0.41
41:1p:121:ARG:HA	41:1p:121:ARG:NH1	2.35	0.41
42:1q:85:GLU:OE1	42:1q:85:GLU:N	2.42	0.41
1:1A:75:LEU:HD12	8:1H:151:LEU:HD21	2.01	0.41
2:1B:38:ASN:O	2:1B:42:ARG:HG2	2.20	0.41
2:1B:144:ILE:HG13	9:1I:141:THR:O	2.21	0.41
4:1D:19:MET:HE3	4:1D:20:TYR:HB3	2.02	0.41
4:1D:87:THR:HG23	4:1D:102:TYR:CD1	2.56	0.41
4:1D:141:PHE:CD2	4:1D:144:ILE:HD11	2.55	0.41
4:1D:284:ASP:OD2	4:1D:284:ASP:N	2.52	0.41
5:1E:173:ILE:O	5:1E:177:LYS:HG3	2.21	0.41
6:1F:139:ARG:HD3	6:1F:141:GLU:HB2	2.02	0.41
6:1F:409:ASP:OD1	6:1F:409:ASP:N	2.54	0.41
12:1L:106:TRP:CH2	12:1L:450:LEU:HD22	2.56	0.41
12:1L:261:ILE:HG13	12:1L:262:ARG:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:264:TYR:CZ	12:1L:322:PRO:HG3	2.56	0.41
12:1L:500:LEU:HA	12:1L:503:GLU:OE1	2.21	0.41
13:1M:349:GLN:HE22	13:1M:417:GLY:H	1.68	0.41
13:1M:411:LEU:O	13:1M:416:ARG:N	2.50	0.41
14:1N:55:ALA:HB2	14:1N:121:GLY:HA3	2.02	0.41
14:1N:219:LEU:HD23	14:1N:219:LEU:HA	1.76	0.41
15:1O:70:ASP:OD2	15:1O:71:VAL:N	2.54	0.41
17:1Q:72:TRP:HA	17:1Q:72:TRP:CE3	2.56	0.41
21:1V:59:LYS:HE2	21:1V:59:LYS:HB2	1.71	0.41
31:1f:22:PHE:O	31:1f:26:LEU:HD12	2.20	0.41
31:1f:46:ARG:HH11	31:1f:48:LEU:HA	1.85	0.41
34:1i:10:ARG:HG2	39:1n:155:PRO:HB3	2.02	0.41
34:1i:84:TYR:O	34:1i:89:VAL:HG23	2.20	0.41
35:1j:8:GLU:OE1	36:1k:11:SER:N	2.54	0.41
37:1l:138:LEU:CB	37:1l:142:ARG:HB2	2.51	0.41
39:1n:100:GLU:O	39:1n:121:ARG:NH1	2.54	0.41
40:1o:67:LYS:HZ2	40:1o:70:ARG:NH1	2.19	0.41
43:1r:45:SER:HA	43:1r:51:ASN:HD21	1.84	0.41
3:1C:93:VAL:HG22	3:1C:108:LYS:HD2	2.02	0.41
3:1C:151:ILE:HG23	3:1C:152:LEU:HG	2.02	0.41
4:1D:20:TYR:CE2	12:1L:571:MET:HG3	2.55	0.41
4:1D:347:HIS:O	4:1D:351:LEU:HB2	2.21	0.41
5:1E:40:GLU:HG3	44:1s:67:SER:HA	2.01	0.41
6:1F:53:PRO:HB3	6:1F:128:ALA:HA	2.02	0.41
8:1H:284:GLN:O	8:1H:288:LEU:N	2.42	0.41
12:1L:19:ILE:HD13	12:1L:19:ILE:HA	1.82	0.41
12:1L:34:ASN:ND2	12:1L:105:MET:HE1	2.36	0.41
12:1L:121:LEU:O	12:1L:124:PHE:HB3	2.20	0.41
12:1L:138:PHE:O	12:1L:142:ILE:HG13	2.21	0.41
12:1L:166:THR:HG22	12:1L:170:GLN:HE22	1.85	0.41
12:1L:298:ILE:HD12	12:1L:343:SER:HB2	2.02	0.41
12:1L:362:LEU:HB3	12:1L:431:PHE:HD1	1.84	0.41
12:1L:477:VAL:HG22	40:1o:54:GLN:HG2	2.03	0.41
12:1L:486:MET:HA	12:1L:489:THR:CG2	2.49	0.41
13:1M:8:THR:HG21	13:1M:103:GLN:OE1	2.20	0.41
13:1M:107:ILE:HG13	13:1M:108:MET:N	2.35	0.41
14:1N:112:HIS:CE1	14:1N:164:ILE:HG21	2.56	0.41
14:1N:275:SER:HB2	24:1Y:136:ALA:HB3	2.02	0.41
15:1O:306:PRO:HB2	28:1c:7:PRO:HB3	2.02	0.41
23:1X:150:ASN:OD1	23:1X:150:ASN:N	2.52	0.41
29:1d:118:PRO:HB2	29:1d:120:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:93:PRO:HG3	41:1p:4:TRP:HB3	2.03	0.41
39:1n:96:TYR:O	39:1n:98:VAL:HG12	2.21	0.41
1:1A:54:LYS:NZ	4:1D:72:MET:SD	2.89	0.41
1:1A:106:TRP:CZ3	27:1b:18:LEU:HD21	2.56	0.41
2:1B:68:ASP:OD2	2:1B:71:ARG:N	2.53	0.41
3:1C:57:VAL:O	3:1C:61:LEU:HB2	2.21	0.41
3:1C:147:ASP:OD2	3:1C:149:ARG:NH1	2.54	0.41
4:1D:2:ARG:HD2	15:1O:287:HIS:CD2	2.56	0.41
4:1D:51:PHE:CZ	4:1D:57:ALA:HB3	2.56	0.41
4:1D:335:ARG:HE	4:1D:335:ARG:HB3	1.63	0.41
4:1D:347:HIS:NE2	7:1G:126:ASP:HA	2.35	0.41
7:1G:55:CYS:SG	7:1G:68:ALA:N	2.93	0.41
7:1G:79:ILE:HG22	7:1G:81:THR:HG22	2.02	0.41
7:1G:460:ARG:HE	7:1G:460:ARG:HB3	1.55	0.41
8:1H:98:MET:HE1	8:1H:104:PHE:CG	2.56	0.41
8:1H:119:SER:HB2	8:1H:215:TYR:CE2	2.56	0.41
9:1I:116:CYS:HB3	45:1I:201:SF4:S3	2.59	0.41
10:1J:57:PHE:CE1	10:1J:61:LEU:HD11	2.56	0.41
11:1K:11:ALA:O	11:1K:14:ILE:HD12	2.21	0.41
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.20	0.41
12:1L:117:PHE:O	12:1L:120:TYR:HB2	2.20	0.41
12:1L:151:SER:O	12:1L:155:ILE:HG23	2.21	0.41
12:1L:197:ASP:OD1	12:1L:197:ASP:N	2.53	0.41
12:1L:388:GLY:O	12:1L:392:LYS:N	2.53	0.41
12:1L:586:LEU:O	12:1L:590:SER:OG	2.38	0.41
14:1N:313:MET:HE2	15:1O:59:ALA:HB2	2.03	0.41
16:1P:100:GLU:OE1	16:1P:106:PHE:N	2.54	0.41
16:1P:319:ARG:NH1	22:1W:51:GLN:OE1	2.54	0.41
19:1S:36:ILE:HA	19:1S:40:TYR:HB2	2.03	0.41
19:1S:69:ALA:O	19:1S:70:PHE:C	2.64	0.41
20:1T:46:ASP:HA	20:1T:49:GLU:OE1	2.21	0.41
23:1X:18:LYS:H	26:1a:69:ILE:HG22	1.86	0.41
23:1X:43:MET:HA	23:1X:46:ARG:HB2	2.03	0.41
23:1X:150:ASN:HD22	33:1h:124:GLN:HE22	1.69	0.41
24:1Y:13:GLU:HA	24:1Y:20:LYS:HZ2	1.85	0.41
25:1Z:111:PHE:HD2	25:1Z:117:VAL:HG11	1.85	0.41
32:1g:56:TRP:HA	32:1g:59:ARG:HD3	2.03	0.41
33:1h:7:ARG:HD2	34:1i:27:LEU:HD23	2.02	0.41
36:1k:12:LYS:HE2	36:1k:12:LYS:HB2	1.85	0.41
36:1k:48:GLU:HG3	36:1k:52:TYR:CE2	2.56	0.41
39:1n:29:TRP:HA	52:1n:202:3PE:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:30:TYR:O	1:1A:32:GLU:N	2.54	0.41
2:1B:119:CYS:HA	2:1B:124:GLY:HA3	2.01	0.41
2:1B:158:TYR:OH	42:1q:78:ASP:OD1	2.39	0.41
3:1C:155:TYR:HB2	22:1W:102:HIS:CD2	2.56	0.41
4:1D:107:ASP:OD2	4:1D:110:SER:HB2	2.21	0.41
4:1D:111:MET:SD	4:1D:111:MET:N	2.93	0.41
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.53	0.41
5:1E:38:TYR:N	5:1E:38:TYR:CD2	2.88	0.41
5:1E:100:ILE:HB	5:1E:139:LEU:HA	2.02	0.41
5:1E:147:ALA:HA	6:1F:105:CYS:SG	2.61	0.41
6:1F:74:PRO:HG2	6:1F:77:LEU:HD21	2.03	0.41
6:1F:189:GLU:CD	6:1F:190:THR:HG23	2.46	0.41
8:1H:241:LEU:HD12	8:1H:241:LEU:HA	1.90	0.41
8:1H:283:ASP:OD1	8:1H:283:ASP:C	2.64	0.41
11:1K:23:ARG:CG	11:1K:24:SER:H	2.33	0.41
11:1K:44:SER:HA	11:1K:47:ILE:HD12	2.03	0.41
12:1L:210:ASN:O	12:1L:214:ILE:HG12	2.20	0.41
12:1L:271:LYS:HB2	12:1L:271:LYS:HE2	1.88	0.41
13:1M:23:ILE:HG23	13:1M:24:TRP:H	1.86	0.41
13:1M:293:HIS:CE1	13:1M:366:ASN:HD21	2.38	0.41
13:1M:303:ILE:HG12	13:1M:388:TRP:CG	2.56	0.41
13:1M:305:THR:HG22	13:1M:307:TRP:N	2.35	0.41
13:1M:322:THR:H	13:1M:322:THR:HG1	1.60	0.41
13:1M:353:PRO:O	13:1M:357:THR:HG23	2.21	0.41
13:1M:367:LEU:HD11	13:1M:408:LEU:HD11	2.02	0.41
14:1N:240:ILE:HD11	29:1d:48:ILE:HG23	2.03	0.41
15:1O:40:ARG:NH1	15:1O:50:HIS:CG	2.89	0.41
15:1O:135:LEU:HD21	15:1O:149:VAL:HG22	2.02	0.41
18:1R:23:TYR:CE1	18:1R:24:ARG:HD3	2.56	0.41
20:1T:35:HIS:CD2	20:1T:37:MET:H	2.37	0.41
20:1T:58:PHE:HB2	20:1T:60:PHE:HE2	1.84	0.41
21:1V:76:ILE:HD13	21:1V:76:ILE:HA	1.93	0.41
22:1W:62:LYS:HA	22:1W:62:LYS:HD2	1.67	0.41
29:1d:106:LYS:O	29:1d:106:LYS:HG3	2.20	0.41
33:1h:8:LEU:HD21	34:1i:22:LEU:HD22	2.02	0.41
33:1h:62:GLU:HG3	33:1h:64:TRP:NE1	2.35	0.41
33:1h:67:PHE:HB2	33:1h:73:ARG:HG2	2.02	0.41
33:1h:130:LYS:O	33:1h:133:ILE:HG12	2.21	0.41
34:1i:11:LEU:HD23	34:1i:11:LEU:HA	1.92	0.41
34:1i:102:ARG:H	34:1i:102:ARG:HG2	1.61	0.41
35:1j:22:LEU:HD13	35:1j:22:LEU:HA	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:97:SER:HB2	38:1m:6:LYS:N	2.36	0.41
38:1m:106:THR:O	38:1m:110:LYS:HG2	2.21	0.41
39:1n:21:ARG:H	39:1n:21:ARG:HG2	1.56	0.41
39:1n:50:HIS:O	39:1n:53:GLU:HG2	2.20	0.41
39:1n:54:LYS:HD2	39:1n:55:ASP:OD1	2.21	0.41
1:1A:73:LEU:HD13	8:1H:103:LEU:HD11	2.02	0.41
4:1D:309:ARG:HG2	25:1Z:21:TYR:CG	2.56	0.41
4:1D:428:VAL:HG13	4:1D:429:ASP:OD1	2.21	0.41
5:1E:30:ARG:HH12	44:1s:49:TYR:HB3	1.86	0.41
5:1E:169:ILE:H	5:1E:169:ILE:HG13	1.73	0.41
6:1F:19:ASP:HA	6:1F:241:TRP:CZ2	2.56	0.41
6:1F:432:GLN:O	6:1F:436:GLN:HG3	2.21	0.41
7:1G:152:ARG:NH1	7:1G:704:CYS:O	2.52	0.41
7:1G:254:MET:HE3	7:1G:254:MET:HB2	1.99	0.41
7:1G:269:PHE:O	7:1G:684:MET:HE2	2.21	0.41
7:1G:331:LEU:HD22	7:1G:525:LEU:HG	2.03	0.41
9:1I:169:ILE:O	9:1I:173:TYR:HB3	2.20	0.41
10:1J:56:VAL:HB	11:1K:41:PHE:CE2	2.56	0.41
12:1L:4:PHE:H	12:1L:7:LEU:HD12	1.85	0.41
12:1L:187:ALA:O	12:1L:191:THR:HG23	2.21	0.41
12:1L:234:PRO:HG3	12:1L:304:PHE:CE1	2.40	0.41
13:1M:24:TRP:CZ3	13:1M:80:SER:HB2	2.56	0.41
13:1M:203:PHE:HD1	13:1M:239:GLY:HA2	1.85	0.41
14:1N:62:THR:HG21	14:1N:114:TRP:HB3	2.03	0.41
14:1N:102:LEU:HA	14:1N:105:LYS:HG3	2.03	0.41
14:1N:180:ALA:O	14:1N:184:ILE:HG13	2.21	0.41
15:1O:182:ARG:O	15:1O:182:ARG:NE	2.54	0.41
17:1Q:124:TRP:O	44:1s:68:SER:OG	2.29	0.41
19:1S:19:ARG:HB3	19:1S:65:TRP:HB2	2.02	0.41
20:1T:11:ILE:HG21	20:1T:80:ILE:HD11	2.03	0.41
24:1Y:103:ARG:NH1	24:1Y:103:ARG:O	2.53	0.41
27:1b:77:LEU:HA	27:1b:79:TRP:CD1	2.55	0.41
33:1h:91:MET:HE3	41:1p:86:GLU:OE2	2.20	0.41
34:1i:41:PRO:HD2	34:1i:42:MET:CE	2.50	0.41
37:1l:37:TYR:CD2	37:1l:44:TYR:HD2	2.39	0.41
37:1l:55:GLN:HA	37:1l:58:ARG:CD	2.51	0.41
38:1m:5:TYR:HD2	38:1m:13:LEU:HD12	1.86	0.41
39:1n:106:TRP:CD1	39:1n:110:GLU:HB3	2.56	0.41
41:1p:105:ILE:O	41:1p:109:LEU:N	2.45	0.41
41:1p:143:SER:N	41:1p:157:LYS:HZ3	2.18	0.41
4:1D:164:MET:SD	8:1H:28:LEU:HD21	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:256:SER:OG	4:1D:373:GLU:N	2.45	0.40
6:1F:47:GLU:HA	6:1F:50:LEU:HB2	2.03	0.40
6:1F:360:GLY:N	45:1F:502:SF4:S2	2.94	0.40
7:1G:653:ASN:OD1	7:1G:653:ASN:C	2.64	0.40
8:1H:146:LEU:HD13	8:1H:188:SER:OG	2.21	0.40
8:1H:233:MET:SD	8:1H:233:MET:C	3.04	0.40
9:1I:66:ALA:HB1	9:1I:158:GLY:HA2	2.03	0.40
10:1J:167:VAL:O	10:1J:171:ILE:HG23	2.22	0.40
10:1J:171:ILE:HD13	11:1K:77:LEU:HD23	2.03	0.40
11:1K:22:TYR:CD2	11:1K:90:VAL:HG11	2.56	0.40
12:1L:10:THR:O	12:1L:14:ILE:HG23	2.21	0.40
12:1L:309:GLN:O	12:1L:312:LEU:N	2.46	0.40
12:1L:359:MET:HE2	12:1L:359:MET:C	2.46	0.40
12:1L:384:PRO:HG3	35:1j:47:VAL:HG21	2.03	0.40
12:1L:525:MET:CE	39:1n:76:PRO:HB2	2.51	0.40
13:1M:11:LEU:HB3	13:1M:100:ILE:HG21	2.04	0.40
13:1M:54:LEU:HD23	13:1M:54:LEU:HA	1.80	0.40
18:1R:81:THR:HB	18:1R:92:ARG:HB3	2.02	0.40
19:1S:90:LEU:O	19:1S:94:LEU:HG	2.21	0.40
20:1T:64:ASP:CG	22:1W:33:ARG:HE	2.29	0.40
20:1U:40:LEU:HG	20:1U:42:LEU:H	1.86	0.40
21:1V:95:ARG:CZ	21:1V:95:ARG:HB2	2.51	0.40
22:1W:32:VAL:HG11	57:1W:201:EHZ:O3	2.21	0.40
22:1W:34:GLU:HA	22:1W:37:ARG:CG	2.50	0.40
24:1Y:5:LEU:HD23	24:1Y:5:LEU:H	1.85	0.40
24:1Y:75:ILE:O	24:1Y:79:VAL:HG22	2.21	0.40
29:1d:111:GLU:HA	32:1g:119:GLN:HB3	2.03	0.40
30:1e:27:LYS:HB3	33:1h:138:LYS:HA	2.03	0.40
32:1g:45:HIS:HD2	32:1g:54:ASP:C	2.29	0.40
34:1i:125:GLN:HB3	40:1o:88:TYR:HB3	2.03	0.40
35:1j:19:ARG:HH11	35:1j:23:ILE:HG12	1.86	0.40
36:1k:46:ARG:H	36:1k:46:ARG:NE	2.11	0.40
37:1l:79:TRP:CZ2	38:1m:71:ARG:HA	2.56	0.40
39:1n:85:PRO:HA	39:1n:90:TYR:CD2	2.55	0.40
41:1p:73:ILE:HD11	41:1p:155:LEU:HB2	2.03	0.40
41:1p:112:CYS:O	41:1p:116:GLU:HB2	2.21	0.40
41:1p:159:LYS:HA	41:1p:159:LYS:HD2	1.92	0.40
43:1r:111:TYR:H	43:1r:111:TYR:HD1	1.66	0.40
3:1C:94:TYR:HB2	3:1C:107:VAL:CG2	2.47	0.40
7:1G:140:LYS:HE2	7:1G:150:MET:HG2	2.02	0.40
7:1G:172:LEU:HD23	7:1G:172:LEU:HA	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:334:LEU:HD22	7:1G:600:ILE:HG23	2.03	0.40
8:1H:33:LEU:HD12	8:1H:33:LEU:HA	1.90	0.40
9:1I:43:ARG:HH21	43:1r:24:GLN:HE21	1.69	0.40
10:1J:14:VAL:O	10:1J:18:VAL:N	2.43	0.40
10:1J:46:ASN:O	25:1Z:141:ILE:HD13	2.20	0.40
10:1J:150:GLY:HA2	30:1e:16:TRP:CZ2	2.56	0.40
12:1L:142:ILE:HA	13:1M:370:PRO:HG2	2.03	0.40
12:1L:186:MET:HG2	12:1L:196:TRP:HE1	1.86	0.40
12:1L:357:ARG:HA	39:1n:31:VAL:HG13	2.03	0.40
12:1L:574:SER:O	12:1L:578:SER:N	2.47	0.40
13:1M:10:MET:CE	31:1f:15:LEU:HB2	2.51	0.40
13:1M:237:LYS:HB3	13:1M:316:MET:SD	2.61	0.40
14:1N:166:GLY:HA2	14:1N:289:ASN:ND2	2.36	0.40
15:1O:37:ARG:H	15:1O:37:ARG:CD	2.34	0.40
15:1O:176:VAL:HG12	15:1O:180:GLN:OE1	2.22	0.40
15:1O:279:LEU:HB2	15:1O:282:ILE:CG2	2.51	0.40
20:1U:43:ASP:OD1	20:1U:44:SER:N	2.50	0.40
23:1X:38:PRO:HB3	23:1X:61:LEU:HD12	2.02	0.40
26:1a:14:ALA:O	26:1a:18:ILE:HG12	2.21	0.40
27:1b:68:HIS:C	27:1b:70:GLN:H	2.29	0.40
31:1f:55:THR:OG1	33:1h:84:GLU:HG3	2.21	0.40
39:1n:154:PRO:O	39:1n:164:PRO:HD2	2.20	0.40
40:1o:116:GLN:O	40:1o:120:GLU:HB2	2.21	0.40
42:1q:7:LEU:HD23	42:1q:7:LEU:HA	1.84	0.40
42:1q:67:GLU:HA	42:1q:67:GLU:OE2	2.21	0.40
1:1A:47:ALA:C	1:1A:48:ARG:HD2	2.46	0.40
2:1B:47:PRO:HD2	2:1B:74:VAL:HB	2.03	0.40
2:1B:158:TYR:CE2	9:1I:138:GLU:HG2	2.55	0.40
5:1E:106:THR:O	5:1E:110:LEU:HG	2.21	0.40
5:1E:162:GLU:C	5:1E:186:PRO:HA	2.46	0.40
6:1F:135:TYR:CD1	6:1F:176:PHE:HB2	2.56	0.40
7:1G:675:ASP:O	7:1G:679:ARG:HG3	2.21	0.40
8:1H:144:VAL:HG13	8:1H:145:THR:HG23	2.03	0.40
9:1I:10:PRO:HB2	9:1I:20:ARG:CZ	2.51	0.40
10:1J:9:LEU:CD1	10:1J:39:VAL:HG23	2.44	0.40
10:1J:25:SER:HB2	10:1J:81:GLU:O	2.21	0.40
12:1L:129:MET:HA	12:1L:132:VAL:HG22	2.02	0.40
12:1L:300:LYS:HB3	12:1L:304:PHE:CZ	2.57	0.40
12:1L:409:LEU:HD12	12:1L:409:LEU:HA	1.85	0.40
12:1L:503:GLU:O	12:1L:507:THR:HG23	2.21	0.40
13:1M:129:THR:HG21	13:1M:235:LEU:HD21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:283:LYS:HD3	13:1M:340:ARG:HD3	2.04	0.40
14:1N:63:GLN:OE1	14:1N:105:LYS:HD2	2.22	0.40
14:1N:125:GLN:HE22	51:1O:403:CDL:PB2	2.43	0.40
14:1N:168:GLY:HA3	14:1N:181:TYR:CE2	2.56	0.40
14:1N:214:ALA:HB2	14:1N:329:MET:HB3	2.02	0.40
14:1N:251:MET:HB3	14:1N:293:TYR:CD2	2.56	0.40
15:1O:51:PHE:HD2	15:1O:51:PHE:HA	1.78	0.40
15:1O:179:ILE:O	15:1O:183:ILE:HG23	2.21	0.40
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.56	0.40
17:1Q:59:PHE:N	17:1Q:59:PHE:CD1	2.90	0.40
17:1Q:69:LEU:HD11	42:1q:126:PRO:HG2	2.02	0.40
18:1R:73:ILE:HD11	18:1R:84:CYS:HB2	2.02	0.40
20:1U:42:LEU:HD23	20:1U:46:ASP:CG	2.47	0.40
20:1U:50:ILE:O	20:1U:54:MET:HG2	2.22	0.40
21:1V:8:THR:HB	21:1V:77:GLU:HG3	2.04	0.40
21:1V:97:LYS:HB3	21:1V:100:GLU:OE2	2.21	0.40
24:1Y:137:GLU:O	24:1Y:139:LYS:N	2.54	0.40
25:1Z:51:MET:HE2	25:1Z:55:ARG:CZ	2.52	0.40
25:1Z:53:TRP:NE1	25:1Z:57:ARG:HD2	2.35	0.40
29:1d:61:GLN:O	29:1d:65:VAL:HG12	2.22	0.40
29:1d:95:LYS:HE3	29:1d:95:LYS:HB3	1.94	0.40
31:1f:26:LEU:O	31:1f:30:SER:N	2.46	0.40
33:1h:60:VAL:HA	33:1h:61:PRO:HD3	1.92	0.40
35:1j:36:ILE:HD12	35:1j:37:LEU:N	2.36	0.40
36:1k:49:ALA:HA	36:1k:52:TYR:CD2	2.55	0.40
37:1l:69:LEU:HD12	37:1l:86:ARG:H	1.86	0.40
37:1l:112:MET:HA	37:1l:115:MET:HG3	2.03	0.40
42:1q:116:ASN:OD1	42:1q:116:ASN:N	2.53	0.40
1:1A:93:PHE:CD2	1:1A:93:PHE:C	2.99	0.40
2:1B:134:ARG:O	2:1B:138:ARG:HD2	2.21	0.40
2:1B:158:TYR:CD2	9:1I:138:GLU:HG2	2.56	0.40
3:1C:28:TYR:O	3:1C:32:ILE:HG12	2.22	0.40
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.21	0.40
5:1E:66:MET:HE1	7:1G:186:TYR:HE2	1.85	0.40
6:1F:184:TYR:CE1	48:1F:501:FMN:H6	2.56	0.40
7:1G:119:GLN:O	7:1G:123:PHE:N	2.46	0.40
50:1H:401:U10:O2	50:1H:401:U10:C3M	2.69	0.40
9:1I:88:PRO:HD2	45:1I:201:SF4:S1	2.62	0.40
9:1I:134:GLY:HA2	9:1I:165:ILE:CD1	2.51	0.40
12:1L:19:ILE:HG13	12:1L:123:LEU:HG	2.03	0.40
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:407:TRP:HB3	12:1L:411:MET:HE2	2.04	0.40
13:1M:123:GLU:OE1	13:1M:123:GLU:C	2.65	0.40
13:1M:430:PHE:HB2	13:1M:433:GLU:OE1	2.22	0.40
14:1N:276:ILE:HG13	14:1N:277:ILE:N	2.36	0.40
17:1Q:77:ASP:OD1	17:1Q:77:ASP:N	2.54	0.40
21:1V:39:LYS:HB3	21:1V:39:LYS:HE3	1.71	0.40
22:1W:114:ARG:HD3	22:1W:114:ARG:HA	1.90	0.40
24:1Y:72:THR:HB	24:1Y:92:GLY:HA2	2.02	0.40
25:1Z:97:ILE:HG22	25:1Z:98:MET:CE	2.49	0.40
25:1Z:128:ARG:HD3	30:1e:97:HIS:CD2	2.52	0.40
27:1b:31:LEU:HD12	27:1b:31:LEU:H	1.86	0.40
29:1d:99:GLU:H	29:1d:99:GLU:CD	2.19	0.40
32:1g:72:LEU:HD23	32:1g:72:LEU:HA	1.92	0.40
32:1g:90:ARG:NE	32:1g:90:ARG:HA	2.37	0.40
33:1h:44:ASN:O	41:1p:55:HIS:NE2	2.52	0.40
38:1m:22:TYR:HD1	39:1n:14:LYS:NZ	2.19	0.40
39:1n:30:CYS:O	39:1n:32:HIS:N	2.54	0.40
41:1p:53:GLN:HA	41:1p:56:ALA:HB3	2.02	0.40
4:1D:265:ILE:HG13	21:1V:10:LEU:HD23	2.03	0.40
4:1D:346:ILE:HG23	7:1G:117:GLN:HG2	2.04	0.40
6:1F:122:CYS:O	6:1F:173:PHE:HE1	2.04	0.40
6:1F:403:THR:OG1	6:1F:405:CYS:O	2.22	0.40
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	2.03	0.40
7:1G:219:PRO:O	7:1G:222:THR:HG22	2.21	0.40
7:1G:243:ARG:N	7:1G:248:MET:HE1	2.36	0.40
7:1G:564:ALA:HB1	7:1G:568:GLU:HB2	2.03	0.40
12:1L:166:THR:O	12:1L:170:GLN:NE2	2.54	0.40
12:1L:538:THR:O	12:1L:542:LEU:HG	2.22	0.40
12:1L:566:THR:O	12:1L:570:GLN:HG2	2.21	0.40
13:1M:437:MET:O	13:1M:441:ILE:HG22	2.22	0.40
14:1N:211:MET:SD	14:1N:251:MET:SD	3.19	0.40
14:1N:215:MET:HE1	14:1N:244:MET:SD	2.61	0.40
14:1N:231:SER:O	14:1N:234:TRP:HD1	2.03	0.40
14:1N:308:THR:HG22	14:1N:311:MET:HB3	2.03	0.40
15:1O:241:LEU:HD23	15:1O:241:LEU:HA	1.90	0.40
17:1Q:91:ASP:C	17:1Q:91:ASP:OD2	2.64	0.40
20:1U:85:ASP:OD1	39:1n:172:ARG:NH2	2.52	0.40
23:1X:39:ASN:HB3	25:1Z:73:PRO:HG2	2.02	0.40
26:1a:70:ASP:OD1	26:1a:70:ASP:N	2.55	0.40
27:1b:15:GLU:OE2	27:1b:18:LEU:N	2.55	0.40
27:1b:31:LEU:HA	27:1b:34:LEU:HD23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:76:SER:O	30:1e:80:ARG:HB2	2.22	0.40
33:1h:42:LEU:O	33:1h:46:PHE:HB2	2.22	0.40
34:1i:50:LEU:HD12	34:1i:58:ASN:ND2	2.37	0.40
35:1j:39:ARG:HA	35:1j:42:HIS:HB3	2.02	0.40
38:1m:76:TYR:CD1	46:1m:201:PC1:H143	2.56	0.40
39:1n:26:LEU:HD23	39:1n:26:LEU:HA	1.90	0.40
40:1o:41:THR:O	40:1o:44:GLU:HB2	2.21	0.40
40:1o:115:GLU:HA	40:1o:118:GLU:HG2	2.03	0.40
43:1r:24:GLN:H	43:1r:24:GLN:HG2	1.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	102 (90%)	10 (9%)	1 (1%)	14	47
2	1B	153/255 (60%)	138 (90%)	14 (9%)	1 (1%)	18	51
3	1C	207/264 (78%)	196 (95%)	11 (5%)	0	100	100
4	1D	427/476 (90%)	407 (95%)	20 (5%)	0	100	100
5	1E	212/249 (85%)	192 (91%)	19 (9%)	1 (0%)	24	57
6	1F	430/464 (93%)	401 (93%)	28 (6%)	1 (0%)	43	74
7	1G	697/727 (96%)	633 (91%)	62 (9%)	2 (0%)	36	67
8	1H	316/318 (99%)	299 (95%)	14 (4%)	3 (1%)	14	47
9	1I	174/239 (73%)	160 (92%)	12 (7%)	2 (1%)	11	43
10	1J	173/175 (99%)	161 (93%)	9 (5%)	3 (2%)	7	35
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	541 (90%)	62 (10%)	1 (0%)	43	74
13	1M	457/459 (100%)	431 (94%)	25 (6%)	1 (0%)	43	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1N	345/347 (99%)	320 (93%)	23 (7%)	2 (1%)	21	54
15	1O	318/357 (89%)	287 (90%)	31 (10%)	0	100	100
16	1P	340/377 (90%)	316 (93%)	24 (7%)	0	100	100
17	1Q	127/175 (73%)	119 (94%)	8 (6%)	0	100	100
18	1R	94/123 (76%)	81 (86%)	13 (14%)	0	100	100
19	1S	85/99 (86%)	68 (80%)	17 (20%)	0	100	100
20	1T	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	14	47
22	1W	113/128 (88%)	107 (95%)	6 (5%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
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%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	112 (96%)	5 (4%)	0	100	100
30	1e	97/106 (92%)	87 (90%)	10 (10%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	5 (9%)	0	100	100
32	1g	98/154 (64%)	84 (86%)	12 (12%)	2 (2%)	6	32
33	1h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	1i	124/128 (97%)	116 (94%)	8 (6%)	0	100	100
35	1j	69/105 (66%)	58 (84%)	11 (16%)	0	100	100
36	1k	79/98 (81%)	71 (90%)	8 (10%)	0	100	100
37	1l	154/186 (83%)	130 (84%)	24 (16%)	0	100	100
38	1m	126/129 (98%)	122 (97%)	4 (3%)	0	100	100
39	1n	170/179 (95%)	157 (92%)	12 (7%)	1 (1%)	21	54
40	1o	120/137 (88%)	114 (95%)	6 (5%)	0	100	100
41	1p	171/176 (97%)	166 (97%)	5 (3%)	0	100	100
42	1q	143/145 (99%)	136 (95%)	6 (4%)	1 (1%)	18	51
43	1r	90/114 (79%)	85 (94%)	4 (4%)	1 (1%)	11	43

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
All	All	8194/9741 (84%)	7570 (92%)	600 (7%)	24 (0%)	37	67

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	46	SER
8	1H	92	PRO
8	1H	196	ALA
10	1J	113	VAL
10	1J	122	LEU
13	1M	23	ILE
14	1N	324	LYS
14	1N	323	MET
5	1E	157	ASN
7	1G	256	GLU
12	1L	4	PHE
7	1G	654	GLN
42	1q	75	TRP
2	1B	172	ARG
8	1H	208	VAL
9	1I	50	TYR
9	1I	51	PRO
32	1g	64	PHE
43	1r	110	PRO
21	1V	112	LYS
32	1g	63	PHE
39	1n	31	VAL
6	1F	207	PRO
10	1J	116	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%)	90 (91%)	9 (9%)	9	32
2	1B	131/209 (63%)	120 (92%)	11 (8%)	10	34
3	1C	190/227 (84%)	178 (94%)	12 (6%)	16	42
4	1D	371/405 (92%)	341 (92%)	30 (8%)	11	35
5	1E	183/207 (88%)	175 (96%)	8 (4%)	25	51
6	1F	346/368 (94%)	334 (96%)	12 (4%)	32	57
7	1G	588/610 (96%)	559 (95%)	29 (5%)	22	48
8	1H	274/274 (100%)	262 (96%)	12 (4%)	25	51
9	1I	151/201 (75%)	141 (93%)	10 (7%)	15	41
10	1J	140/140 (100%)	130 (93%)	10 (7%)	13	38
11	1K	84/84 (100%)	77 (92%)	7 (8%)	10	34
12	1L	539/539 (100%)	512 (95%)	27 (5%)	22	48
13	1M	408/408 (100%)	380 (93%)	28 (7%)	14	39
14	1N	310/310 (100%)	294 (95%)	16 (5%)	21	47
15	1O	283/307 (92%)	272 (96%)	11 (4%)	28	54
16	1P	296/323 (92%)	273 (92%)	23 (8%)	11	36
17	1Q	117/152 (77%)	112 (96%)	5 (4%)	26	51
18	1R	79/97 (81%)	76 (96%)	3 (4%)	29	55
19	1S	77/82 (94%)	70 (91%)	7 (9%)	9	32
20	1T	79/133 (59%)	74 (94%)	5 (6%)	16	42
20	1U	79/133 (59%)	71 (90%)	8 (10%)	7	28
21	1V	100/101 (99%)	93 (93%)	7 (7%)	14	39
22	1W	107/112 (96%)	101 (94%)	6 (6%)	19	46
23	1X	153/154 (99%)	147 (96%)	6 (4%)	28	54
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	28	54
25	1Z	123/124 (99%)	116 (94%)	7 (6%)	18	45
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	57
27	1b	69/70 (99%)	66 (96%)	3 (4%)	26	51
28	1c	45/66 (68%)	43 (96%)	2 (4%)	25	51
29	1d	107/109 (98%)	99 (92%)	8 (8%)	12	37
30	1e	87/94 (93%)	82 (94%)	5 (6%)	18	45
31	1f	54/113 (48%)	51 (94%)	3 (6%)	19	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	1g	92/129 (71%)	88 (96%)	4 (4%)	26	51
33	1h	121/158 (77%)	118 (98%)	3 (2%)	42	63
34	1i	119/120 (99%)	114 (96%)	5 (4%)	26	52
35	1j	62/84 (74%)	58 (94%)	4 (6%)	15	42
36	1k	63/76 (83%)	61 (97%)	2 (3%)	34	59
37	1l	141/161 (88%)	135 (96%)	6 (4%)	26	51
38	1m	113/114 (99%)	106 (94%)	7 (6%)	16	43
39	1n	156/160 (98%)	151 (97%)	5 (3%)	34	59
40	1o	110/120 (92%)	103 (94%)	7 (6%)	16	42
41	1p	154/156 (99%)	150 (97%)	4 (3%)	40	62
42	1q	131/131 (100%)	124 (95%)	7 (5%)	20	47
43	1r	85/98 (87%)	82 (96%)	3 (4%)	32	57
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7219/8269 (87%)	6826 (95%)	393 (5%)	21	46

All (393) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	17	LEU
1	1A	33	LYS
1	1A	39	CYS
1	1A	49	LEU
1	1A	58	VAL
1	1A	60	ILE
1	1A	96	ILE
1	1A	107	THR
1	1A	113	TRP
2	1B	30	VAL
2	1B	54	CYS
2	1B	55	CYS
2	1B	75	VAL
2	1B	79	SER
2	1B	82	GLN
2	1B	87	ILE
2	1B	103	VAL
2	1B	137	ASP
2	1B	140	VAL

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Mol	Chain	Res	Type
2	1B	146	VAL
3	1C	7	THR
3	1C	42	VAL
3	1C	43	SER
3	1C	57	VAL
3	1C	71	GLN
3	1C	81	VAL
3	1C	103	SER
3	1C	109	THR
3	1C	131	GLU
3	1C	190	LEU
3	1C	198	ASP
3	1C	199	LEU
4	1D	20	TYR
4	1D	42	THR
4	1D	43	LEU
4	1D	65	VAL
4	1D	72	MET
4	1D	73	VAL
4	1D	75	LYS
4	1D	83	LEU
4	1D	109	VAL
4	1D	124	LYS
4	1D	128	ILE
4	1D	145	THR
4	1D	156	THR
4	1D	178	PHE
4	1D	199	VAL
4	1D	215	SER
4	1D	239	THR
4	1D	244	VAL
4	1D	246	THR
4	1D	256	SER
4	1D	284	ASP
4	1D	299	CYS
4	1D	323	ILE
4	1D	324	LYS
4	1D	331	SER
4	1D	338	MET
4	1D	358	VAL
4	1D	399	LEU
4	1D	407	LYS

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Mol	Chain	Res	Type
4	1D	411	LEU
5	1E	18	ASP
5	1E	48	LEU
5	1E	80	VAL
5	1E	105	THR
5	1E	126	ILE
5	1E	128	VAL
5	1E	131	THR
5	1E	201	SER
6	1F	14	SER
6	1F	147	SER
6	1F	242	PHE
6	1F	268	VAL
6	1F	280	ILE
6	1F	287	VAL
6	1F	331	THR
6	1F	341	THR
6	1F	359	CYS
6	1F	415	VAL
6	1F	418	LEU
6	1F	438	GLN
7	1G	17	SER
7	1G	25	THR
7	1G	33	VAL
7	1G	65	VAL
7	1G	83	SER
7	1G	123	PHE
7	1G	154	ILE
7	1G	156	CYS
7	1G	201	ASP
7	1G	215	PHE
7	1G	216	THR
7	1G	229	ASP
7	1G	231	MET
7	1G	234	VAL
7	1G	236	SER
7	1G	309	SER
7	1G	371	VAL
7	1G	402	ASN
7	1G	425	SER
7	1G	434	SER
7	1G	511	VAL

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Mol	Chain	Res	Type
7	1G	541	CYS
7	1G	592	LEU
7	1G	632	ARG
7	1G	636	VAL
7	1G	659	ASP
7	1G	681	SER
7	1G	698	VAL
7	1G	703	ILE
8	1H	45	LEU
8	1H	87	VAL
8	1H	123	SER
8	1H	152	SER
8	1H	157	ASN
8	1H	161	THR
8	1H	165	LEU
8	1H	225	MET
8	1H	256	THR
8	1H	271	LEU
8	1H	282	TYR
8	1H	296	LEU
9	1I	13	ASP
9	1I	18	THR
9	1I	25	LEU
9	1I	30	LEU
9	1I	40	TYR
9	1I	67	LEU
9	1I	122	CYS
9	1I	132	VAL
9	1I	143	THR
9	1I	169	ILE
10	1J	10	SER
10	1J	17	PHE
10	1J	35	VAL
10	1J	82	VAL
10	1J	130	THR
10	1J	137	SER
10	1J	161	LEU
10	1J	165	VAL
10	1J	168	ILE
10	1J	171	ILE
11	1K	4	VAL
11	1K	29	SER

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Mol	Chain	Res	Type
11	1K	54	THR
11	1K	55	LEU
11	1K	75	LEU
11	1K	78	LEU
11	1K	88	ASP
12	1L	10	THR
12	1L	24	SER
12	1L	45	THR
12	1L	63	ILE
12	1L	70	THR
12	1L	73	THR
12	1L	92	VAL
12	1L	100	ILE
12	1L	127	THR
12	1L	241	THR
12	1L	247	LEU
12	1L	257	VAL
12	1L	261	ILE
12	1L	290	LEU
12	1L	341	MET
12	1L	425	ARG
12	1L	477	VAL
12	1L	481	THR
12	1L	508	THR
12	1L	519	THR
12	1L	526	LEU
12	1L	550	SER
12	1L	553	LEU
12	1L	576	MET
12	1L	590	SER
12	1L	593	ILE
12	1L	594	THR
13	1M	10	MET
13	1M	23	ILE
13	1M	41	LEU
13	1M	50	LEU
13	1M	83	HIS
13	1M	88	THR
13	1M	90	THR
13	1M	99	LEU
13	1M	130	LEU
13	1M	175	ASN

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Mol	Chain	Res	Type
13	1M	189	SER
13	1M	228	SER
13	1M	243	MET
13	1M	247	THR
13	1M	254	THR
13	1M	274	SER
13	1M	280	THR
13	1M	289	SER
13	1M	291	VAL
13	1M	292	SER
13	1M	298	ILE
13	1M	302	MET
13	1M	341	THR
13	1M	376	ILE
13	1M	389	SER
13	1M	390	ASN
13	1M	420	THR
13	1M	434	ASN
14	1N	23	SER
14	1N	38	LEU
14	1N	43	VAL
14	1N	47	ASN
14	1N	72	MET
14	1N	85	THR
14	1N	93	VAL
14	1N	125	GLN
14	1N	140	SER
14	1N	161	SER
14	1N	194	LEU
14	1N	219	LEU
14	1N	246	VAL
14	1N	271	THR
14	1N	276	ILE
14	1N	277	ILE
15	1O	42	ILE
15	1O	48	LEU
15	1O	83	TYR
15	1O	88	SER
15	1O	199	LEU
15	1O	218	CYS
15	1O	221	LEU
15	1O	230	ASP

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Mol	Chain	Res	Type
15	1O	269	VAL
15	1O	289	SER
15	1O	309	ASN
16	1P	30	LEU
16	1P	87	HIS
16	1P	101	THR
16	1P	105	ASP
16	1P	134	HIS
16	1P	135	LEU
16	1P	140	LYS
16	1P	141	SER
16	1P	148	SER
16	1P	155	GLU
16	1P	156	VAL
16	1P	184	SER
16	1P	201	VAL
16	1P	210	VAL
16	1P	214	ILE
16	1P	231	VAL
16	1P	234	ASN
16	1P	288	HIS
16	1P	302	ASP
16	1P	323	THR
16	1P	339	THR
16	1P	340	VAL
16	1P	342	ILE
17	1Q	13	VAL
17	1Q	19	ILE
17	1Q	52	THR
17	1Q	81	ASN
17	1Q	117	SER
18	1R	12	THR
18	1R	58	SER
18	1R	83	THR
19	1S	13	LEU
19	1S	15	LEU
19	1S	18	ILE
19	1S	41	VAL
19	1S	47	ASN
19	1S	76	VAL
19	1S	86	VAL
20	1T	7	THR

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Mol	Chain	Res	Type
20	1T	34	SER
20	1T	40	LEU
20	1T	62	ILE
20	1T	86	VAL
20	1U	15	VAL
20	1U	21	LEU
20	1U	23	ASP
20	1U	24	LYS
20	1U	42	LEU
20	1U	44	SER
20	1U	50	ILE
20	1U	71	MET
21	1V	18	THR
21	1V	26	LEU
21	1V	45	LYS
21	1V	50	ILE
21	1V	71	LEU
21	1V	80	ILE
21	1V	91	ARG
22	1W	32	VAL
22	1W	52	LEU
22	1W	60	ARG
22	1W	73	VAL
22	1W	101	THR
22	1W	126	HIS
23	1X	6	LEU
23	1X	45	CYS
23	1X	61	LEU
23	1X	117	VAL
23	1X	130	VAL
23	1X	170	THR
24	1Y	3	THR
24	1Y	15	THR
24	1Y	36	SER
24	1Y	124	VAL
25	1Z	7	LYS
25	1Z	20	ASP
25	1Z	31	SER
25	1Z	51	MET
25	1Z	87	LEU
25	1Z	117	VAL
25	1Z	133	ILE

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Mol	Chain	Res	Type
26	1a	3	PHE
26	1a	49	GLU
27	1b	17	VAL
27	1b	19	VAL
27	1b	39	ASN
28	1c	40	LEU
28	1c	48	LEU
29	1d	-1	MET
29	1d	32	VAL
29	1d	34	MET
29	1d	41	SER
29	1d	44	ILE
29	1d	55	SER
29	1d	100	ASP
29	1d	108	THR
30	1e	5	VAL
30	1e	19	ILE
30	1e	63	VAL
30	1e	70	LYS
30	1e	72	MET
31	1f	3	VAL
31	1f	7	VAL
31	1f	14	ILE
32	1g	55	LEU
32	1g	107	LEU
32	1g	111	ASN
32	1g	114	ASP
33	1h	18	ASP
33	1h	45	VAL
33	1h	74	TRP
34	1i	3	TYR
34	1i	76	ILE
34	1i	112	THR
34	1i	116	ILE
34	1i	126	HIS
35	1j	14	PHE
35	1j	44	SER
35	1j	64	LEU
35	1j	67	LEU
36	1k	31	VAL
36	1k	78	VAL
37	1l	8	MET

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Mol	Chain	Res	Type
37	1l	97	SER
37	1l	120	GLU
37	1l	140	LEU
37	1l	148	LYS
37	1l	154	VAL
38	1m	8	SER
38	1m	12	THR
38	1m	56	LEU
38	1m	59	ILE
38	1m	75	ILE
38	1m	106	THR
38	1m	108	ARG
39	1n	21	ARG
39	1n	48	ASP
39	1n	89	SER
39	1n	98	VAL
39	1n	139	LEU
40	1o	19	LEU
40	1o	23	THR
40	1o	41	THR
40	1o	58	CYS
40	1o	64	GLN
40	1o	72	SER
40	1o	79	CYS
41	1p	32	LEU
41	1p	44	VAL
41	1p	104	ILE
41	1p	139	GLN
42	1q	4	VAL
42	1q	6	VAL
42	1q	55	PHE
42	1q	94	THR
42	1q	120	THR
42	1q	129	THR
42	1q	141	SER
43	1r	10	LEU
43	1r	49	SER
43	1r	54	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (73) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	108	GLN
2	1B	61	HIS
3	1C	104	GLN
3	1C	211	GLN
4	1D	129	GLN
4	1D	190	HIS
5	1E	67	ASN
5	1E	91	ASN
5	1E	101	GLN
5	1E	214	GLN
6	1F	431	GLN
6	1F	436	GLN
7	1G	36	GLN
7	1G	100	ASN
7	1G	101	HIS
7	1G	459	GLN
7	1G	476	ASN
7	1G	517	ASN
7	1G	618	GLN
9	1I	170	GLN
10	1J	120	ASN
12	1L	34	ASN
12	1L	109	HIS
12	1L	199	GLN
12	1L	248	HIS
12	1L	579	ASN
13	1M	144	ASN
13	1M	366	ASN
14	1N	112	HIS
14	1N	204	ASN
15	1O	107	GLN
15	1O	309	ASN
16	1P	36	ASN
16	1P	180	ASN
16	1P	321	HIS
17	1Q	46	GLN
18	1R	36	ASN
20	1T	33	ASN
20	1T	35	HIS
20	1T	47	GLN
21	1V	110	GLN
23	1X	34	GLN
23	1X	72	GLN

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Mol	Chain	Res	Type
25	1Z	8	GLN
25	1Z	76	GLN
25	1Z	130	ASN
26	1a	68	ASN
27	1b	61	ASN
28	1c	35	HIS
29	1d	88	HIS
29	1d	117	HIS
30	1e	44	HIS
32	1g	45	HIS
33	1h	124	GLN
34	1i	25	GLN
34	1i	47	ASN
36	1k	20	GLN
37	1l	104	HIS
39	1n	32	HIS
39	1n	107	HIS
39	1n	140	GLN
39	1n	168	HIS
41	1p	54	GLN
41	1p	114	GLN
41	1p	122	GLN
41	1p	130	GLN
41	1p	148	HIS
42	1q	87	HIS
43	1r	12	ASN
43	1r	24	GLN
43	1r	35	GLN
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
10	FME	1J	1	10	8,9,10	0.56	0	8,9,11	0.89	1 (12%)
14	FME	1N	1	14,10	8,9,10	0.59	0	8,9,11	0.95	1 (12%)
34	SAC	1i	1	-	7,8,9	0.58	0	7,9,11	1.15	1 (14%)
11	FME	1K	1	11	8,9,10	0.51	0	8,9,11	1.00	1 (12%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	1.00	1 (12%)
12	FME	1L	1	12	8,9,10	0.57	0	8,9,11	0.94	1 (12%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.89	1 (12%)
8	FME	1H	1	8	8,9,10	0.54	0	8,9,11	1.11	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
10	FME	1J	1	10	-	1/7/9/11	-
14	FME	1N	1	14,10	-	3/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
12	FME	1L	1	12	-	1/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-

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	-2.96	117.15	124.77
8	1H	1	FME	O-C-CA	-2.81	117.56	124.77
11	1K	1	FME	O-C-CA	-2.64	117.99	124.77
12	1L	1	FME	O-C-CA	-2.58	118.12	124.77
1	1A	1	FME	O-C-CA	-2.56	118.19	124.77
14	1N	1	FME	O-C-CA	-2.49	118.37	124.77
10	1J	1	FME	O-C-CA	-2.46	118.43	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
13	1M	1	FME	O-C-CA	-2.33	118.77	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	1K	1	FME	O1-CN-N-CA
14	1N	1	FME	O1-CN-N-CA
14	1N	1	FME	N-CA-CB-CG
14	1N	1	FME	C-CA-CB-CG
10	1J	1	FME	N-CA-CB-CG
13	1M	1	FME	N-CA-CB-CG
12	1L	1	FME	CA-CB-CG-SD

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	1J	1	FME	1	0
34	1i	1	SAC	1	0
11	1K	1	FME	1	0
1	1A	1	FME	1	0
13	1M	1	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	PC1	1q	201	42	47,47,53	0.37	0	53,55,61	0.55	1 (1%)
47	FES	1E	301	5	0,4,4	-	-	-		
57	EHZ	1W	201	-	31,36,37	0.19	0	36,44,47	1.27	1 (2%)
52	3PE	1N	401	-	37,37,50	0.32	0	40,42,55	0.39	0
46	PC1	1m	201	38,12	45,45,53	0.28	0	51,53,61	0.36	0
57	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.21	1 (2%)
53	GTP	1O	401	54	33,34,34	0.60	0	50,54,54	0.64	0
45	SF4	1I	202	9	0,12,12	-	-	-		
50	U10	1H	401	-	63,63,63	0.58	2 (3%)	78,79,79	0.85	5 (6%)
45	SF4	1B	201	2	0,12,12	-	-	-		
47	FES	1G	803	7	0,4,4	-	-	-		
46	PC1	1Y	201	24	34,34,53	0.32	0	40,42,61	0.37	0
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.66	1 (2%)
52	3PE	1n	202	39,12	41,41,50	0.29	0	44,46,55	0.43	0
52	3PE	1g	201	32	50,50,50	0.28	0	53,55,55	0.99	3 (5%)
46	PC1	1h	201	-	33,33,53	0.31	0	39,41,61	0.45	0
51	CDL	1O	403	14,15	66,66,99	0.37	0	72,78,111	0.54	1 (1%)
45	SF4	1G	801	7	0,12,12	-	-	-		
46	PC1	1d	201	14,30,29	38,38,53	0.31	0	44,46,61	0.51	0
51	CDL	1a	101	26	60,60,99	0.33	0	66,72,111	0.54	0
52	3PE	1Y	202	24	34,34,50	0.31	0	37,39,55	0.56	1 (2%)
55	NDP	1P	501	-	51,52,52	0.51	0	71,80,80	0.79	2 (2%)
58	MYR	1l	201	-	13,14,15	0.30	0	12,13,15	0.30	0
46	PC1	1B	202	-	33,33,53	0.32	0	39,41,61	0.33	0
45	SF4	1I	201	9	0,12,12	-	-	-		
45	SF4	1G	802	7	0,12,12	-	-	-		
45	SF4	1F	502	6	0,12,12	-	-	-		
51	CDL	1H	402	-	50,50,99	0.36	0	56,62,111	0.55	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
46	PC1	1q	201	42	-	15/51/51/57	-
47	FES	1E	301	5	-	-	0/1/1/1
57	EHZ	1W	201	-	-	16/42/44/45	-
46	PC1	1m	201	38,12	-	6/49/49/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	EHZ	1n	201	-	-	2/42/44/45	-
53	GTP	1O	401	54	-	3/22/38/38	0/3/3/3
51	CDL	1H	402	-	-	7/61/61/110	-
50	U10	1H	401	-	-	6/63/87/87	0/1/1/1
45	SF4	1I	202	9	-	-	0/6/5/5
45	SF4	1B	201	2	-	-	0/6/5/5
47	FES	1G	803	7	-	-	0/1/1/1
46	PC1	1Y	201	24	-	11/38/38/57	-
48	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
52	3PE	1n	202	39,12	-	6/45/45/54	-
52	3PE	1g	201	32	-	11/54/54/54	-
46	PC1	1h	201	-	-	4/36/36/57	-
51	CDL	1O	403	14,15	-	15/76/76/110	-
45	SF4	1G	801	7	-	-	0/6/5/5
46	PC1	1d	201	14,30,29	-	13/42/42/57	-
51	CDL	1a	101	26	-	17/71/71/110	-
55	NDP	1P	501	-	-	3/34/77/77	0/5/5/5
52	3PE	1Y	202	24	-	13/38/38/54	-
58	MYR	1l	201	-	-	2/12/12/13	-
46	PC1	1B	202	-	-	11/37/37/57	-
45	SF4	1G	802	7	-	-	0/6/5/5
45	SF4	1I	201	9	-	-	0/6/5/5
45	SF4	1F	502	6	-	-	0/6/5/5
52	3PE	1N	401	-	-	4/41/41/54	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	1H	401	U10	C4-C5	-2.48	1.41	1.48
50	1H	401	U10	C4-C3	2.10	1.44	1.36

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1W	201	EHZ	C10-S1-C9	7.08	122.76	101.84
57	1n	201	EHZ	C10-S1-C9	6.84	122.07	101.84
55	1P	501	NDP	P2B-O2B-C2B	-4.77	110.69	123.43
52	1g	201	3PE	O21-C21-C22	4.51	121.23	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1g	201	3PE	O21-C2-C3	3.49	120.86	108.34
52	1g	201	3PE	O21-C21-O22	-2.86	117.01	123.70
50	1H	401	U10	O4-C4-C5	-2.65	107.69	116.64
50	1H	401	U10	O3-C3-C2	2.64	125.54	116.64
50	1H	401	U10	C7-C6-C1	-2.57	120.48	124.89
50	1H	401	U10	C4-C3-C2	-2.34	116.39	120.69
51	1H	402	CDL	OB6-CB5-C51	2.15	116.13	111.48
50	1H	401	U10	O4-C4-C3	2.13	131.70	123.64
48	1F	501	FMN	C4-N3-C2	-2.11	121.90	125.64
52	1Y	202	3PE	O21-C2-C3	2.06	115.72	108.34
46	1q	201	PC1	O21-C21-C22	-2.03	107.09	111.48
55	1P	501	NDP	O4D-C1D-C2D	-2.02	102.29	106.62
51	1O	403	CDL	OB4-PB2-OB3	2.00	121.76	112.44

There are no chirality outliers.

All (167) 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	1Y	201	PC1	C1-O11-P-O14
46	1Y	201	PC1	C1-O11-P-O13
46	1Y	201	PC1	O32-C31-O31-C3
46	1Y	201	PC1	C32-C31-O31-C3
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	1h	201	PC1	C1-O11-P-O12
46	1h	201	PC1	C1-O11-P-O14
46	1h	201	PC1	C1-O11-P-O13
46	1m	201	PC1	C11-O13-P-O14
46	1m	201	PC1	C1-O11-P-O14
46	1q	201	PC1	C11-O13-P-O14
48	1F	501	FMN	N10-C1'-C2'-O2'
48	1F	501	FMN	N10-C1'-C2'-C3'
51	1H	402	CDL	C1-CA2-OA2-PA1
51	1H	402	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	1H	402	CDL	OB7-CB5-OB6-CB4
51	1H	402	CDL	C51-CB5-OB6-CB4
51	1O	403	CDL	CA2-OA2-PA1-OA3
51	1O	403	CDL	CA2-OA2-PA1-OA5
51	1O	403	CDL	CB2-OB2-PB2-OB4
51	1O	403	CDL	CB2-OB2-PB2-OB5
51	1a	101	CDL	CB2-OB2-PB2-OB3
51	1a	101	CDL	CB2-OB2-PB2-OB5
52	1Y	202	3PE	C1-O11-P-O13
52	1g	201	3PE	O22-C21-O21-C2
52	1g	201	3PE	C22-C21-O21-C2
57	1W	201	EHZ	N2-C15-C16-C17
57	1W	201	EHZ	N2-C15-C16-O5
57	1W	201	EHZ	O4-C15-C16-C17
57	1W	201	EHZ	O4-C15-C16-O5
57	1W	201	EHZ	C15-C16-C17-C19
57	1W	201	EHZ	C15-C16-C17-C20
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
58	1l	201	MYR	O1-C1-C2-C3
52	1g	201	3PE	O21-C2-C3-O31
51	1a	101	CDL	CB7-C71-C72-C73
50	1H	401	U10	C4-C3-O3-C3M
51	1O	403	CDL	CB7-C71-C72-C73
53	1O	401	GTP	C4'-C5'-O5'-PA
46	1d	201	PC1	C22-C23-C24-C25
46	1q	201	PC1	C32-C33-C34-C35
52	1Y	202	3PE	C34-C35-C36-C37
46	1q	201	PC1	C3A-C3B-C3C-C3D
46	1q	201	PC1	C33-C34-C35-C36
46	1q	201	PC1	C22-C21-O21-C2
52	1g	201	3PE	C21-C22-C23-C24
46	1m	201	PC1	C25-C26-C27-C28
51	1a	101	CDL	OB5-CB3-CB4-OB6
46	1Y	201	PC1	C2-C1-O11-P
52	1Y	202	3PE	C1-C2-C3-O31
51	1O	403	CDL	C55-C56-C57-C58
50	1H	401	U10	C2-C3-O3-C3M
46	1B	202	PC1	C31-C32-C33-C34
52	1g	201	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
46	1d	201	PC1	C3A-C3B-C3C-C3D
51	1H	402	CDL	OB5-CB3-CB4-OB6
51	1O	403	CDL	C71-C72-C73-C74
51	1O	403	CDL	C52-C53-C54-C55
46	1d	201	PC1	C33-C34-C35-C36
46	1q	201	PC1	O11-C1-C2-C3
51	1a	101	CDL	CB5-C51-C52-C53
50	1H	401	U10	C20-C19-C21-C22
52	1g	201	3PE	C1-C2-C3-O31
57	1W	201	EHZ	O3-C12-C13-C14
51	1O	403	CDL	OB6-CB4-CB6-OB8
52	1n	202	3PE	O21-C2-C3-O31
51	1O	403	CDL	C78-C79-C80-C81
46	1q	201	PC1	C39-C3A-C3B-C3C
57	1W	201	EHZ	C13-C14-N2-C15
51	1H	402	CDL	OB5-CB3-CB4-CB6
51	1a	101	CDL	OB5-CB3-CB4-CB6
50	1H	401	U10	C18-C19-C21-C22
46	1q	201	PC1	O11-C1-C2-O21
52	1g	201	3PE	O11-C1-C2-O21
52	1Y	202	3PE	C32-C33-C34-C35
46	1Y	201	PC1	C1-C2-C3-O31
46	1B	202	PC1	C12-C11-O13-P
52	1Y	202	3PE	C12-C11-O13-P
52	1g	201	3PE	C12-C11-O13-P
52	1n	202	3PE	C12-C11-O13-P
52	1n	202	3PE	C26-C27-C28-C29
52	1n	202	3PE	C21-C22-C23-C24
46	1B	202	PC1	O21-C21-C22-C23
46	1Y	201	PC1	O13-C11-C12-N
46	1m	201	PC1	O13-C11-C12-N
52	1Y	202	3PE	O31-C31-C32-C33
46	1h	201	PC1	C2-C1-O11-P
46	1Y	201	PC1	O21-C2-C3-O31
46	1m	201	PC1	O21-C2-C3-O31
52	1Y	202	3PE	O21-C2-C3-O31
51	1O	403	CDL	CB3-CB4-CB6-OB8
51	1a	101	CDL	CB3-CB4-CB6-OB8
46	1Y	201	PC1	C1-O11-P-O12
46	1q	201	PC1	C1-O11-P-O13
51	1O	403	CDL	CB3-OB5-PB2-OB2
51	1a	101	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	1a	101	CDL	CB3-OB5-PB2-OB3
52	1Y	202	3PE	C1-O11-P-O14
52	1n	202	3PE	C1-O11-P-O14
46	1d	201	PC1	C2-C1-O11-P
51	1a	101	CDL	CB4-CB3-OB5-PB2
55	1P	501	NDP	C2D-C1D-N1N-C6N
52	1N	401	3PE	C2-C1-O11-P
46	1q	201	PC1	C21-C22-C23-C24
51	1O	403	CDL	C71-CB7-OB8-CB6
46	1B	202	PC1	O22-C21-C22-C23
51	1a	101	CDL	CA7-C31-C32-C33
52	1Y	202	3PE	C2-C3-O31-C31
51	1a	101	CDL	CA4-CA3-OA5-PA1
57	1W	201	EHZ	N1-C12-C13-C14
50	1H	401	U10	C5-C4-O4-C4M
52	1Y	202	3PE	C27-C28-C29-C2A
46	1q	201	PC1	C37-C38-C39-C3A
51	1H	402	CDL	CA4-CA3-OA5-PA1
57	1W	201	EHZ	C2-C1-C21-C22
52	1Y	202	3PE	C23-C24-C25-C26
55	1P	501	NDP	O4D-C1D-N1N-C6N
52	1n	202	3PE	C22-C23-C24-C25
55	1P	501	NDP	C2D-C1D-N1N-C2N
51	1O	403	CDL	C53-C54-C55-C56
46	1B	202	PC1	C1-C2-C3-O31
46	1d	201	PC1	C23-C24-C25-C26
46	1B	202	PC1	C36-C37-C38-C39
52	1g	201	3PE	C1-C2-O21-C21
57	1W	201	EHZ	C10-C11-N1-C12
46	1q	201	PC1	C12-C11-O13-P
52	1N	401	3PE	C12-C11-O13-P
57	1W	201	EHZ	C15-C16-C17-C18
57	1W	201	EHZ	O5-C16-C17-C18
52	1N	401	3PE	O11-C1-C2-O21
58	1l	201	MYR	C6-C7-C8-C9
46	1m	201	PC1	C1-C2-C3-O31
57	1W	201	EHZ	S1-C10-C11-N1
50	1H	401	U10	C26-C27-C28-C29
52	1g	201	3PE	C25-C26-C27-C28
52	1Y	202	3PE	C3-C2-O21-C21
53	1O	401	GTP	C3'-C4'-C5'-O5'
51	1a	101	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
46	1Y	201	PC1	C33-C34-C35-C36
52	1N	401	3PE	C33-C34-C35-C36
51	1a	101	CDL	CA5-C11-C12-C13
52	1Y	202	3PE	O32-C31-C32-C33
46	1d	201	PC1	C35-C36-C37-C38
51	1a	101	CDL	C17-C18-C19-C20
52	1g	201	3PE	C38-C39-C3A-C3B
46	1q	201	PC1	O22-C21-C22-C23
46	1q	201	PC1	C22-C23-C24-C25
51	1a	101	CDL	C19-C20-C21-C22
46	1Y	201	PC1	C34-C35-C36-C37
51	1a	101	CDL	C12-C11-CA5-OA6
51	1O	403	CDL	C51-C52-C53-C54
53	1O	401	GTP	O4'-C4'-C5'-O5'
46	1d	201	PC1	O31-C31-C32-C33
46	1q	201	PC1	O31-C31-C32-C33
46	1d	201	PC1	O32-C31-C32-C33

There are no ring outliers.

27 monomers are involved in 90 short contacts:

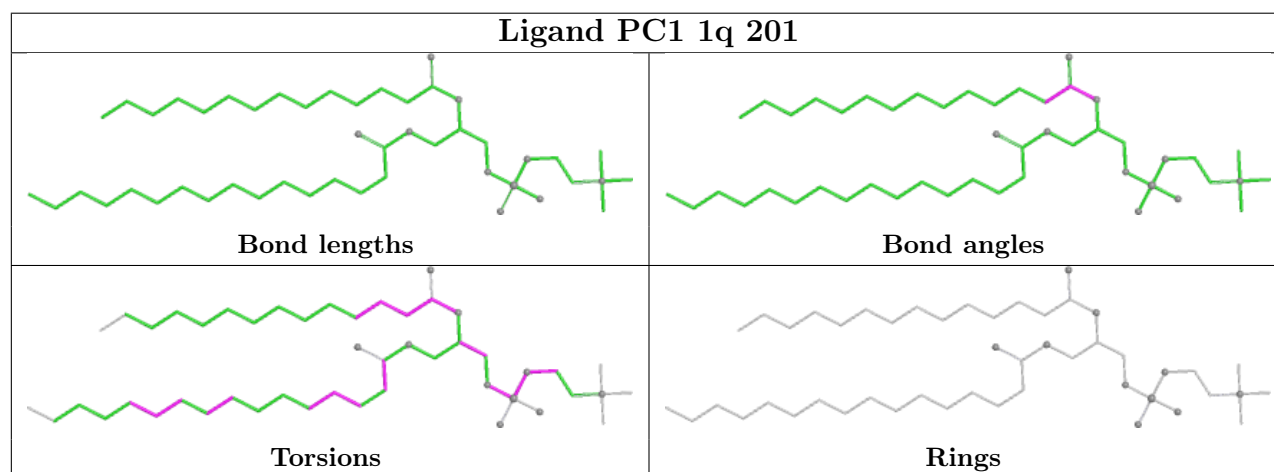
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1q	201	PC1	2	0
47	1E	301	FES	1	0
57	1W	201	EHZ	1	0
52	1N	401	3PE	6	0
46	1m	201	PC1	6	0
53	1O	401	GTP	3	0
45	1I	202	SF4	2	0
50	1H	401	U10	11	0
45	1B	201	SF4	1	0
47	1G	803	FES	1	0
46	1Y	201	PC1	2	0
48	1F	501	FMN	2	0
52	1n	202	3PE	4	0
52	1g	201	3PE	5	0
46	1h	201	PC1	2	0
51	1O	403	CDL	8	0
45	1G	801	SF4	3	0
46	1d	201	PC1	9	0
51	1a	101	CDL	4	0
52	1Y	202	3PE	2	0

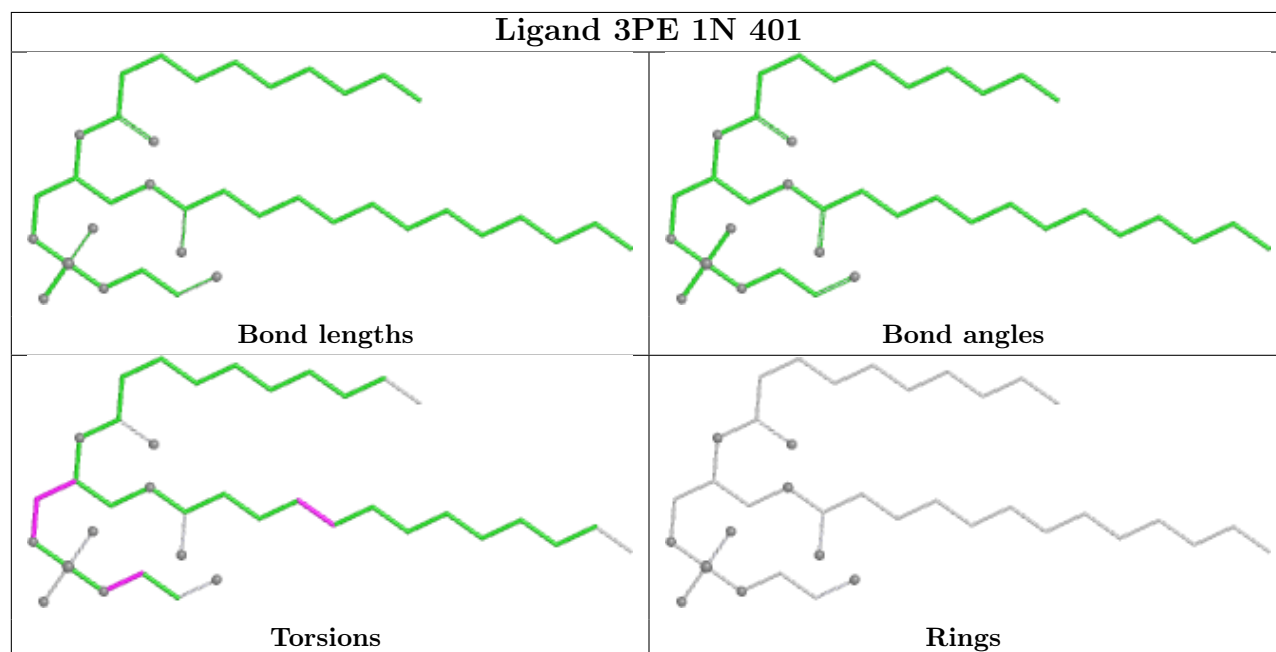
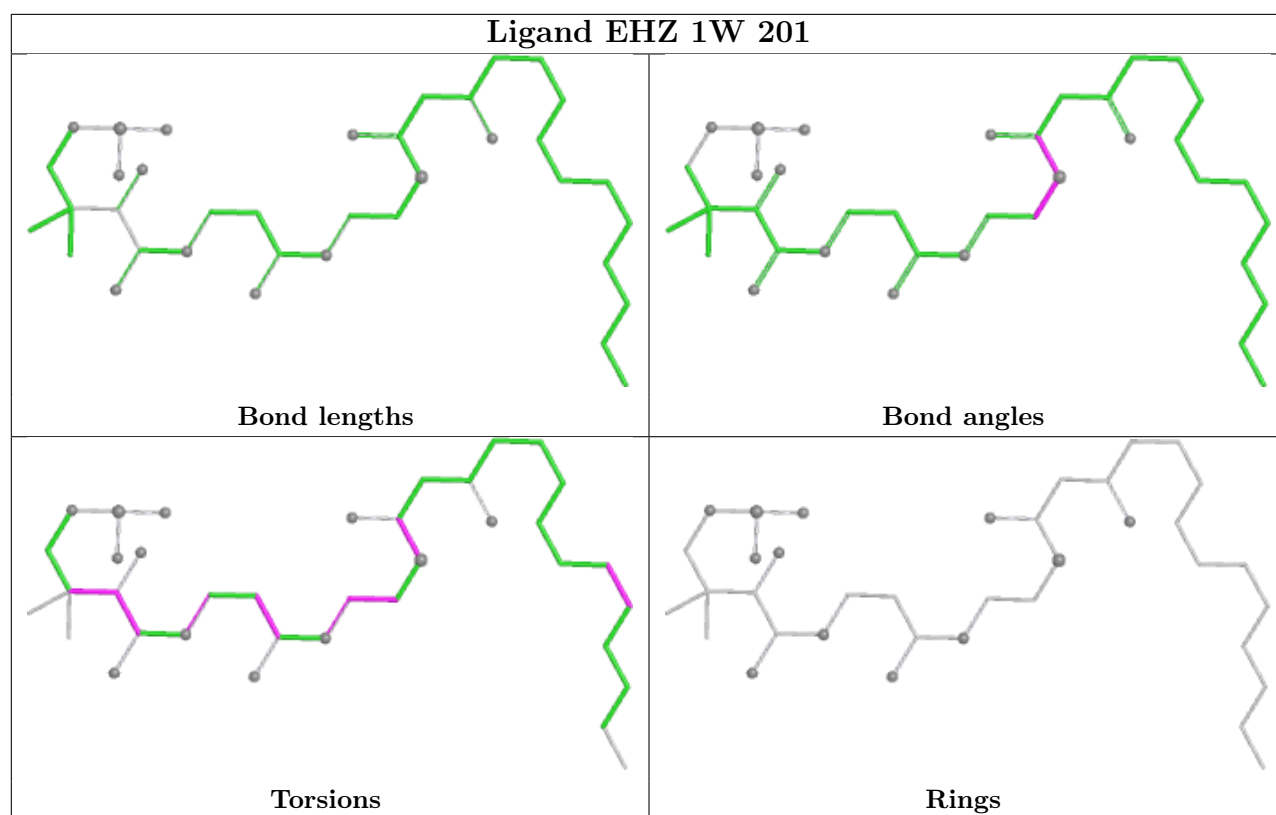
Continued on next page...

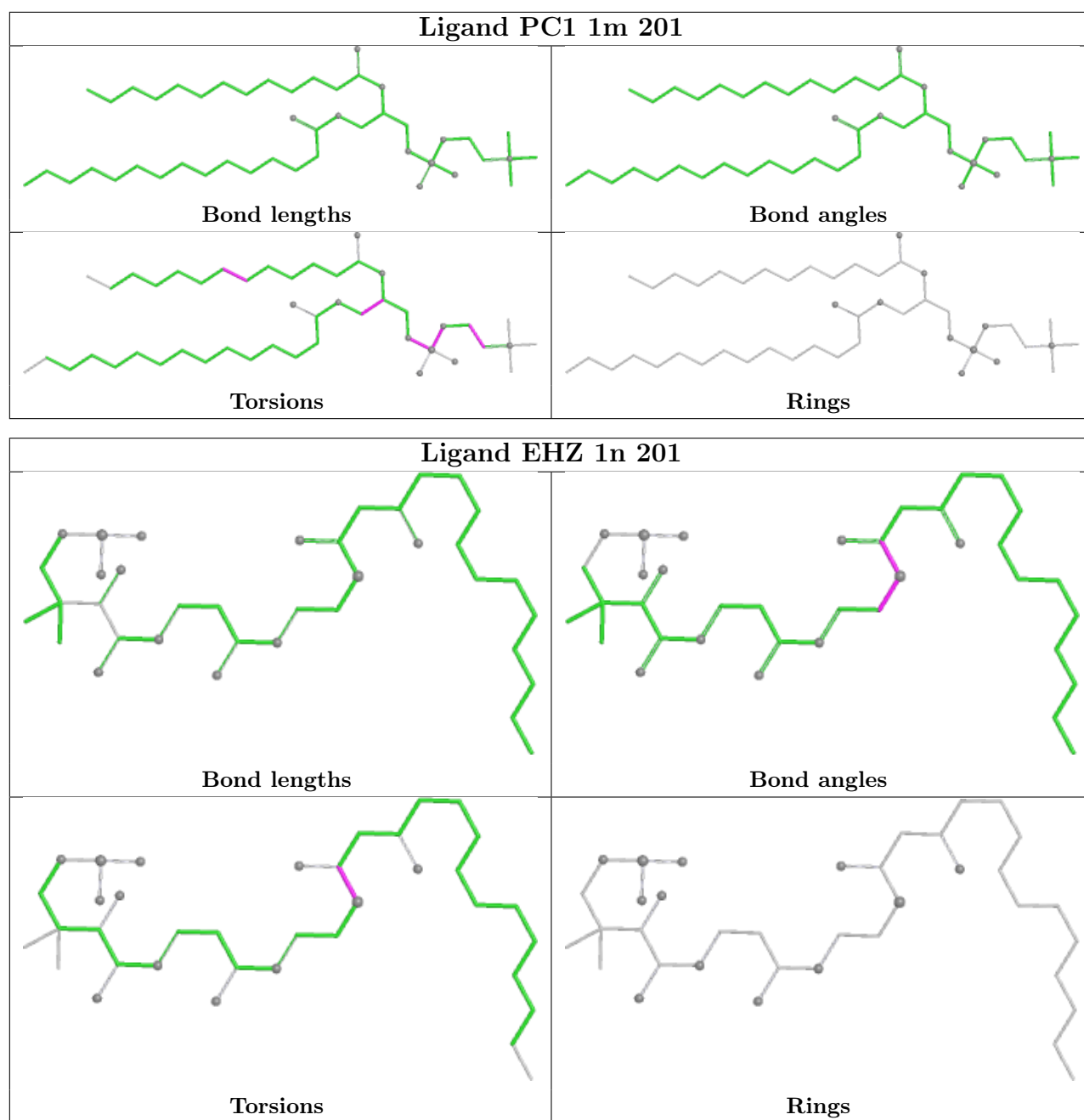
Continued from previous page...

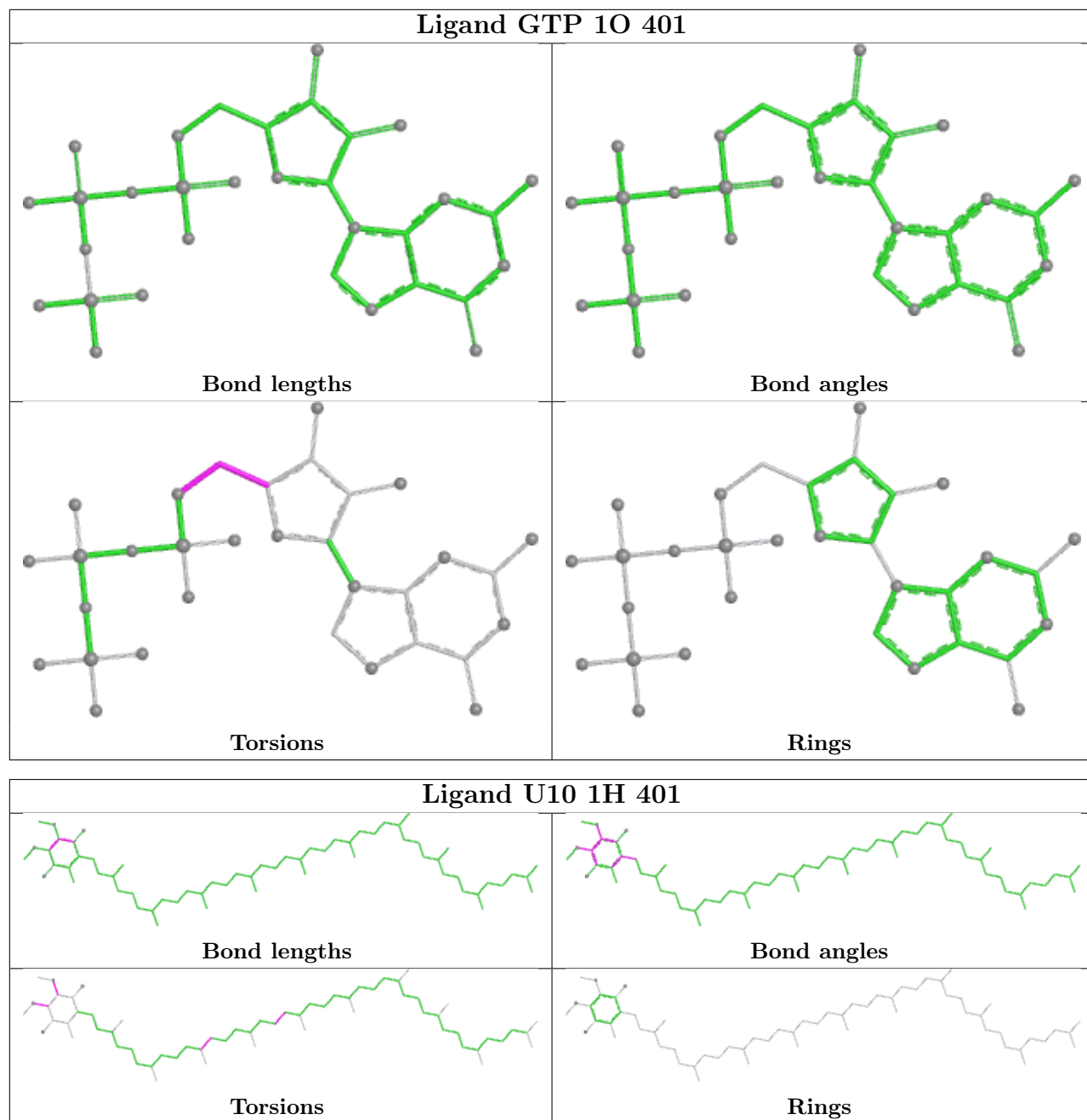
Mol	Chain	Res	Type	Clashes	Symm-Clashes
55	1P	501	NDP	1	0
58	1I	201	MYR	1	0
46	1B	202	PC1	1	0
45	1I	201	SF4	2	0
45	1G	802	SF4	5	0
45	1F	502	SF4	3	0
51	1H	402	CDL	2	0

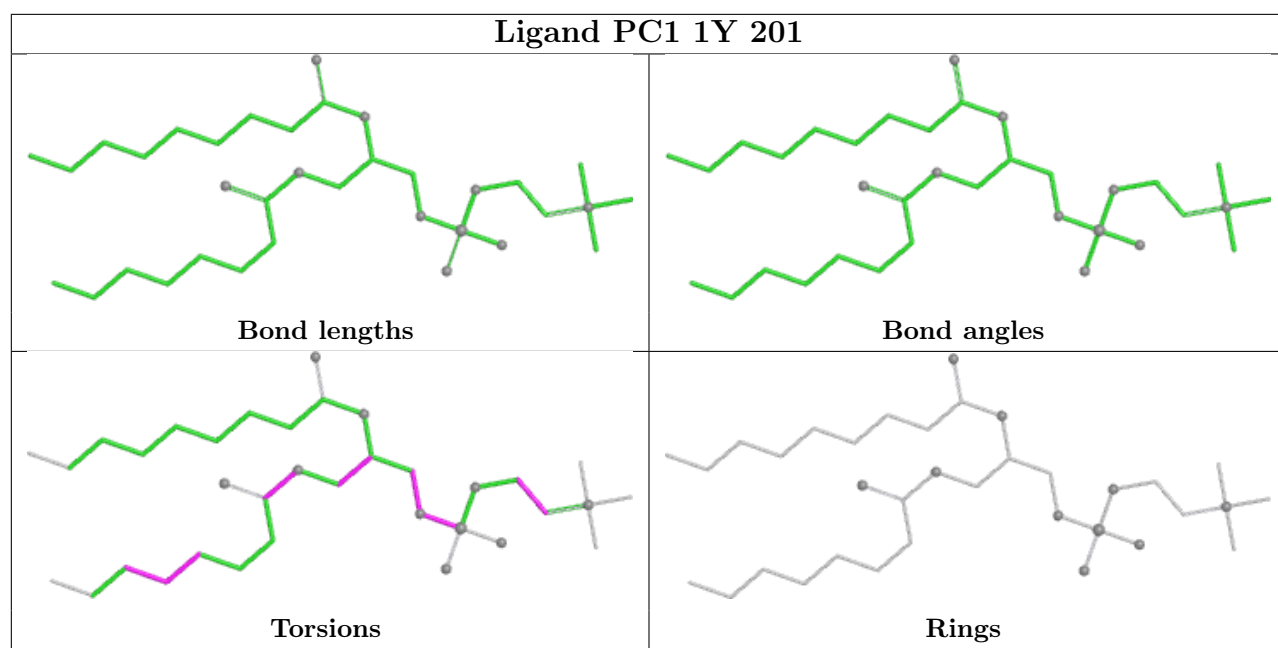
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



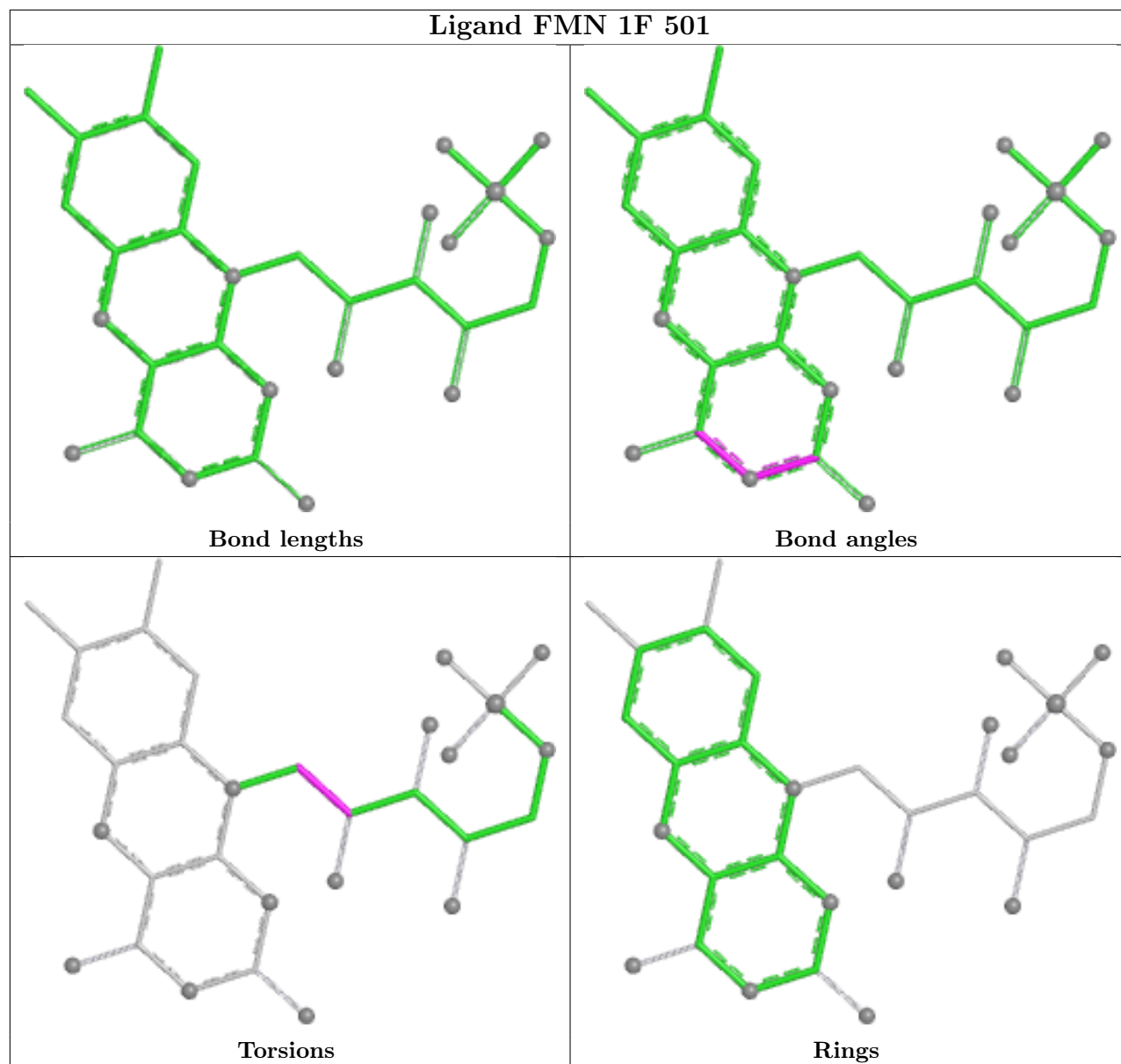


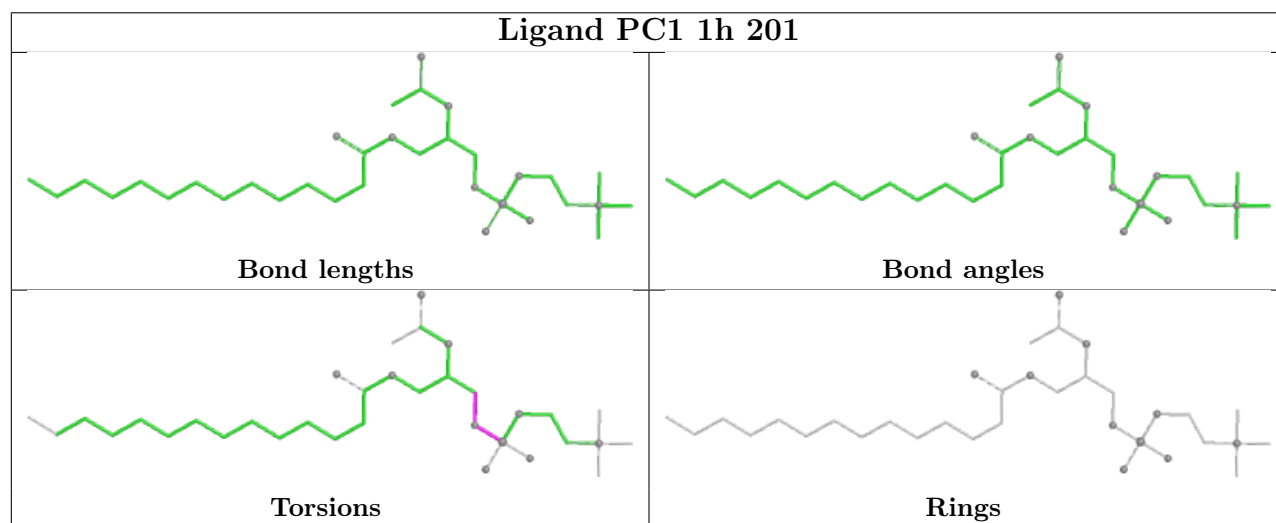
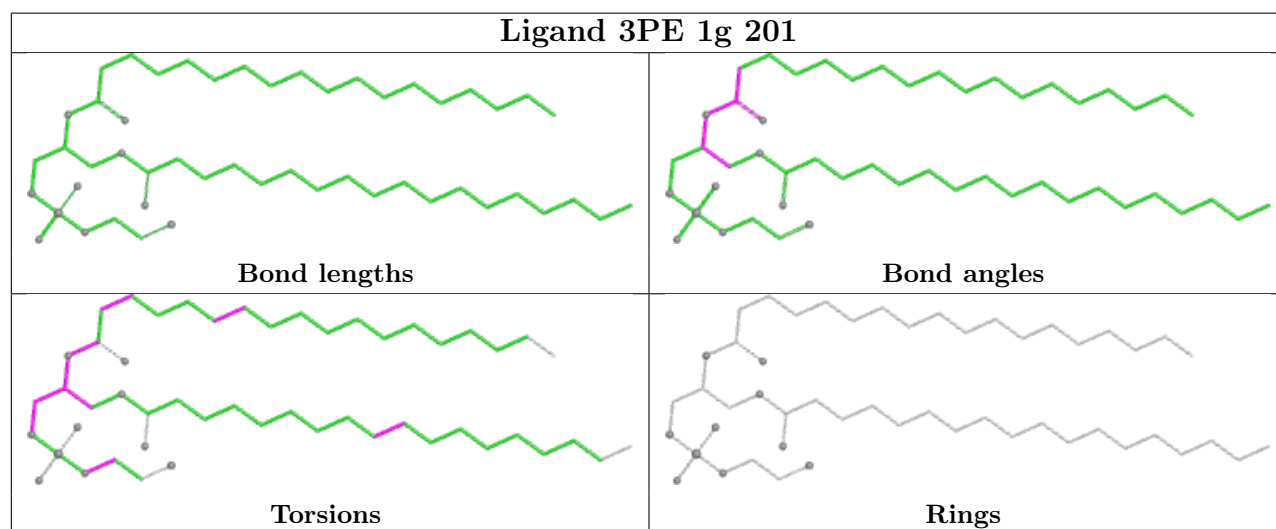
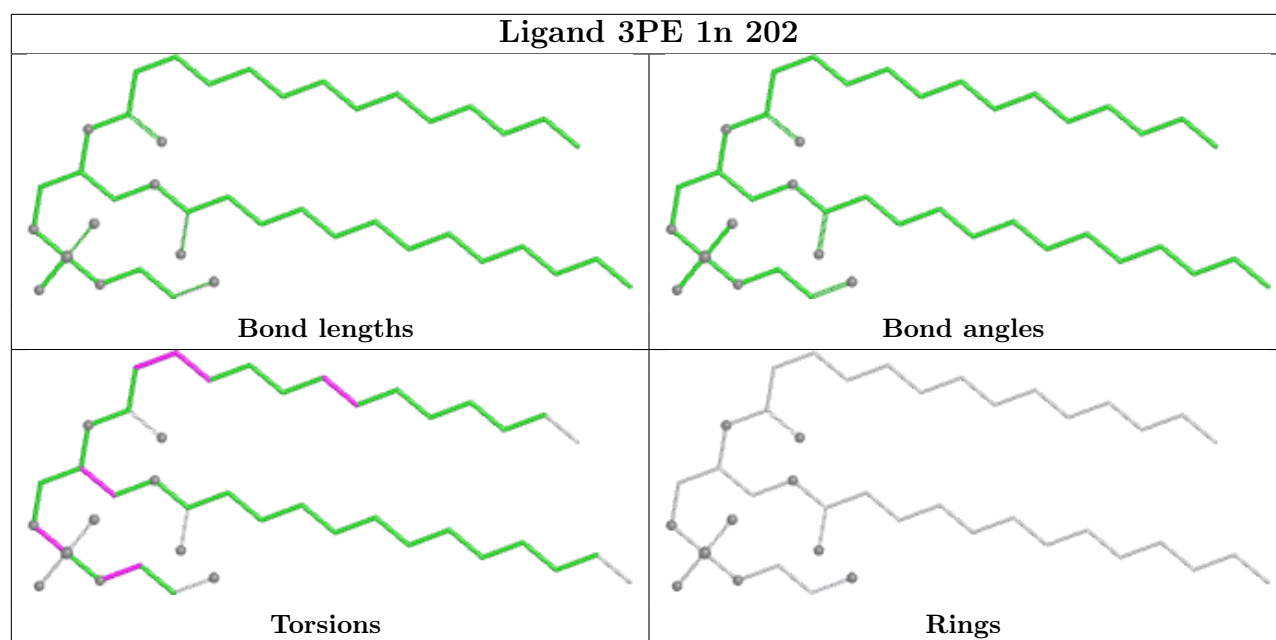


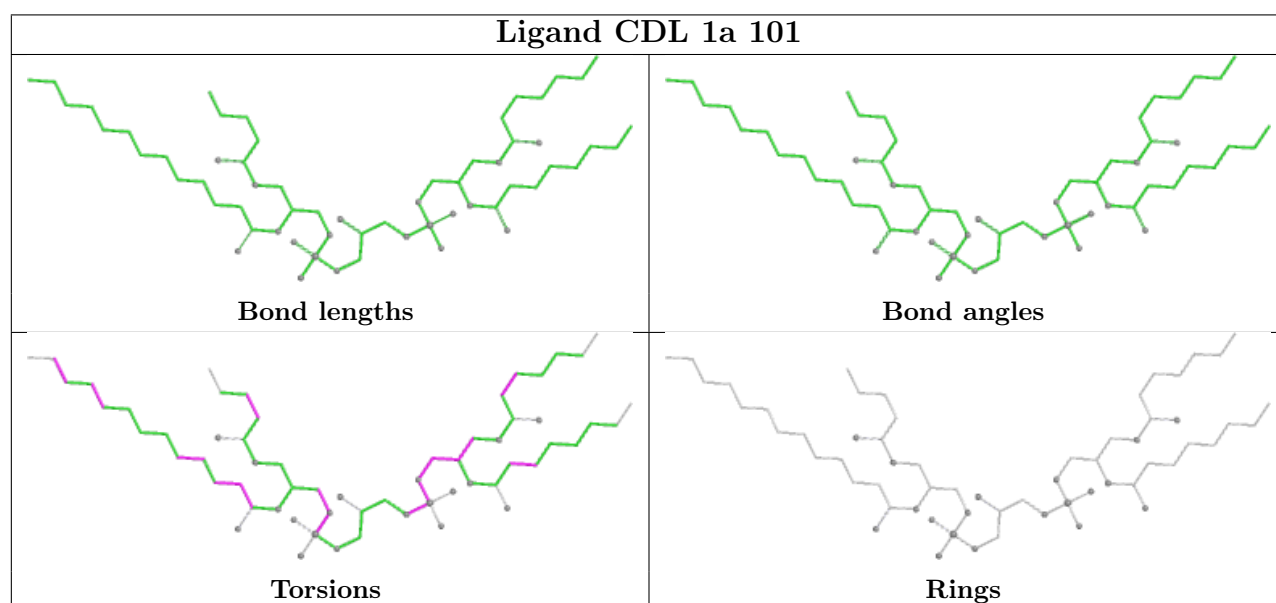
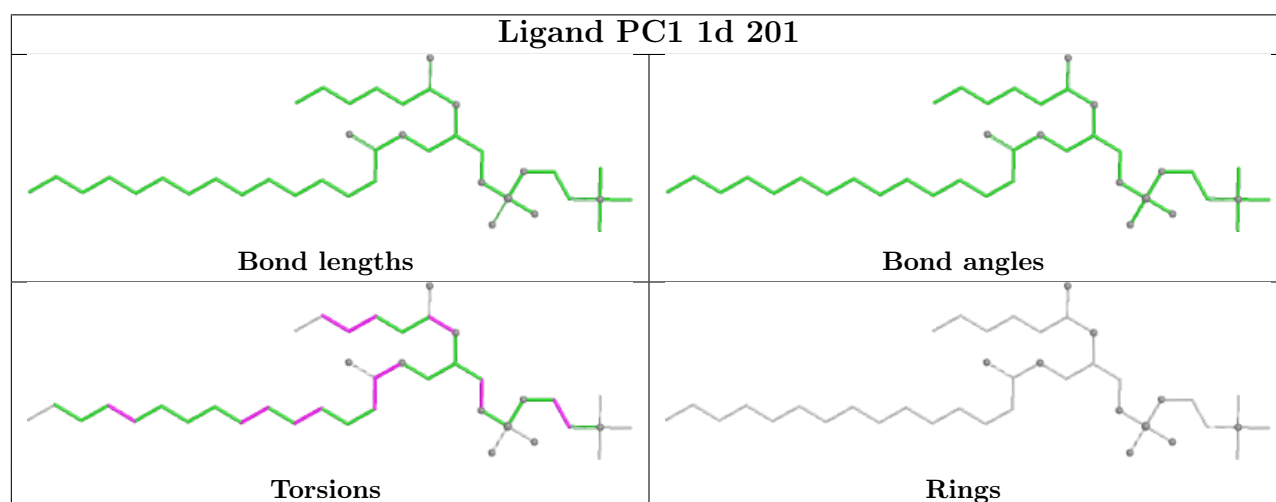
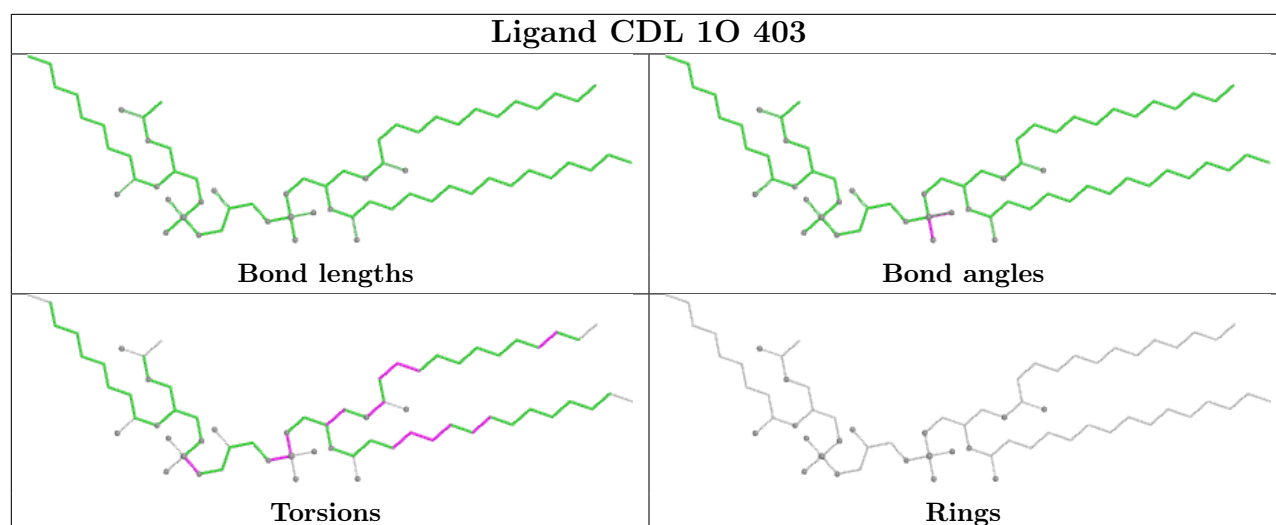


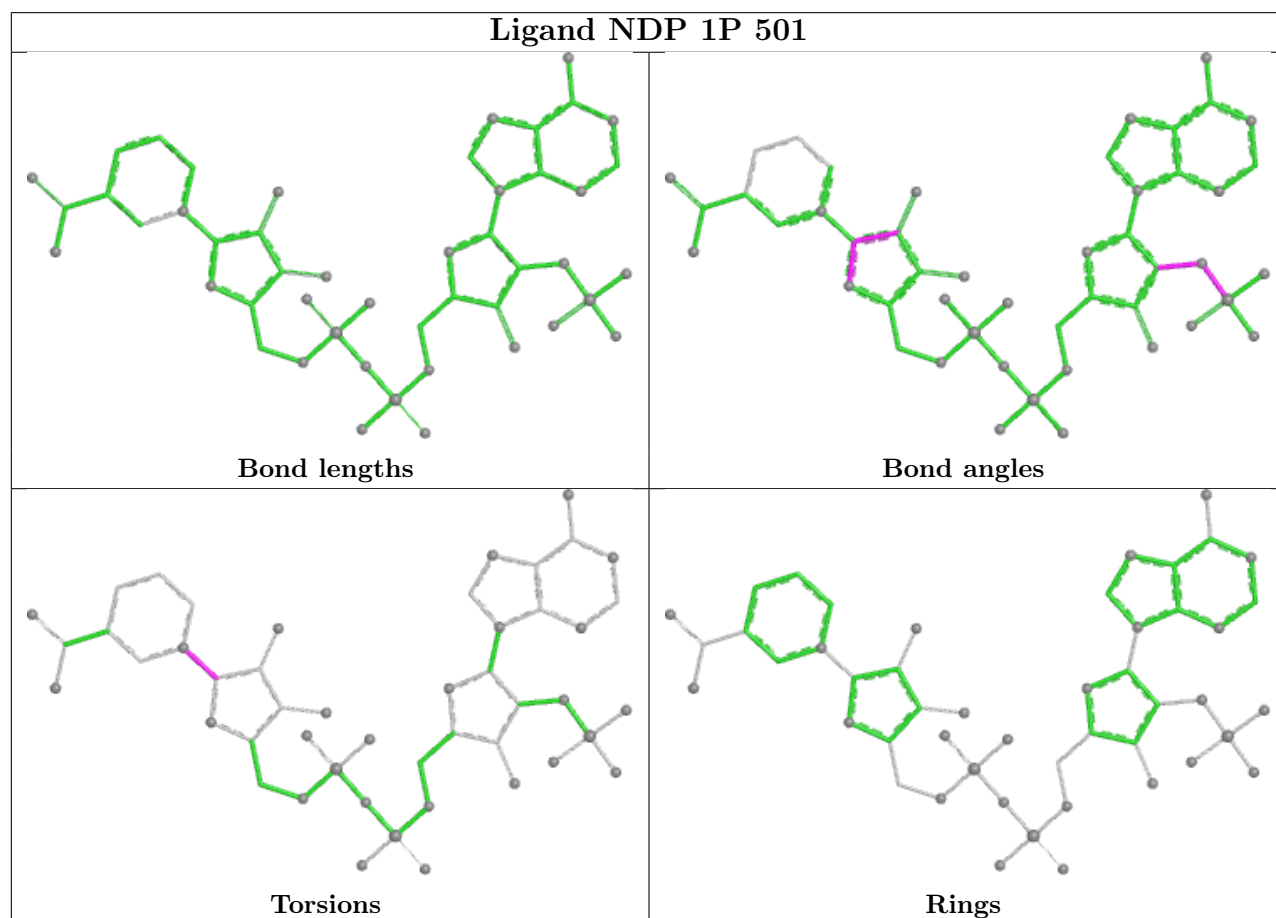
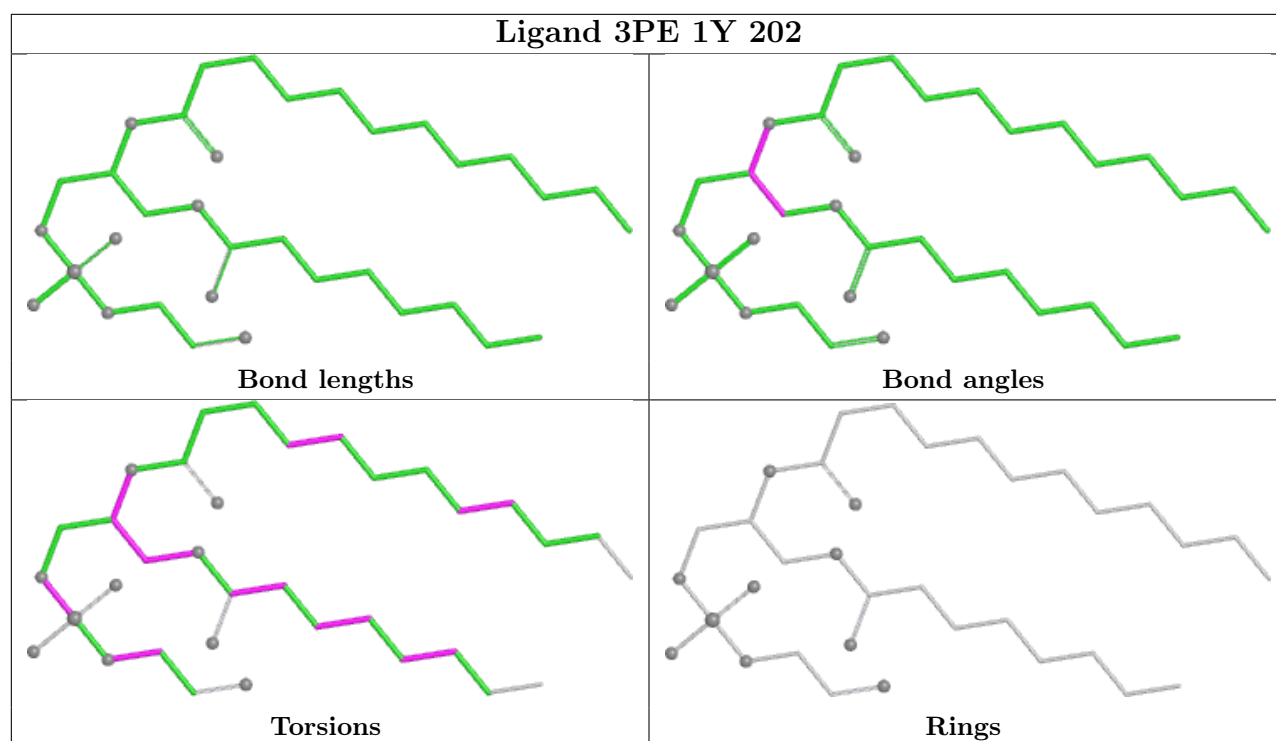


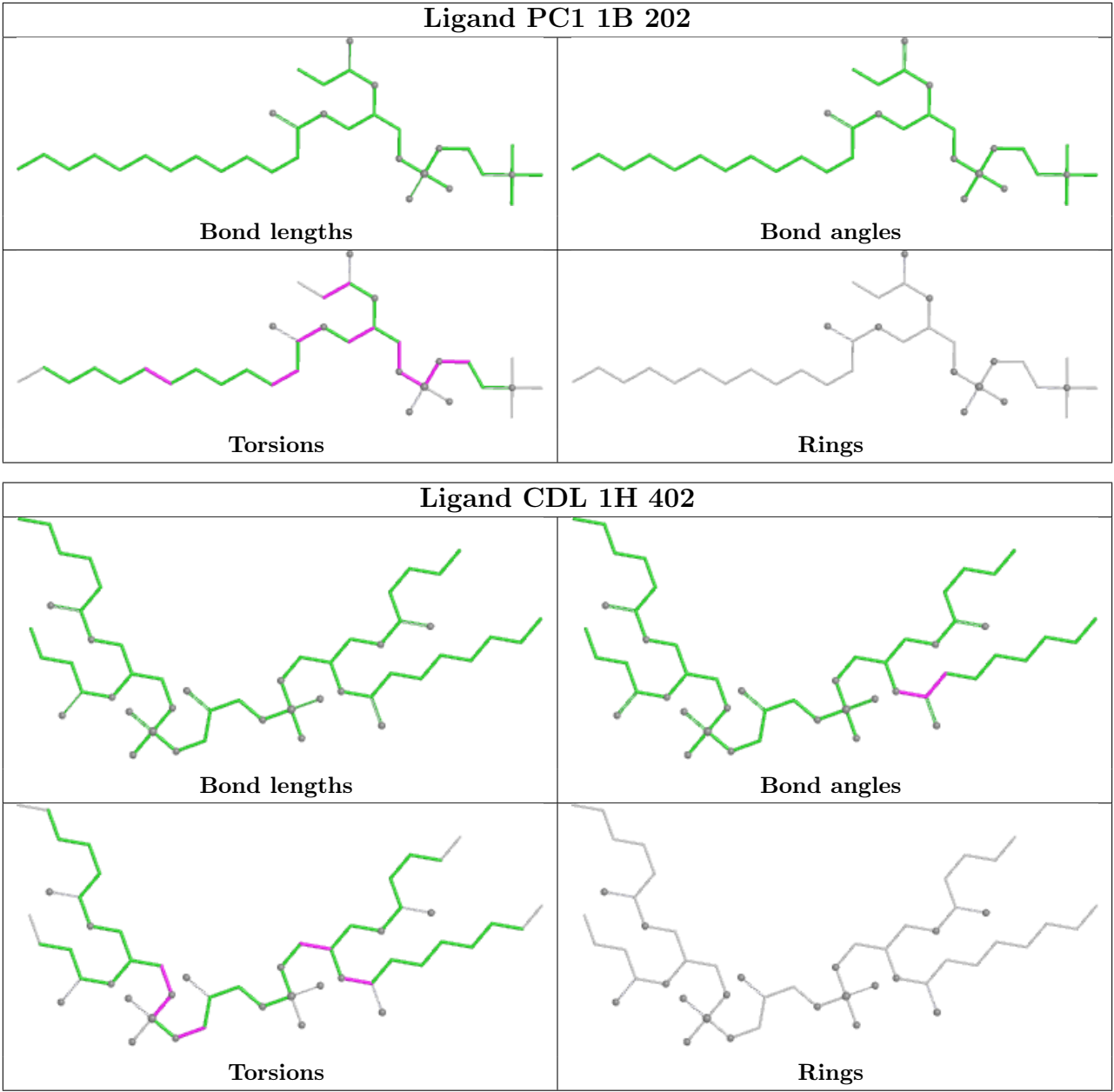
Ligand FMN 1F 501











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	7.02
1	1i	1:SAC	C	2:GLY	N	4.04

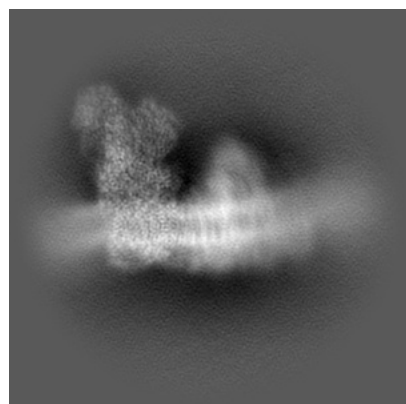
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42168. These allow visual inspection of the internal detail of the map and identification of artifacts.

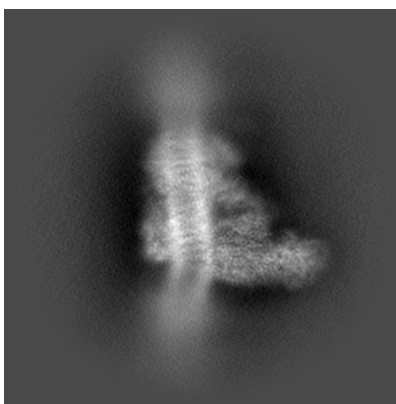
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

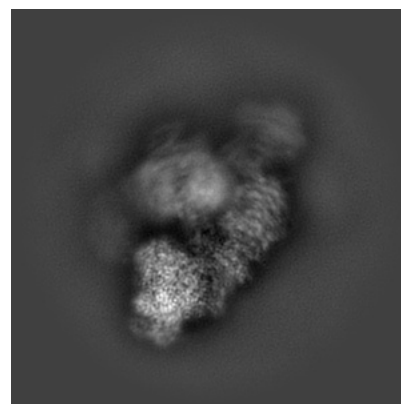
6.1.1 Primary map



X

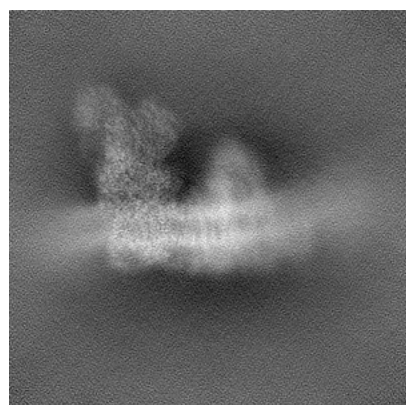


Y

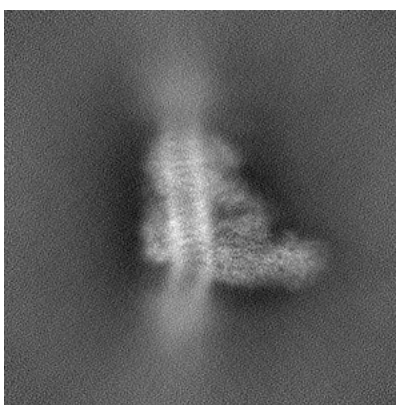


Z

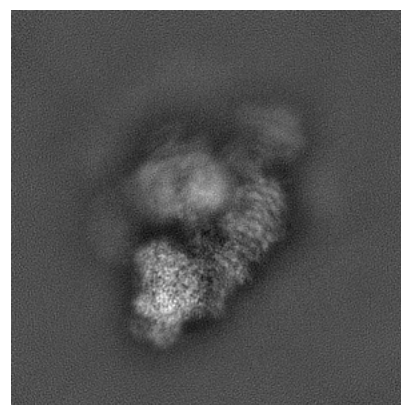
6.1.2 Raw map



X



Y

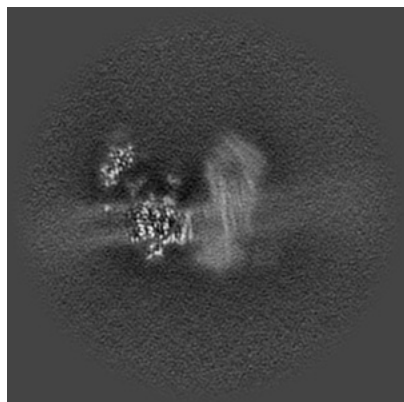


Z

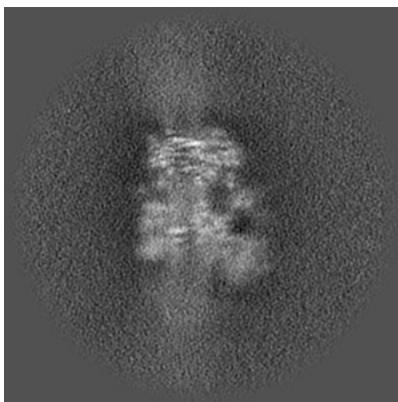
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

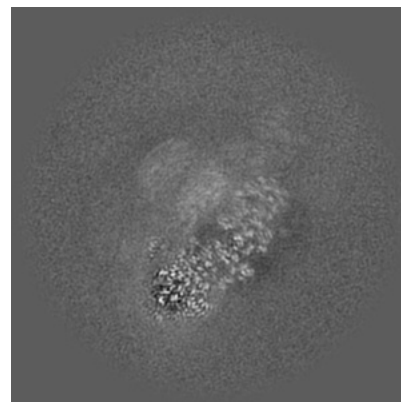
6.2.1 Primary map



X Index: 160

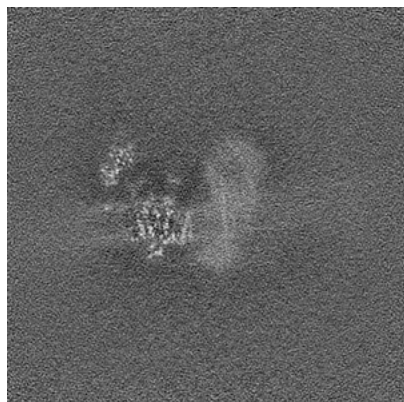


Y Index: 160

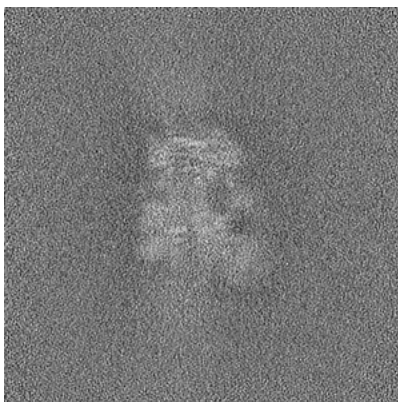


Z Index: 160

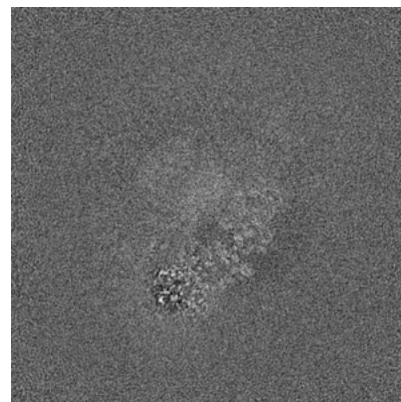
6.2.2 Raw map



X Index: 160



Y Index: 160

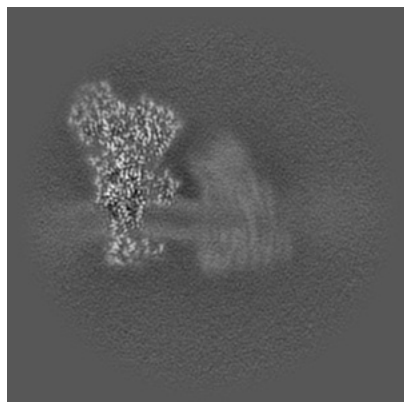


Z Index: 160

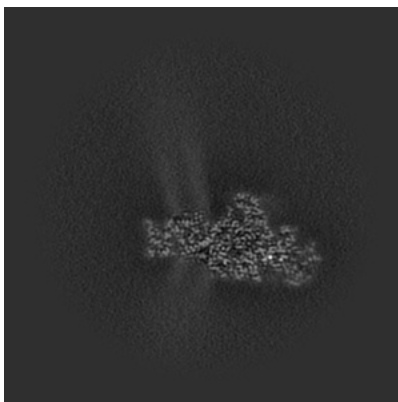
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

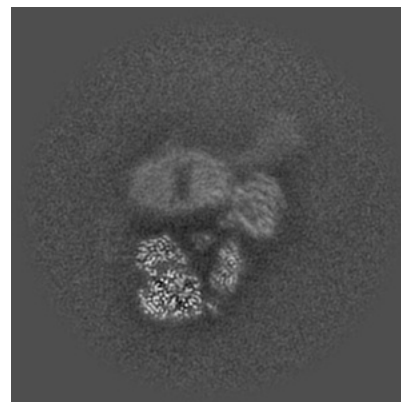
6.3.1 Primary map



X Index: 123

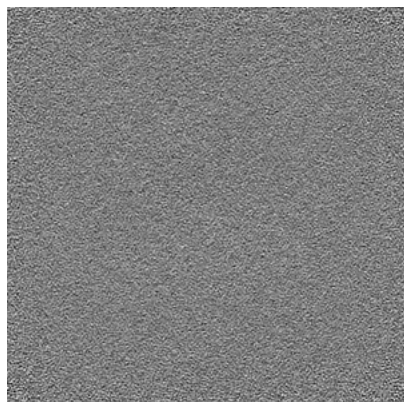


Y Index: 87

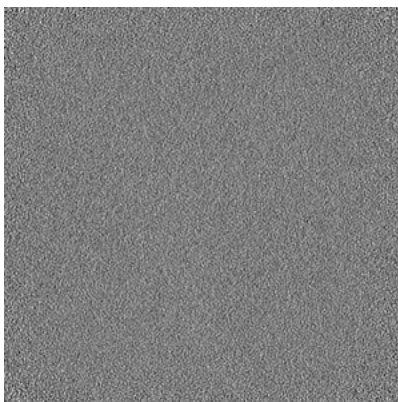


Z Index: 177

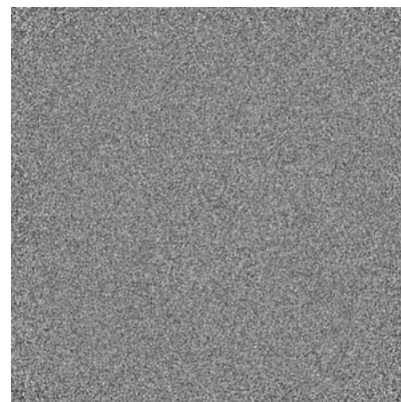
6.3.2 Raw map



X Index: 0



Y Index: 0

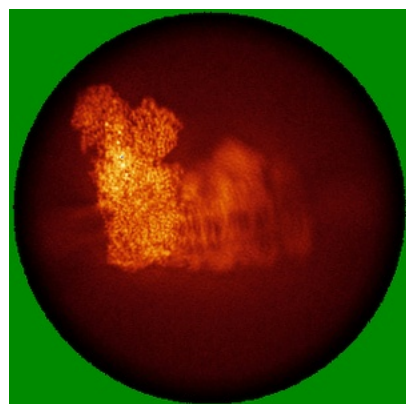


Z Index: 0

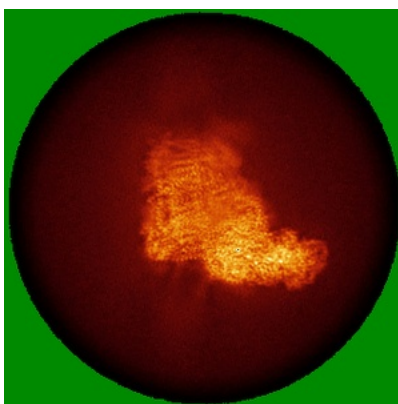
The images above show the largest variance slices of the map in three orthogonal directions.

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

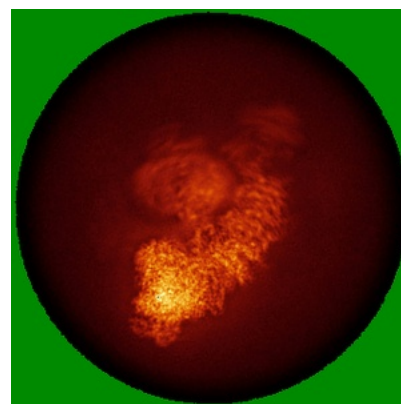
6.4.1 Primary map



X

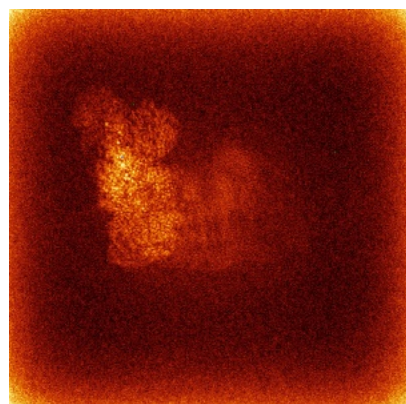


Y

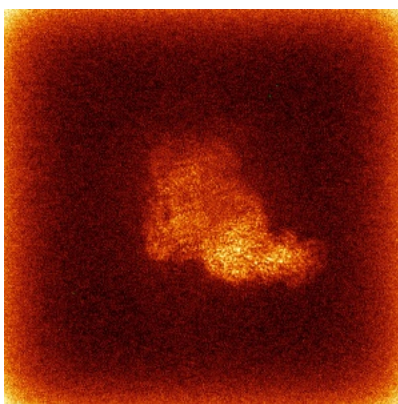


Z

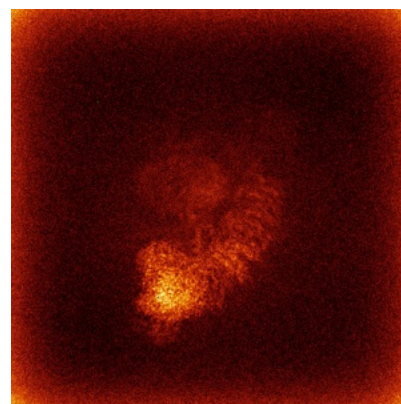
6.4.2 Raw map



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.

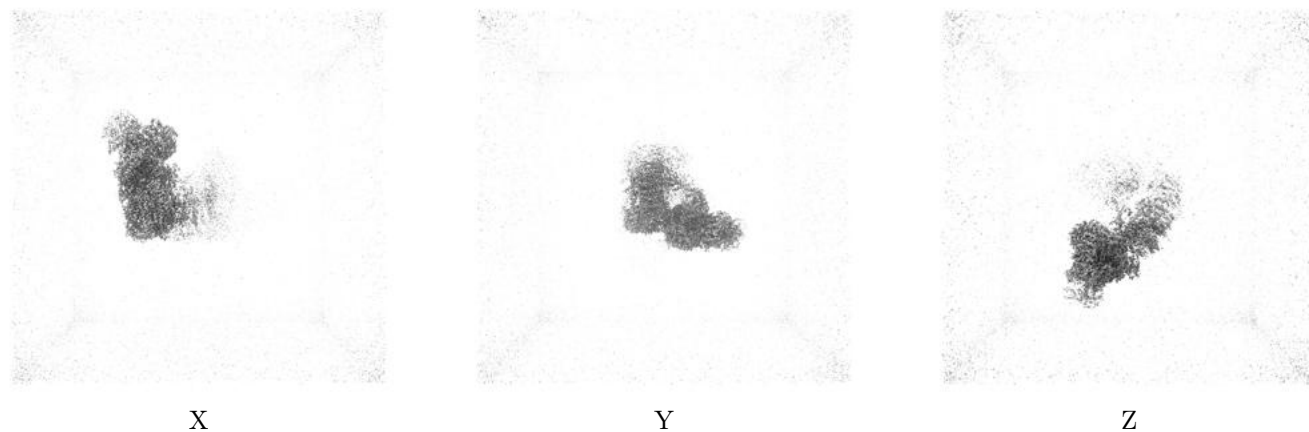
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

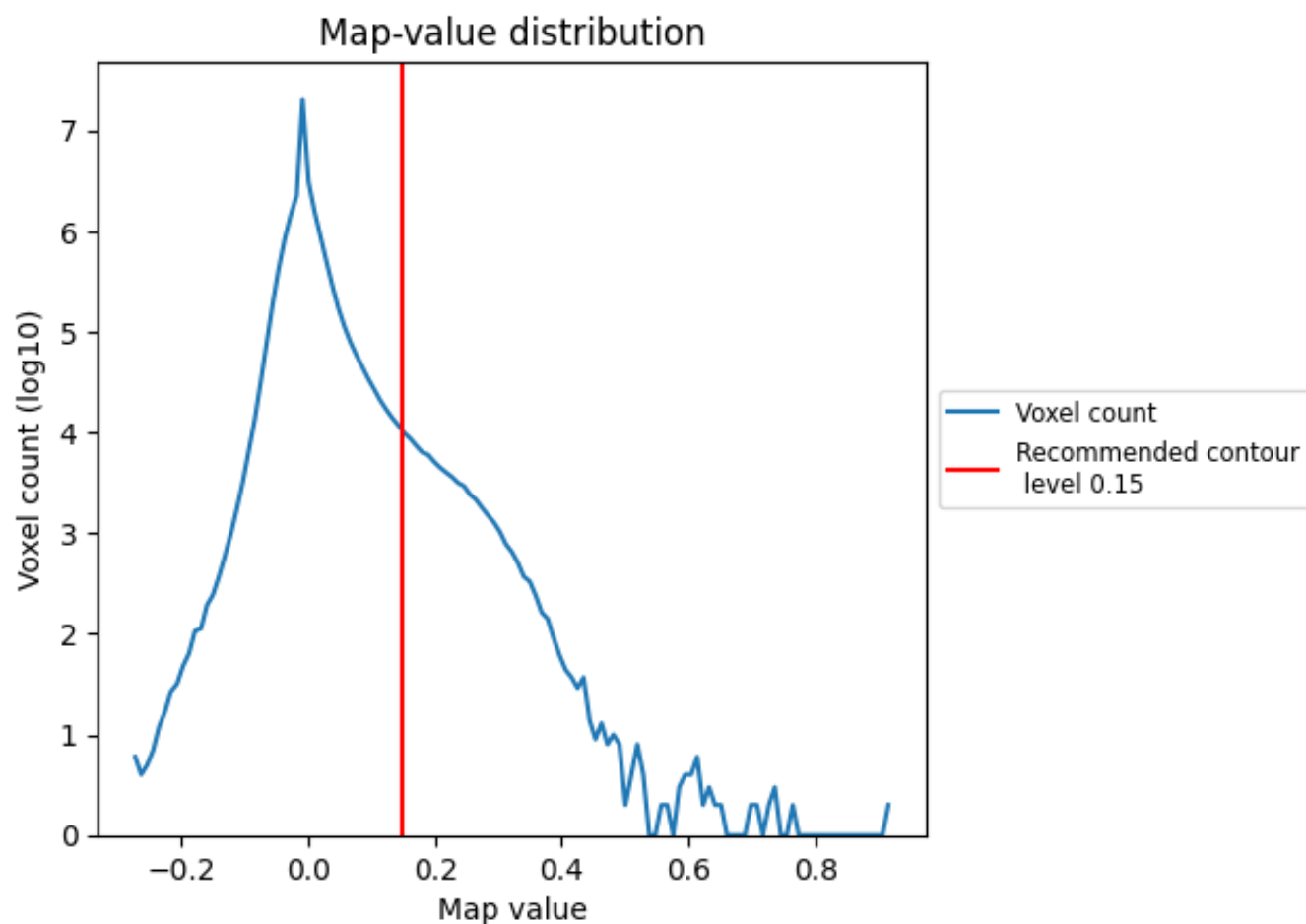
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

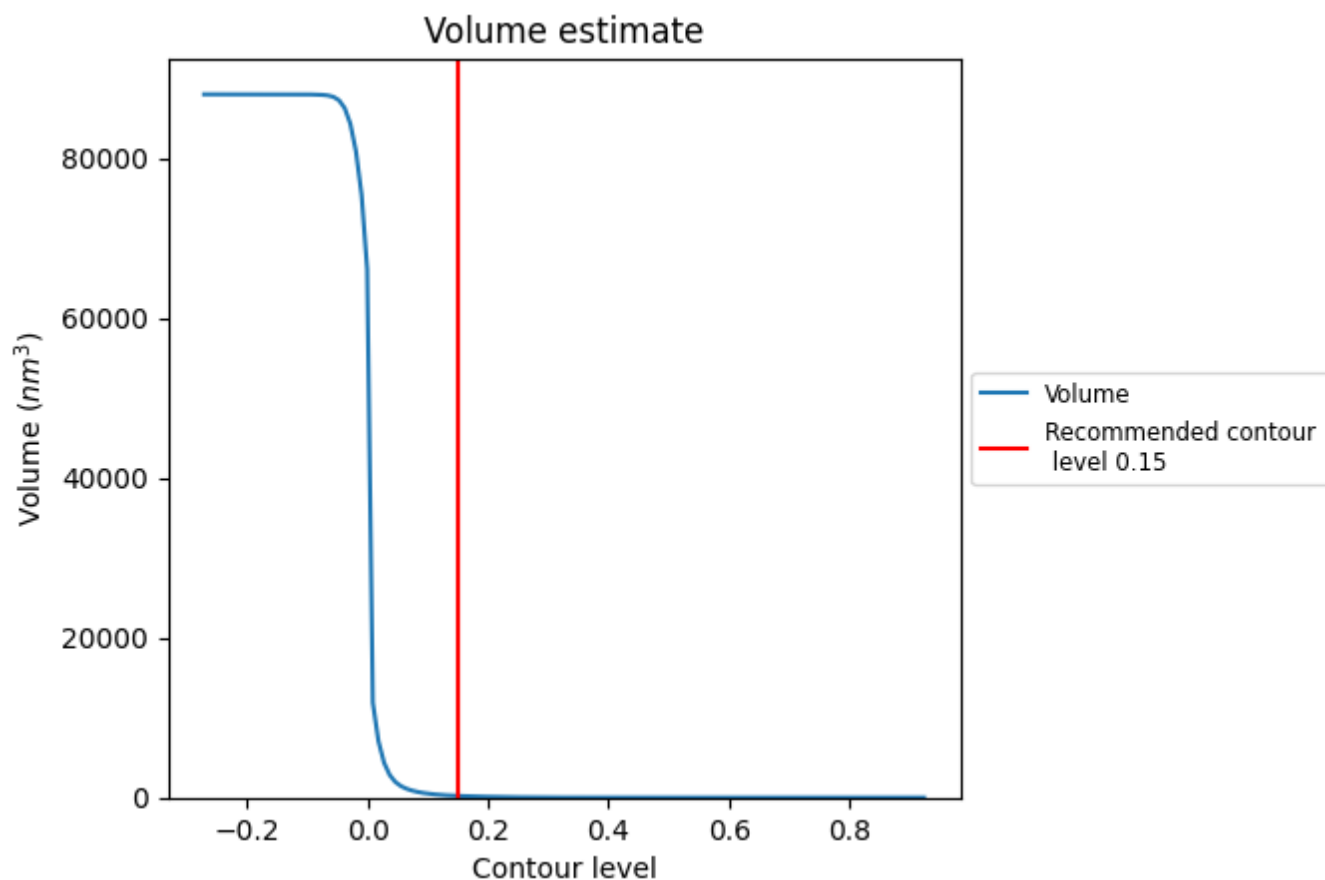
This section contains the results of statistical analysis of the map.

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.

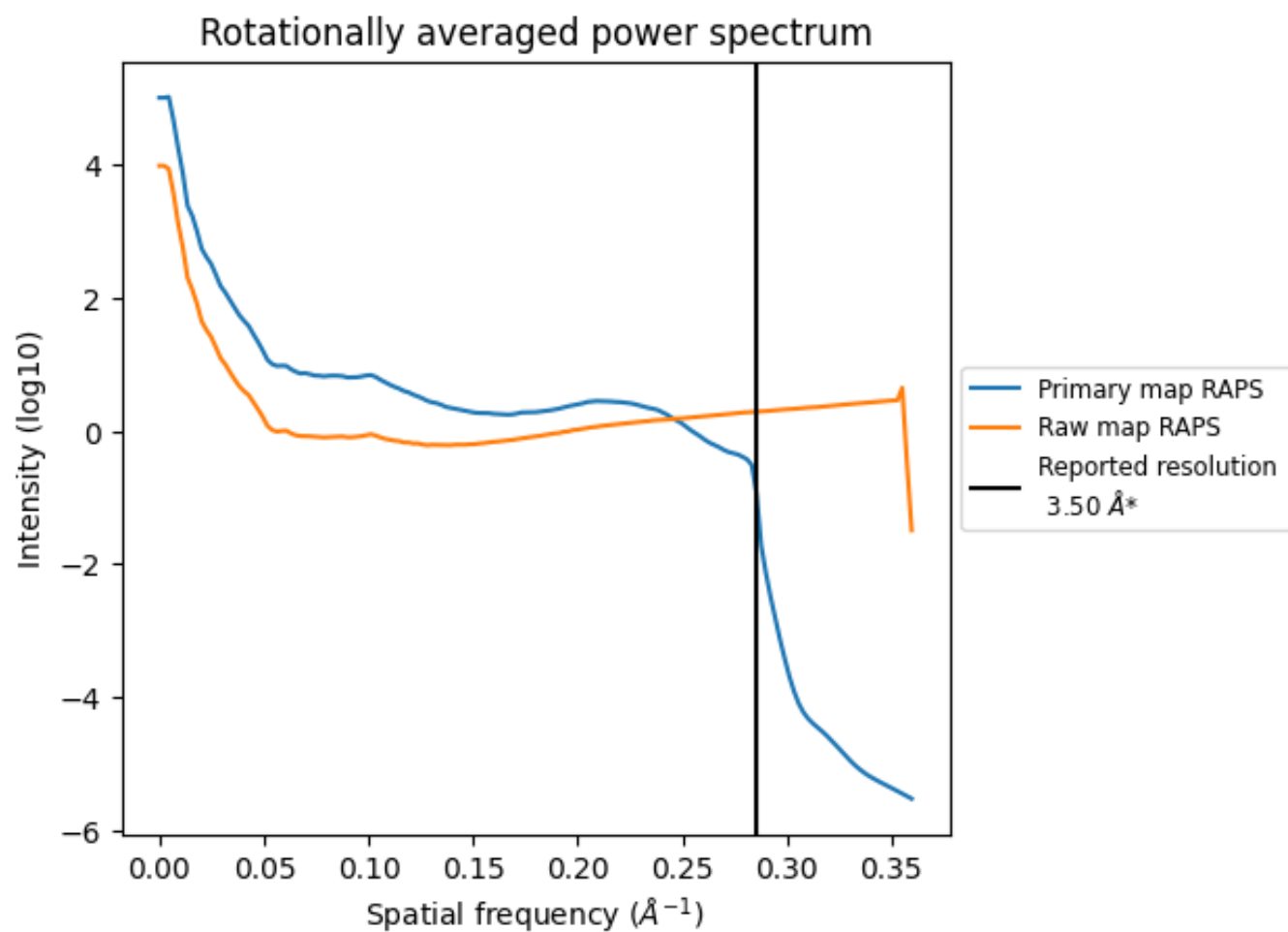
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

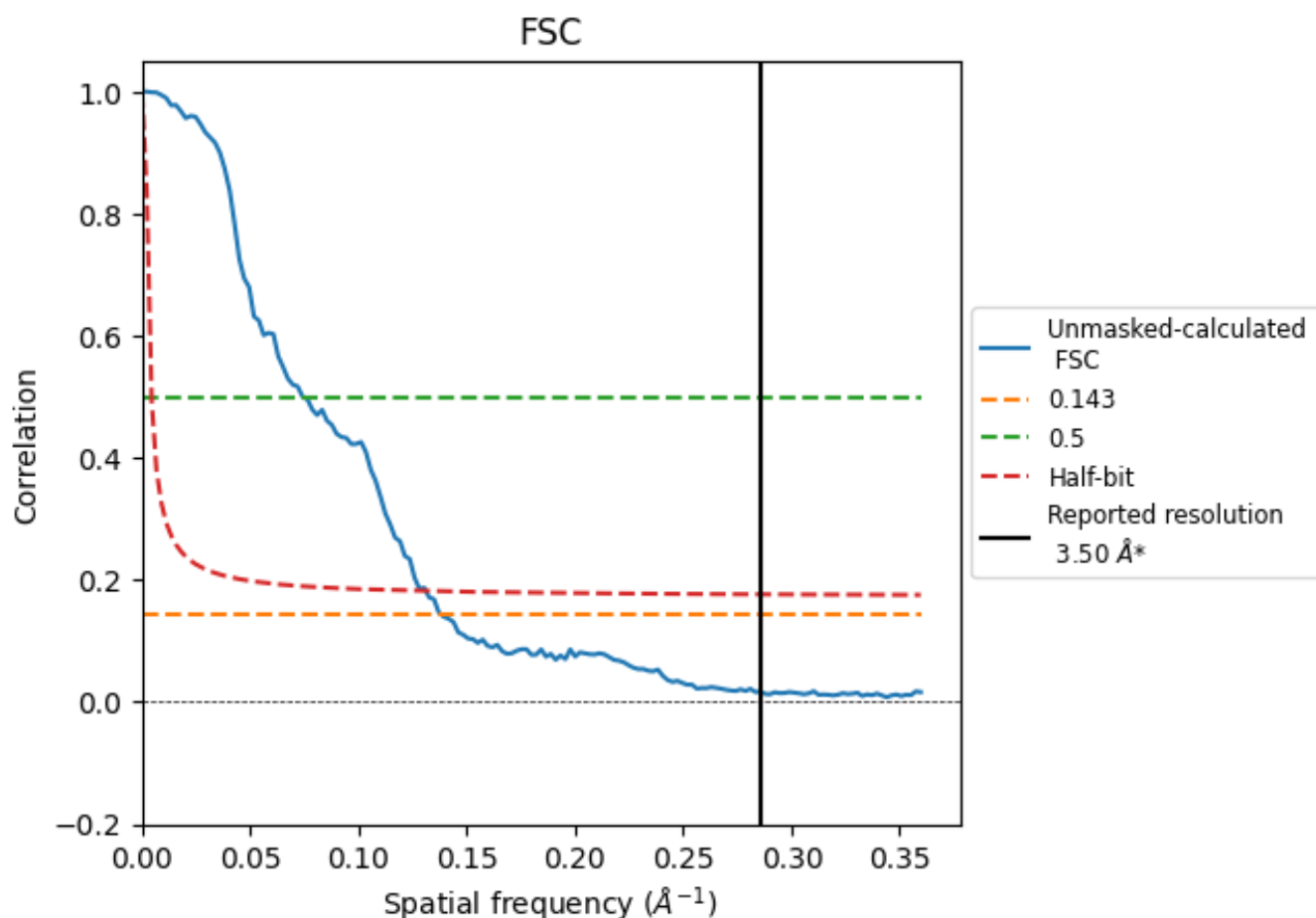


*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

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](#)

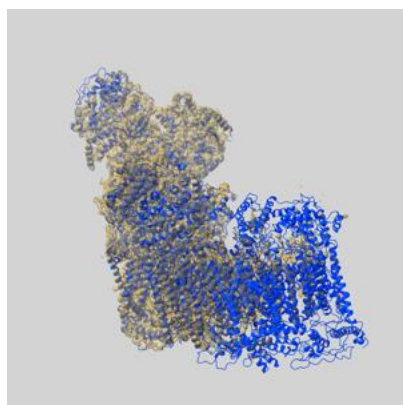
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.24	13.48	7.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.24 differs from the reported value 3.5 by more than 10 %

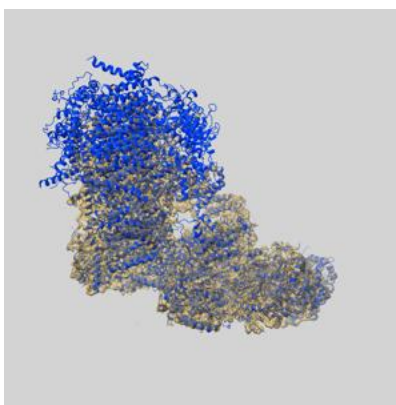
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42168 and PDB model 8UER. Per-residue inclusion information can be found in section 3 on page 21.

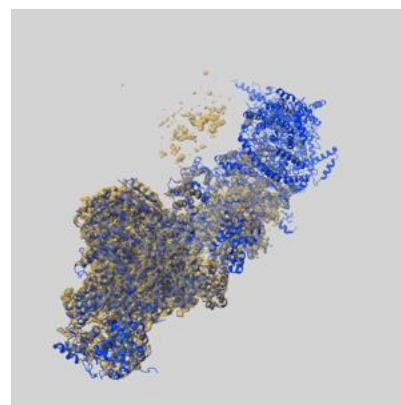
9.1 Map-model overlay [i](#)



X



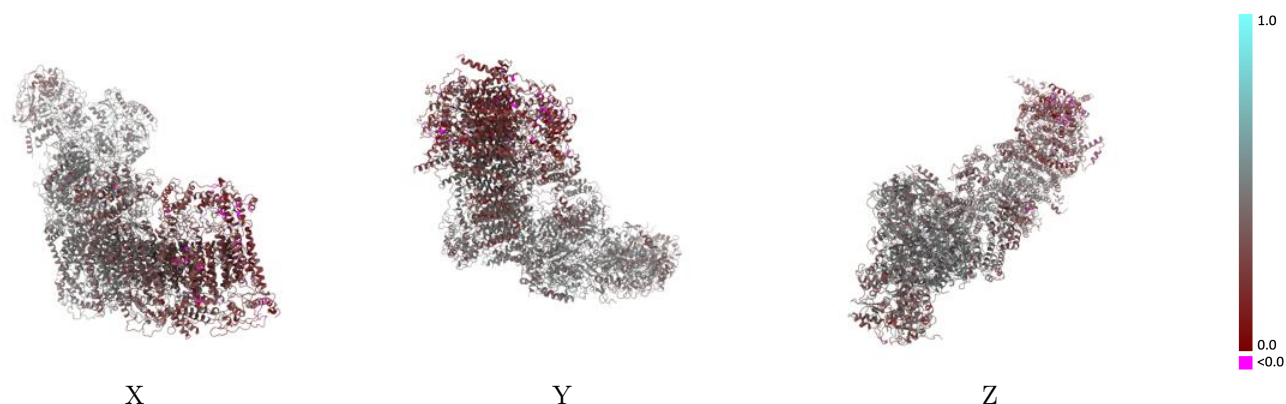
Y



Z

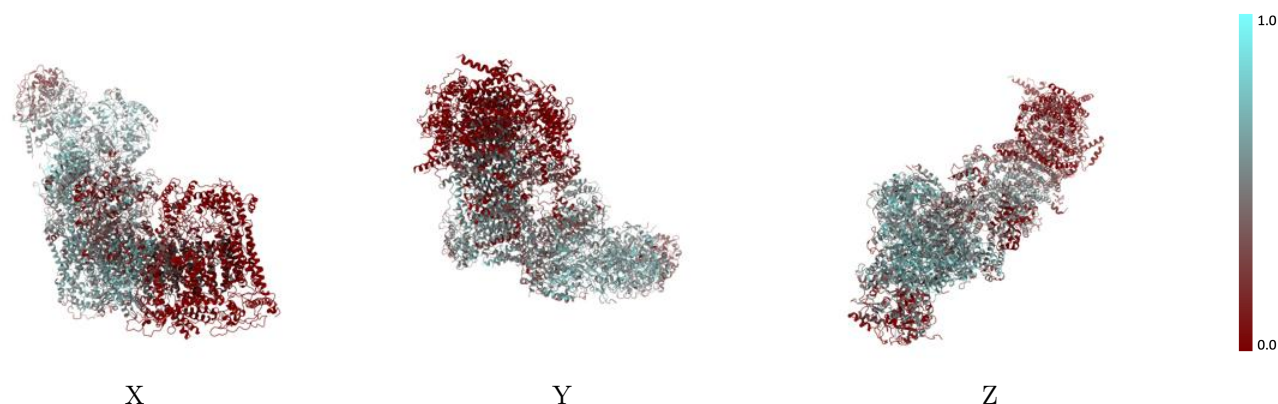
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



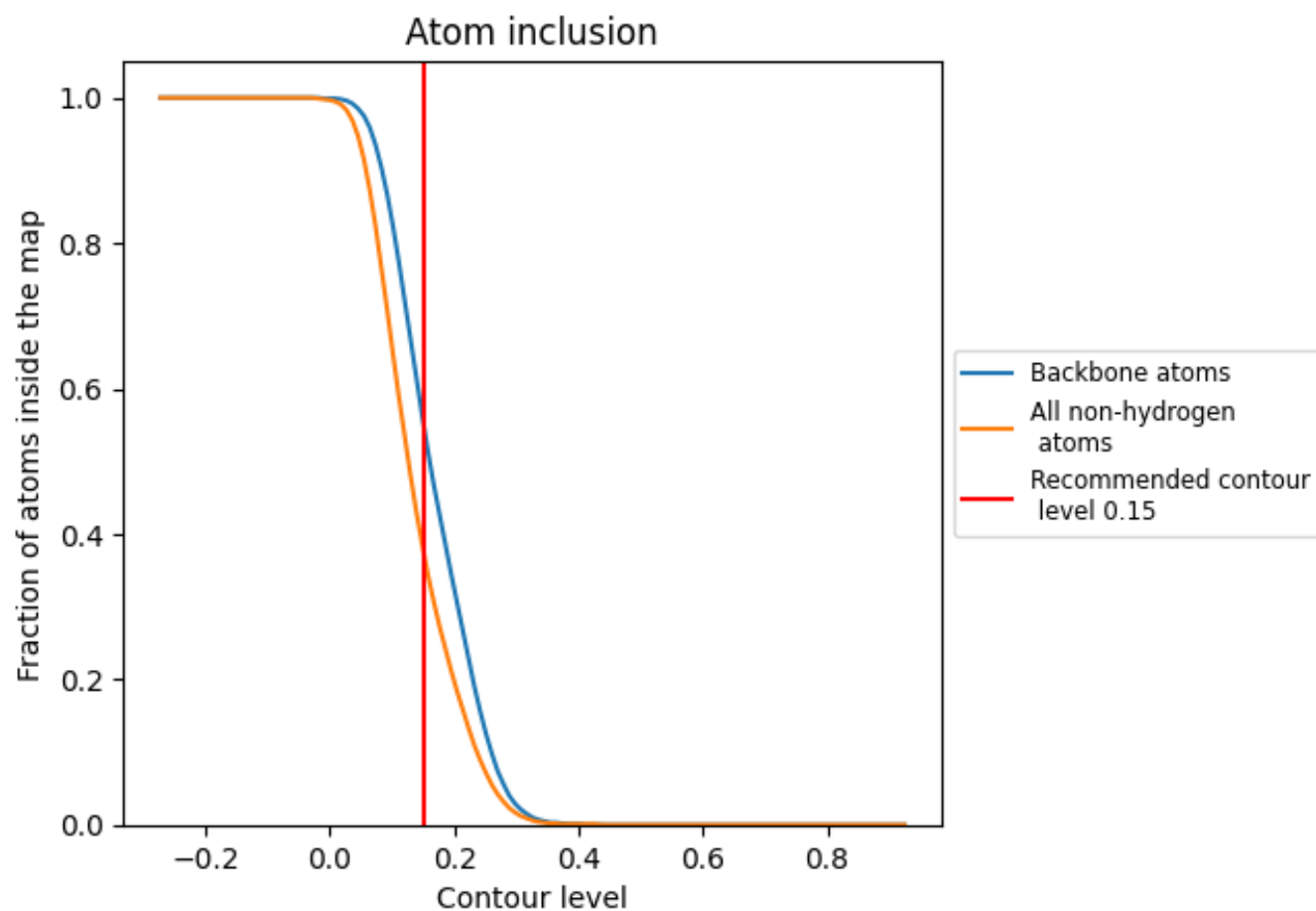
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.15).

9.4 Atom inclusion ⓘ



At the recommended contour level, 56% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3800	 0.3880
1A	 0.4340	 0.4320
1B	 0.6100	 0.4560
1C	 0.5770	 0.4740
1D	 0.5810	 0.4590
1E	 0.3490	 0.3930
1F	 0.3610	 0.3930
1G	 0.5870	 0.4470
1H	 0.5560	 0.4510
1I	 0.6800	 0.4600
1J	 0.4030	 0.4130
1K	 0.4480	 0.4110
1L	 0.1050	 0.2710
1M	 0.3520	 0.3820
1N	 0.5370	 0.4410
1O	 0.2470	 0.3480
1P	 0.5000	 0.4580
1Q	 0.4720	 0.4510
1R	 0.5400	 0.4590
1S	 0.5320	 0.4170
1T	 0.2300	 0.3430
1U	 0.0020	 0.2200
1V	 0.4610	 0.4300
1W	 0.4200	 0.4200
1X	 0.5060	 0.4250
1Y	 0.2750	 0.3430
1Z	 0.5740	 0.4340
1a	 0.5880	 0.4480
1b	 0.4780	 0.4270
1c	 0.3100	 0.3700
1d	 0.4660	 0.4150
1e	 0.5380	 0.4350
1f	 0.2250	 0.3370
1g	 0.1330	 0.3280
1h	 0.2770	 0.3750



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Chain	Atom inclusion	Q-score
1i	 0.0090	 0.2600
1j	 0.0000	 0.2620
1k	 0.0000	 0.2080
1l	 0.0550	 0.2770
1m	 0.1150	 0.2940
1n	 0.0290	 0.2450
1o	 0.0020	 0.2220
1p	 0.0430	 0.3140
1q	 0.6100	 0.4560
1r	 0.5980	 0.4600
1s	 0.2210	 0.3810