



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 08:24 PM EDT

PDB ID : 8UEY / pdb_00008uey
EMDB ID : EMD-42175
Title : In-situ complex I, Deactive class07
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

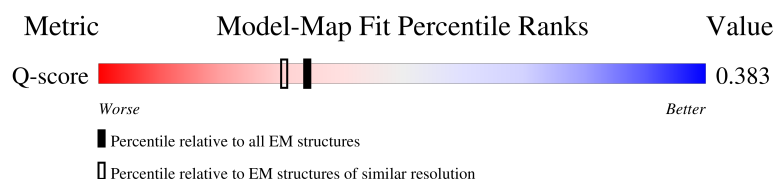
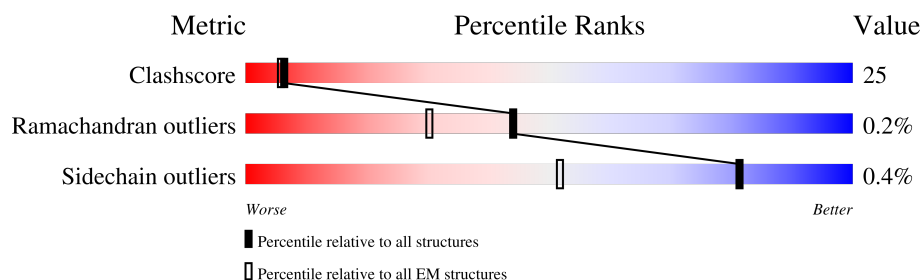
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	10% 36% 40% 23%
2	1B	255	15% 29% 31% 39%
3	1C	264	33% 34% 45% 21%
4	1D	476	15% 46% 37% 17%

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

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 66812 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	88	Total	C	N	O	S	0	0
			707	484	101	117	5		

- 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	394	Total	C	N	O	S	0	0
			3189	2040	547	580	22		

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	293	Total	C	N	O	S	0	0
			2316	1556	355	384	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		

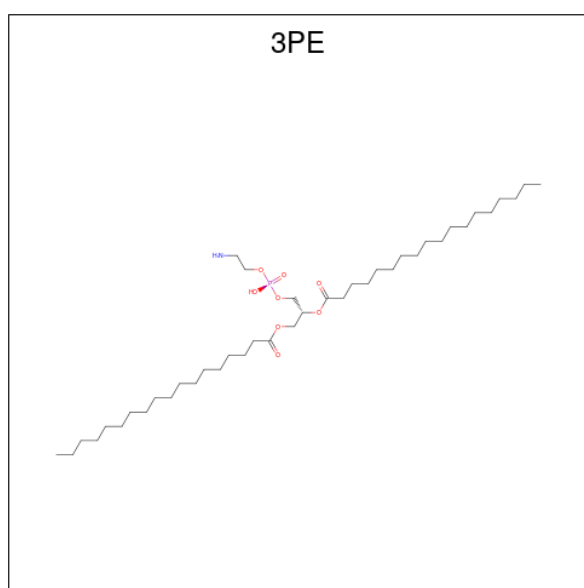
There is a discrepancy between the modelled and reference sequences:

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



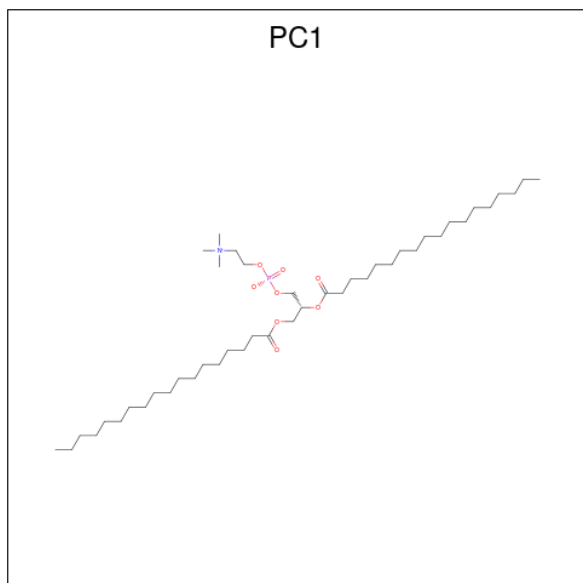
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	

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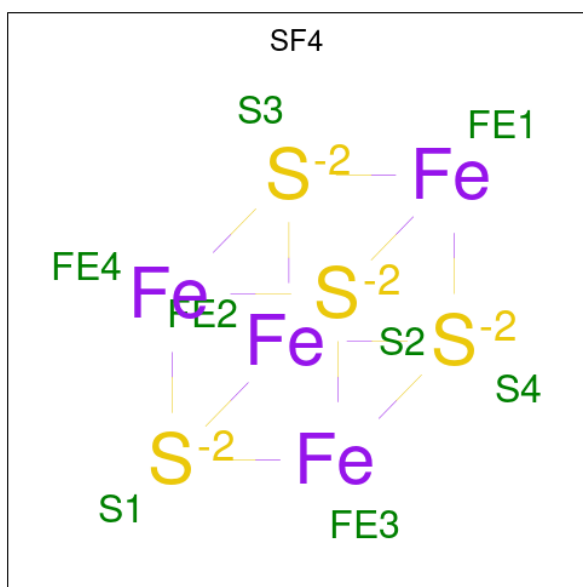
Mol	Chain	Residues	Atoms					AltConf
45	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



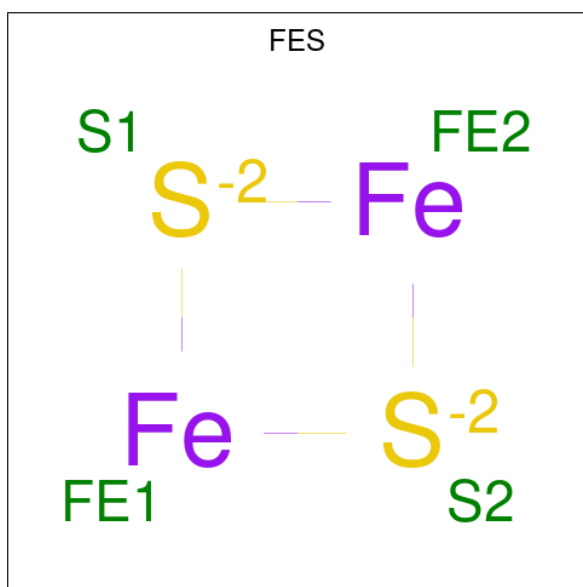
Mol	Chain	Residues	Atoms					AltConf
46	1A	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
46	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
46	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



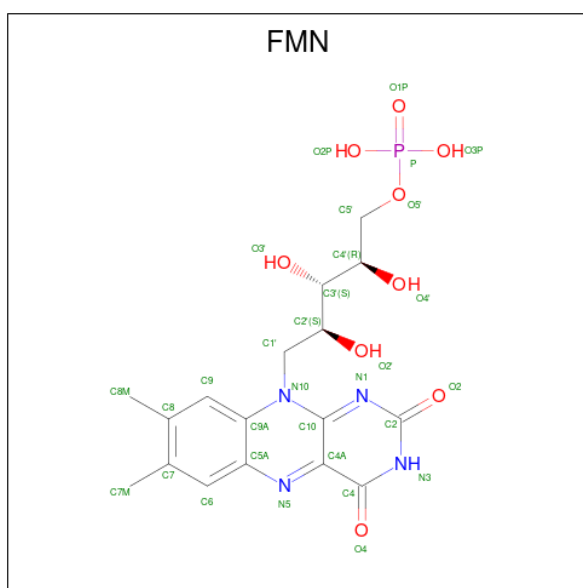
Mol	Chain	Residues	Atoms			AltConf
47	1B	1	Total	Fe	S	0
			8	4	4	
47	1F	1	Total	Fe	S	0
			8	4	4	
47	1G	1	Total	Fe	S	0
			8	4	4	
47	1G	1	Total	Fe	S	0
			8	4	4	
47	1I	1	Total	Fe	S	0
			8	4	4	
47	1I	1	Total	Fe	S	0
			8	4	4	

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



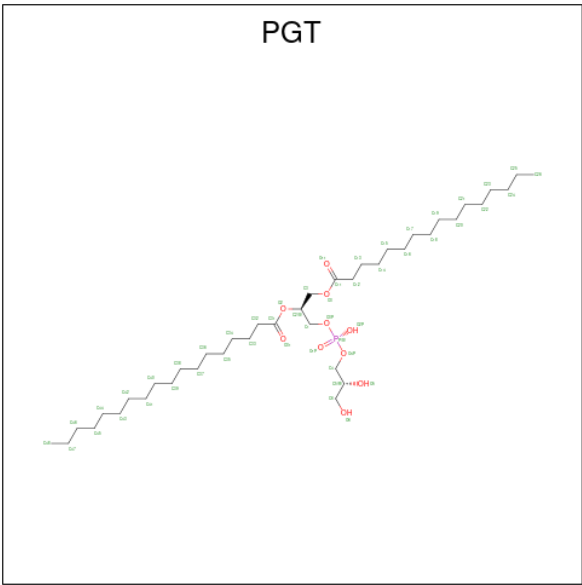
Mol	Chain	Residues	Atoms			AltConf
48	1E	1	Total	Fe	S	0
			4	2	2	
48	1G	1	Total	Fe	S	0
			4	2	2	

- Molecule 49 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



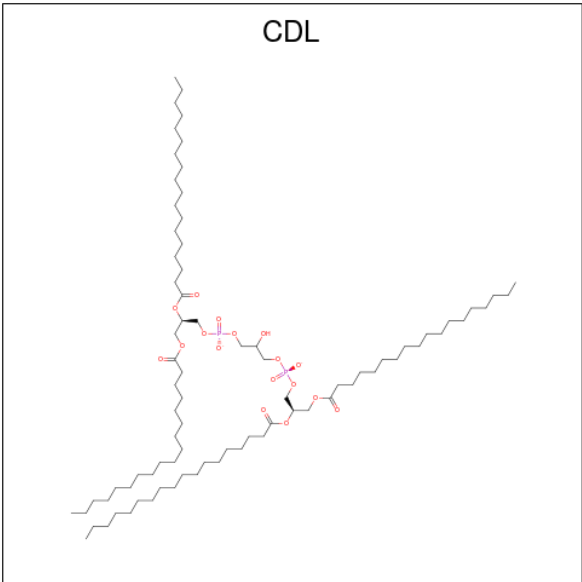
Mol	Chain	Residues	Atoms		AltConf
50	1G	1	Total	K	0
			1	1	

- Molecule 51 is (1S)-2-{{[[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



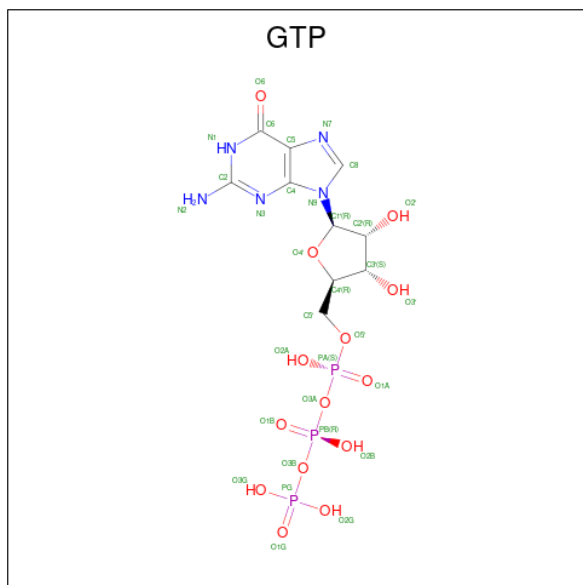
Mol	Chain	Residues	Atoms				AltConf
51	1M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



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

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

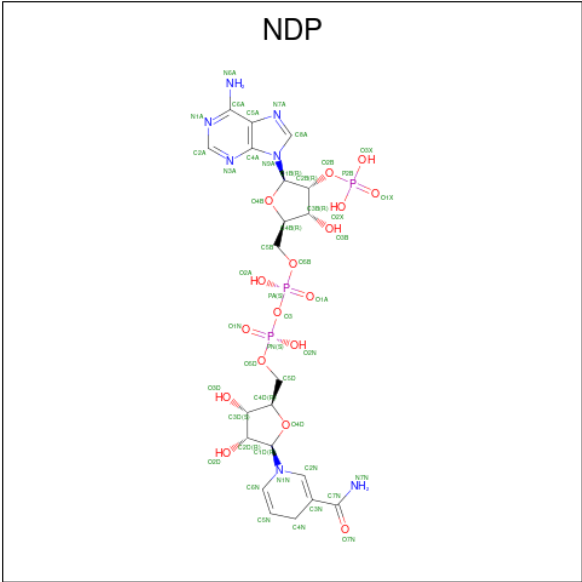


Mol	Chain	Residues	Atoms					AltConf
53	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

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

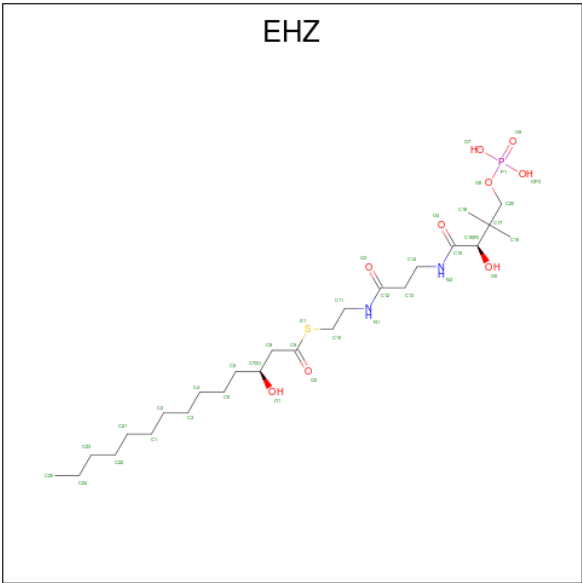


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

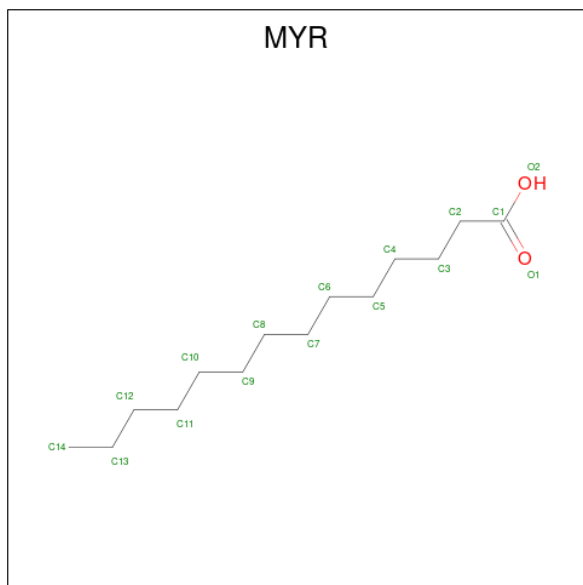
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

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



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

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



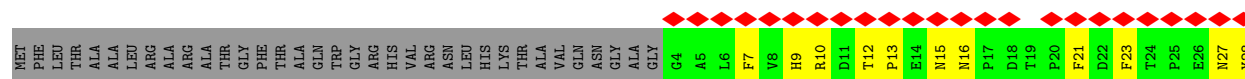
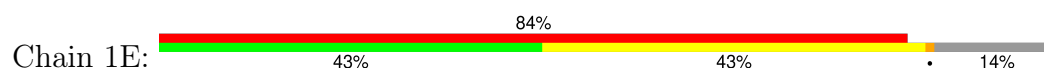
Mol	Chain	Residues	Atoms			AltConf
58	1l	1	Total	C	O	0
			15	14	1	



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

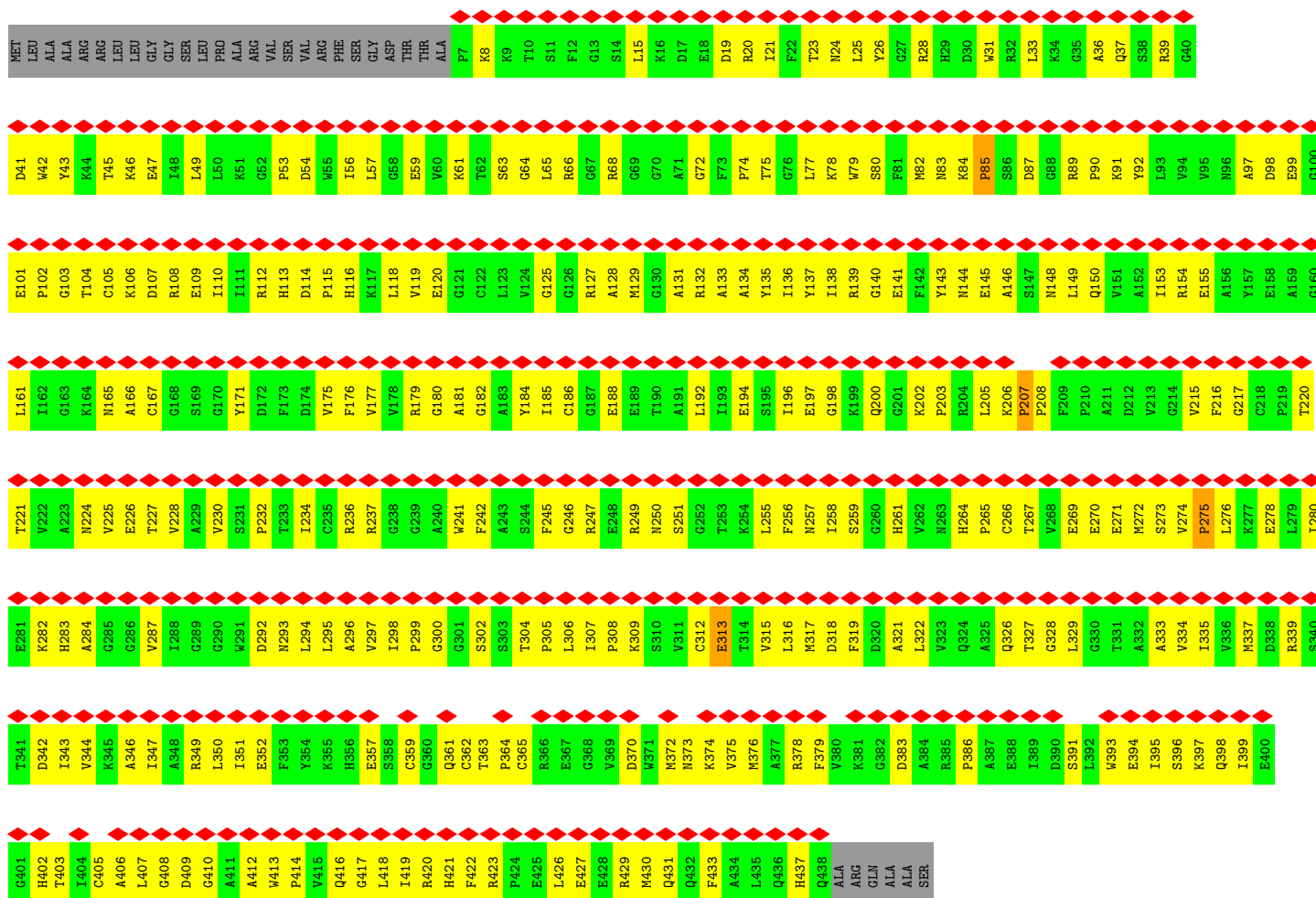
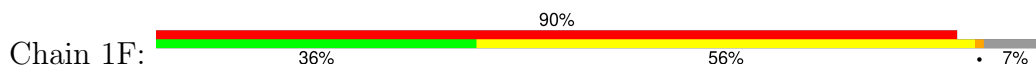


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



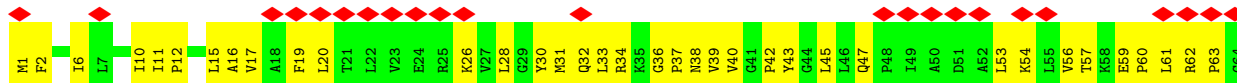
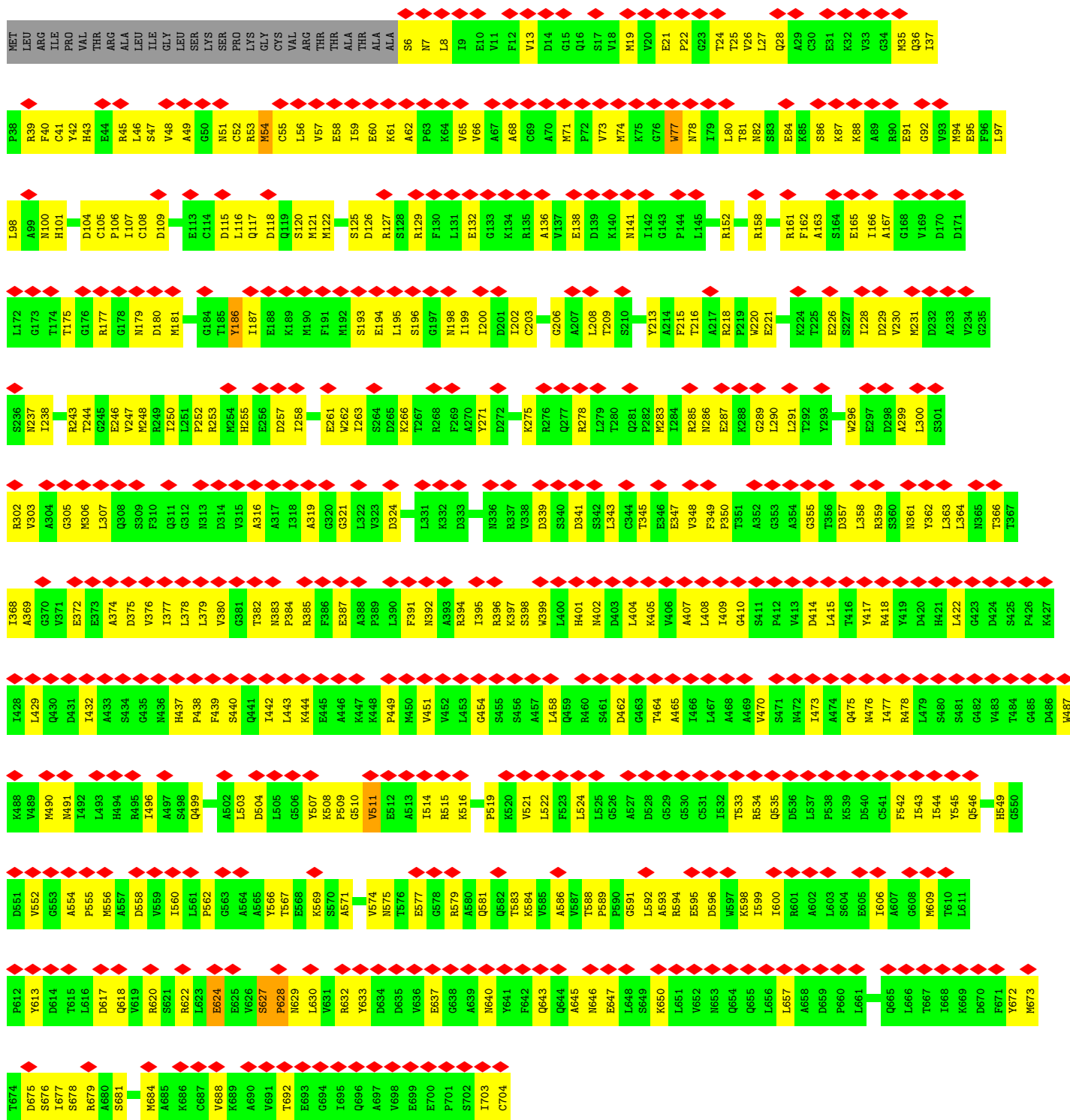


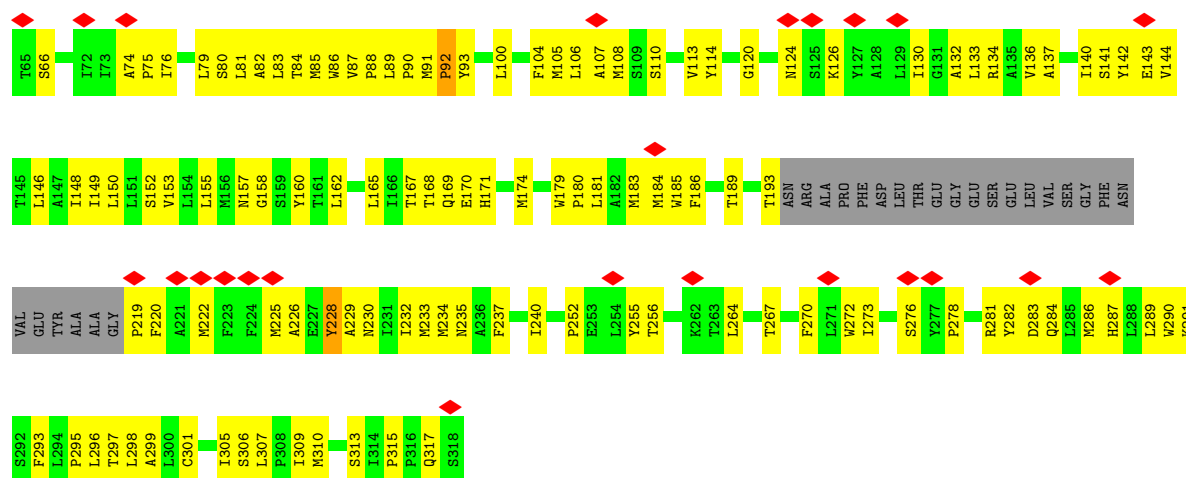
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



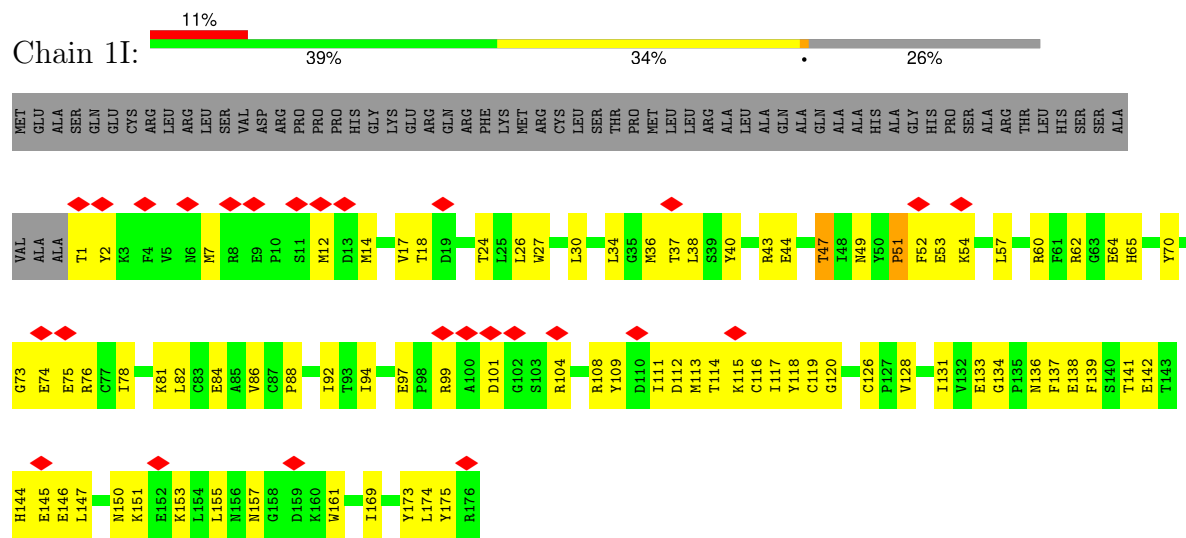
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



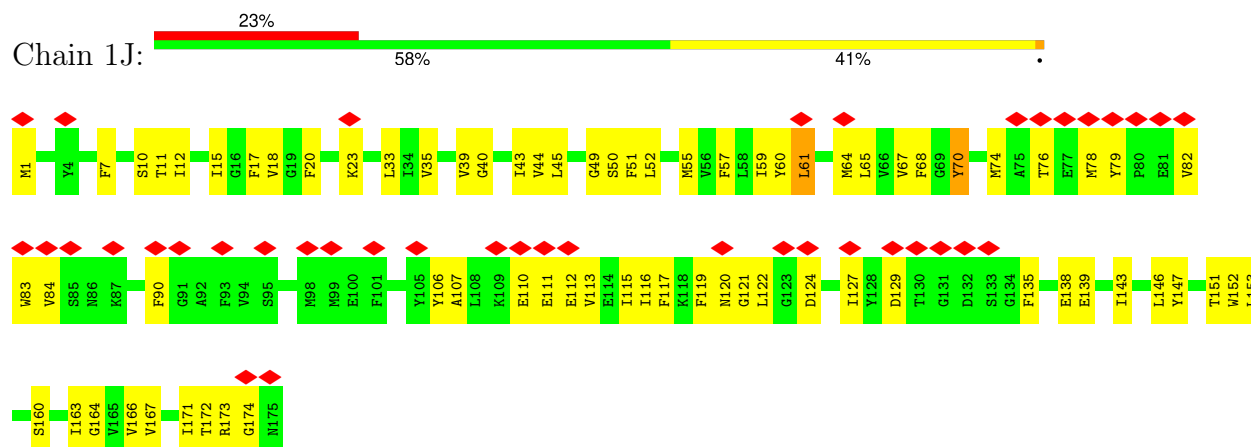




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

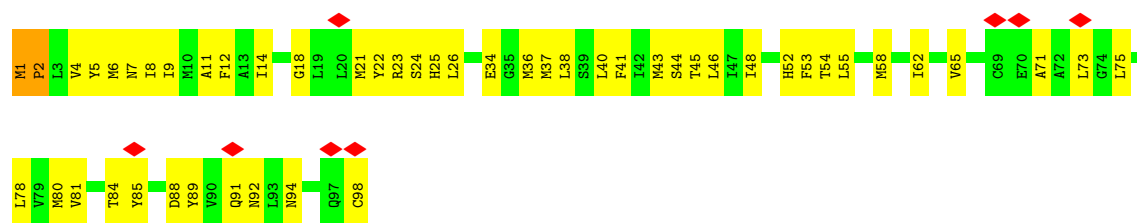


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

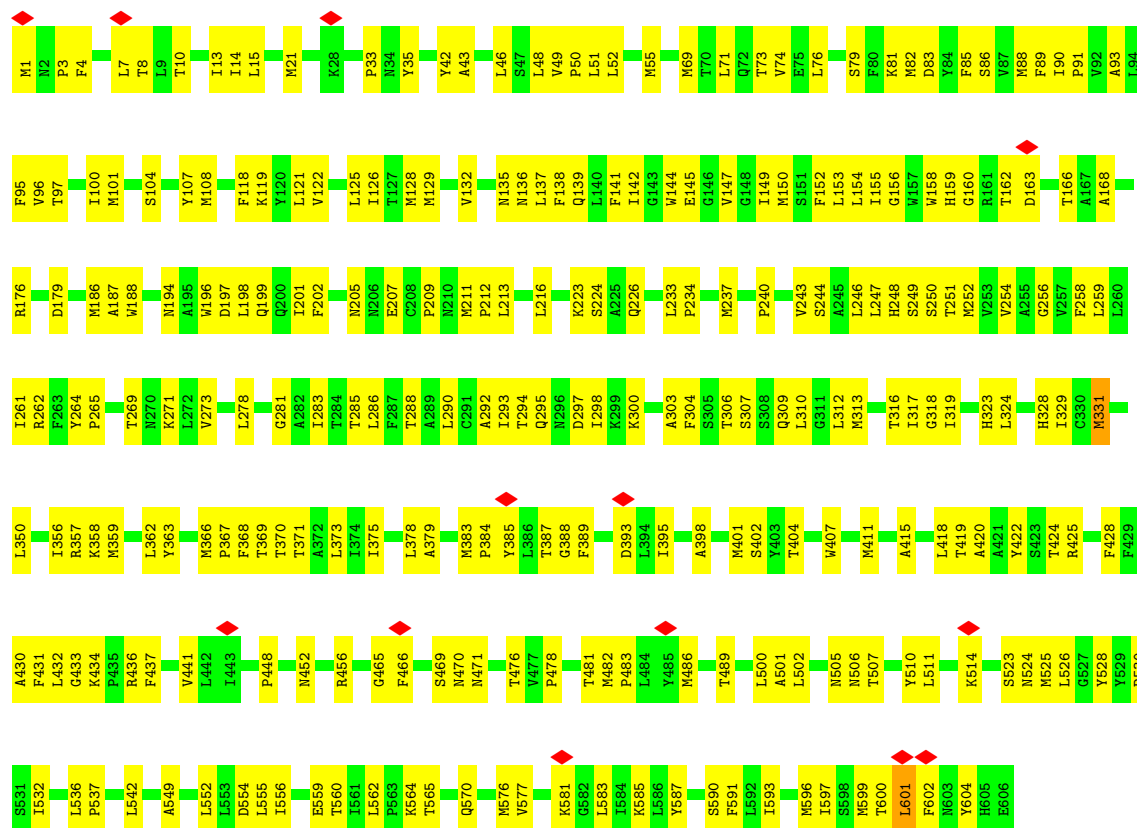


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



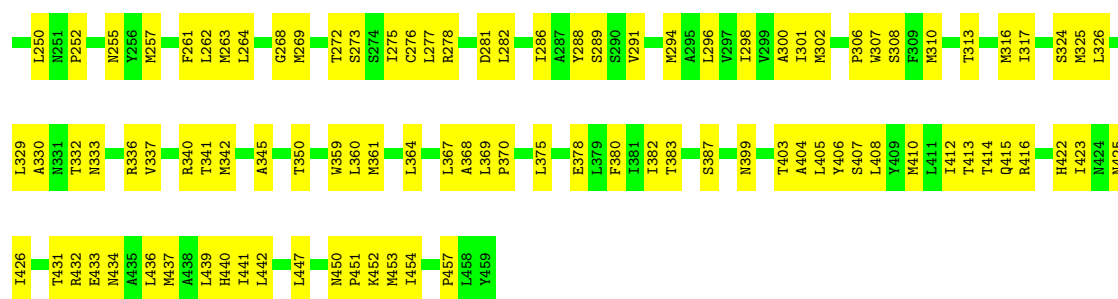


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

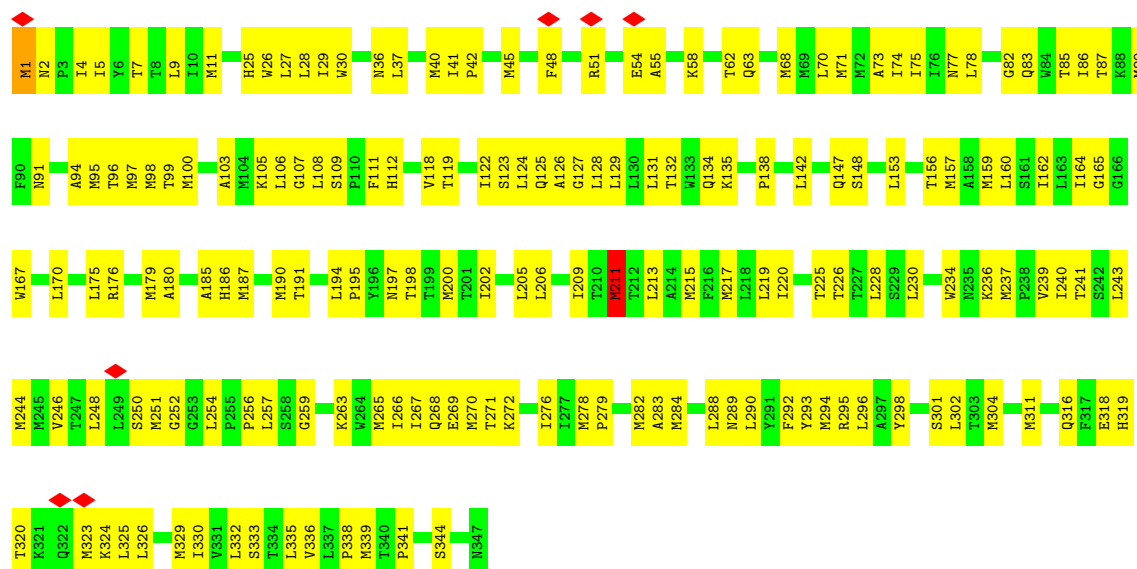


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

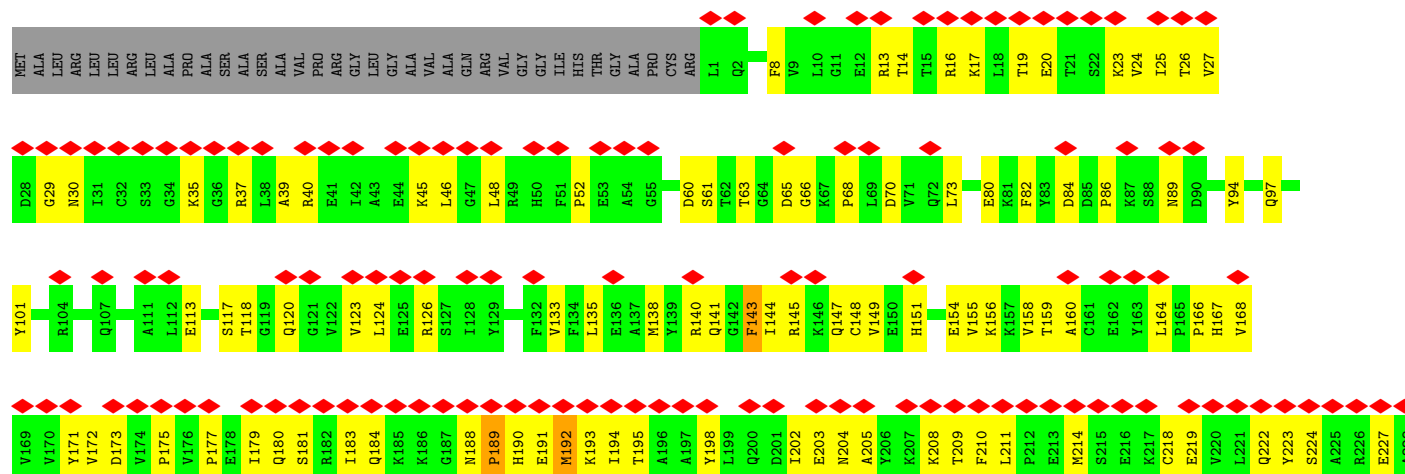




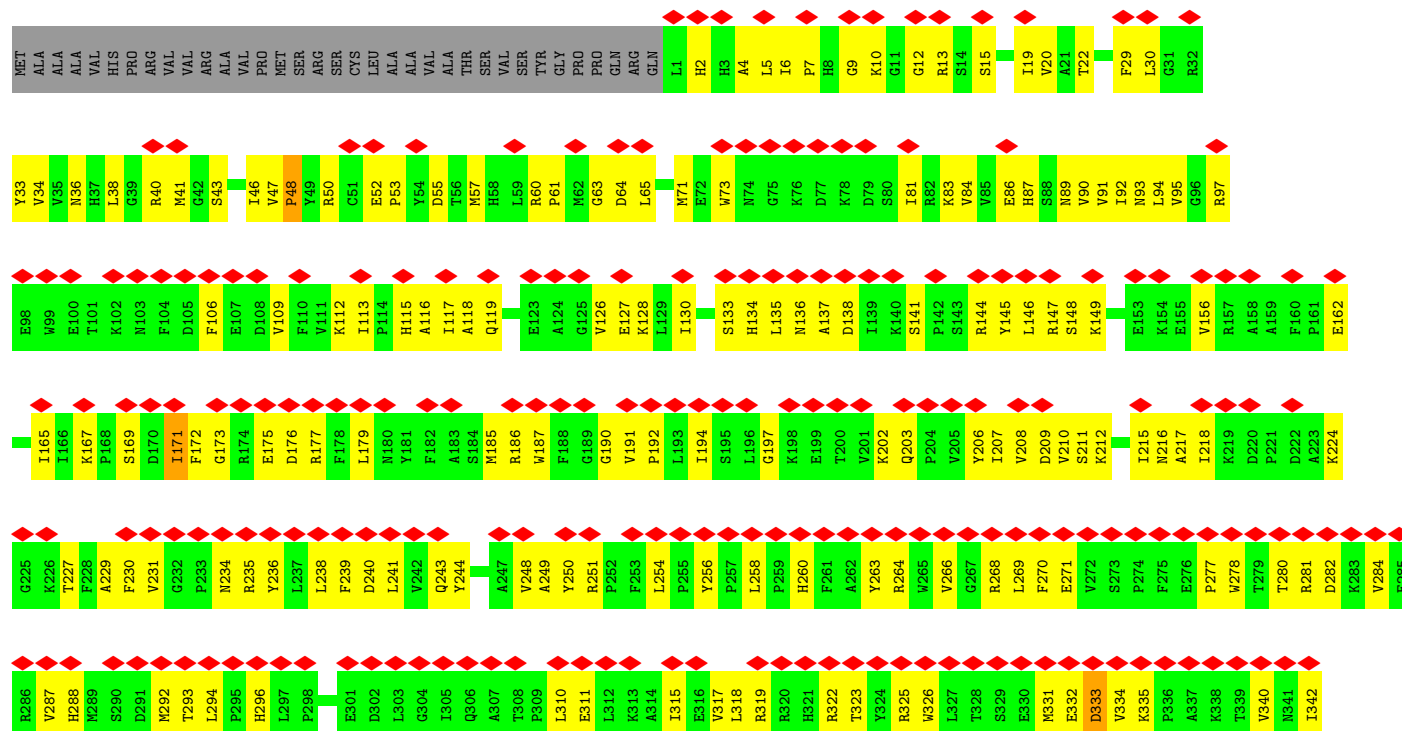
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2



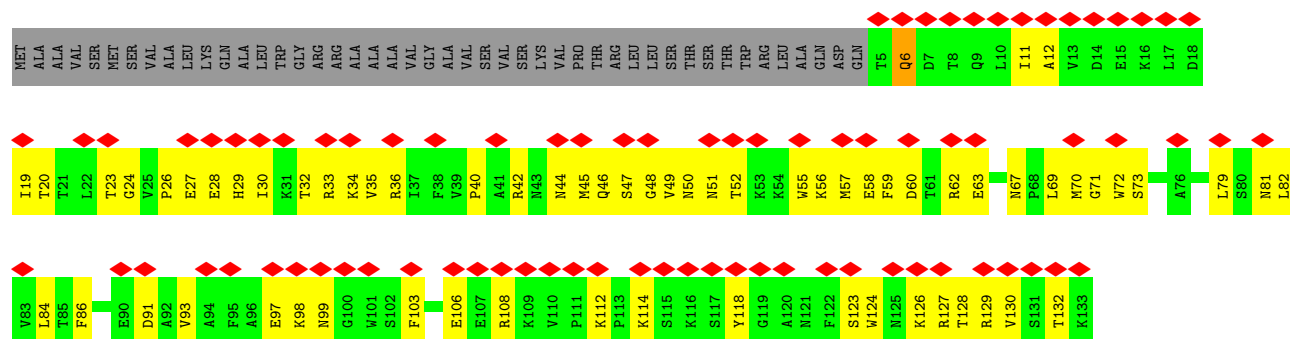
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



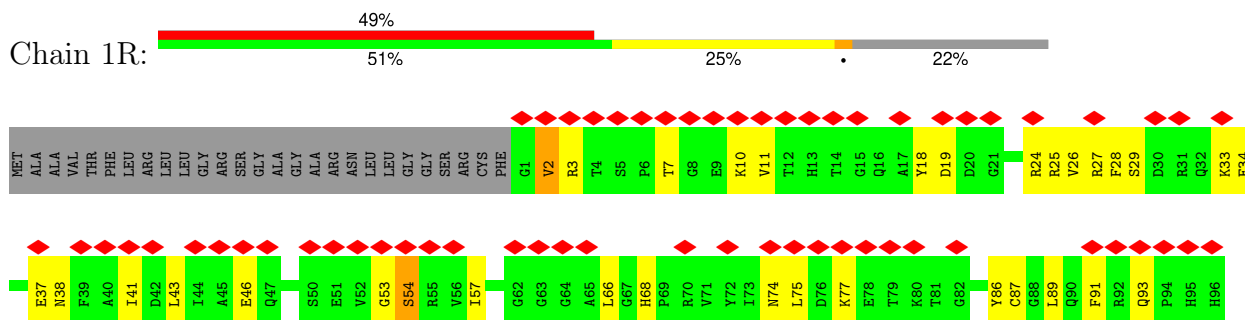
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



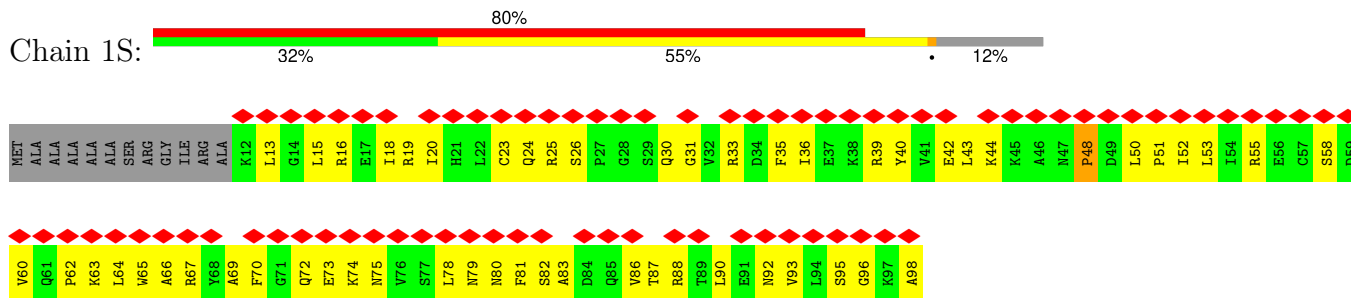
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



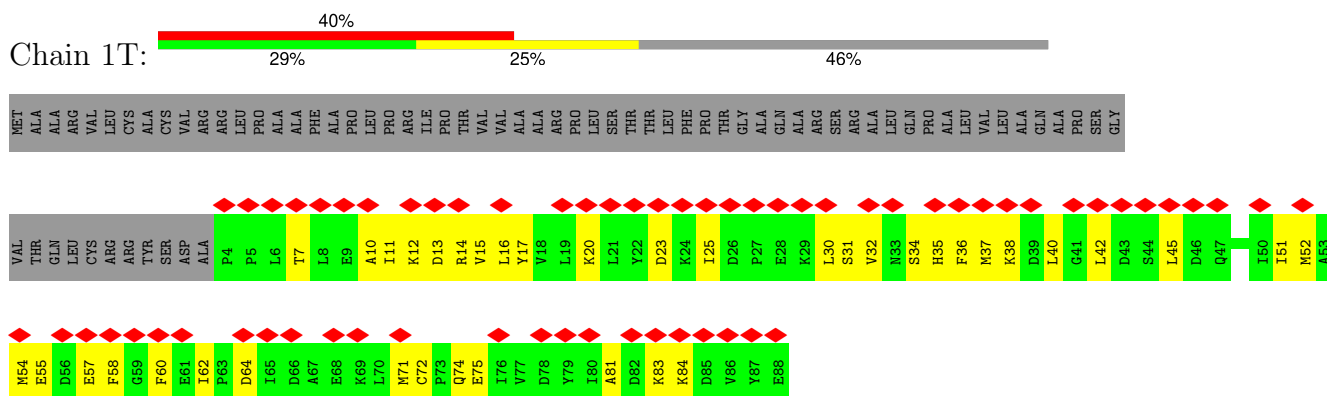
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



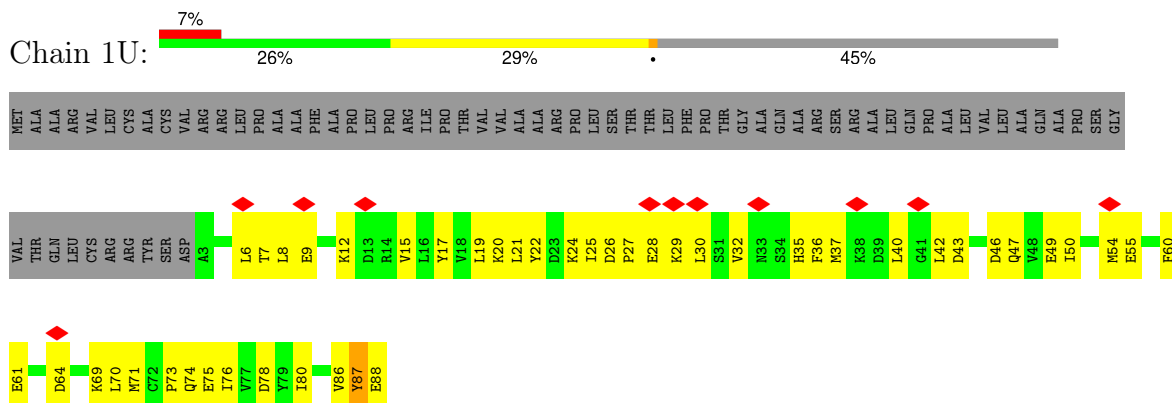
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



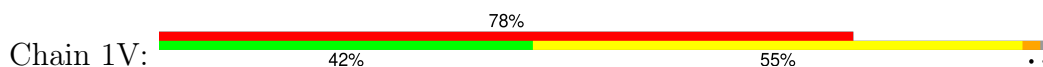
- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

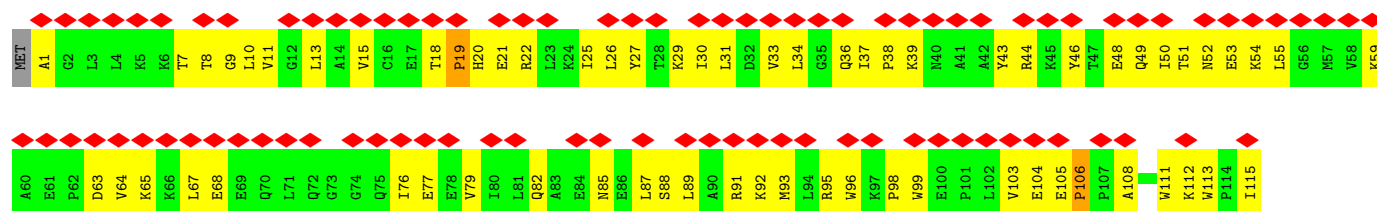


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

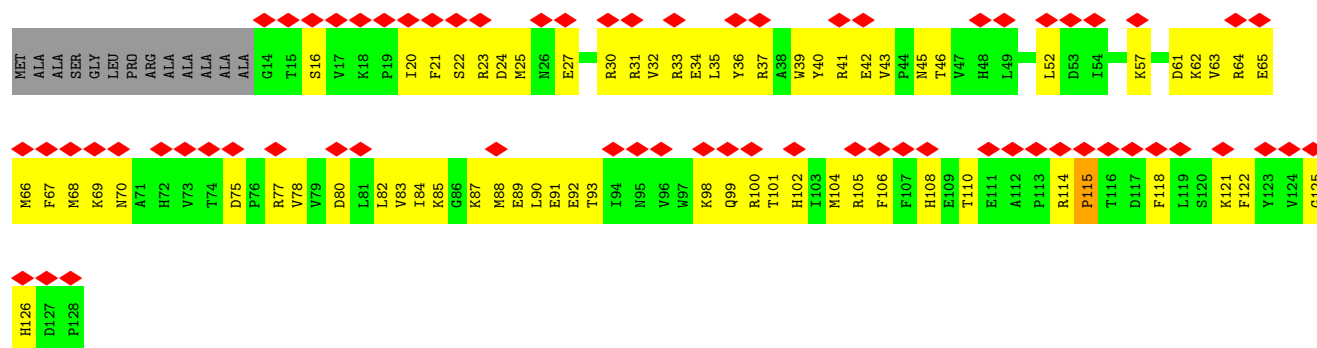


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

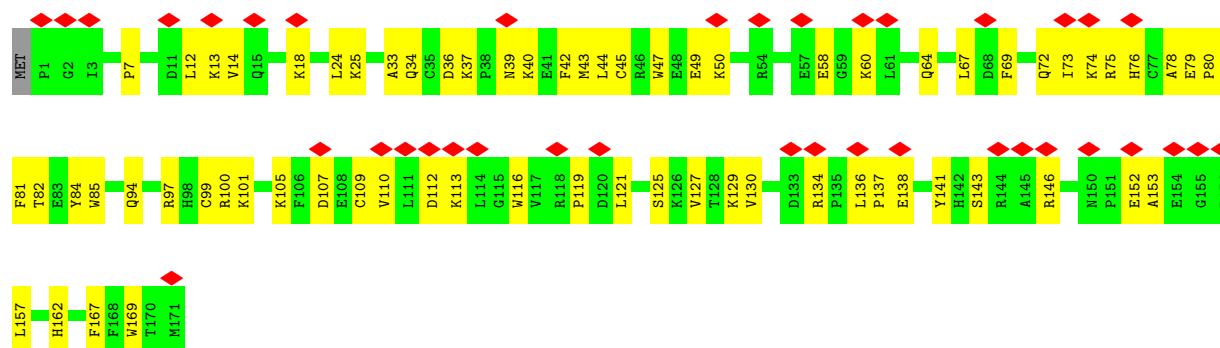




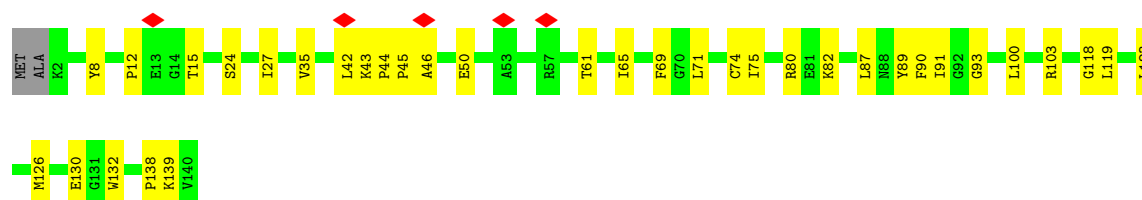
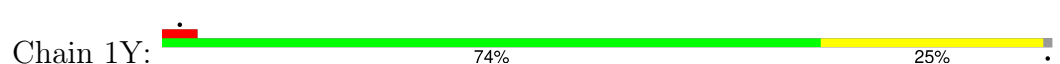
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



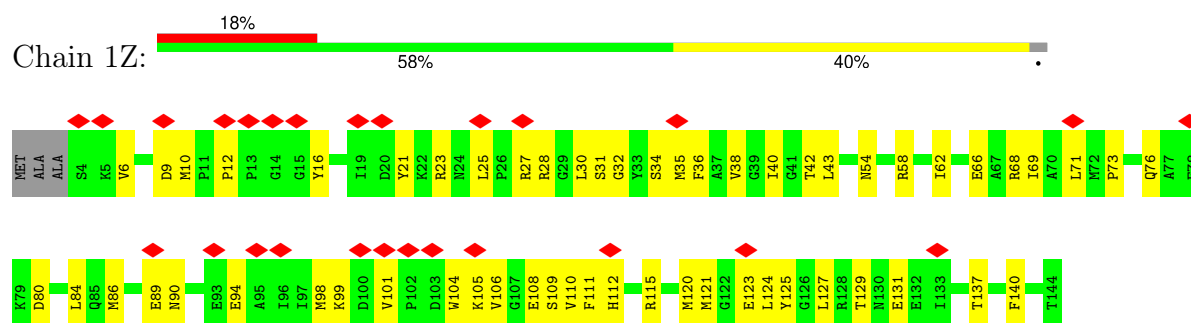
• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



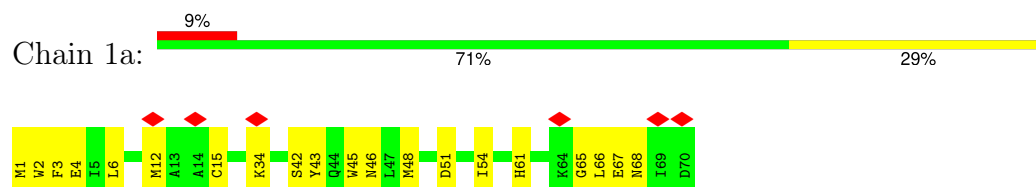
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



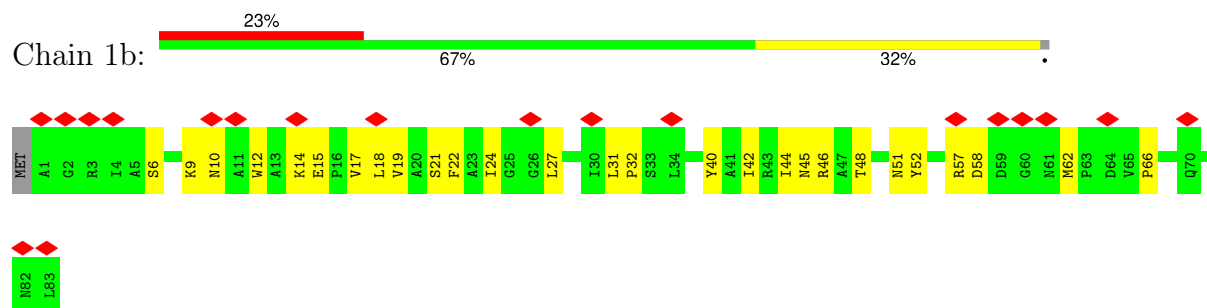
• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



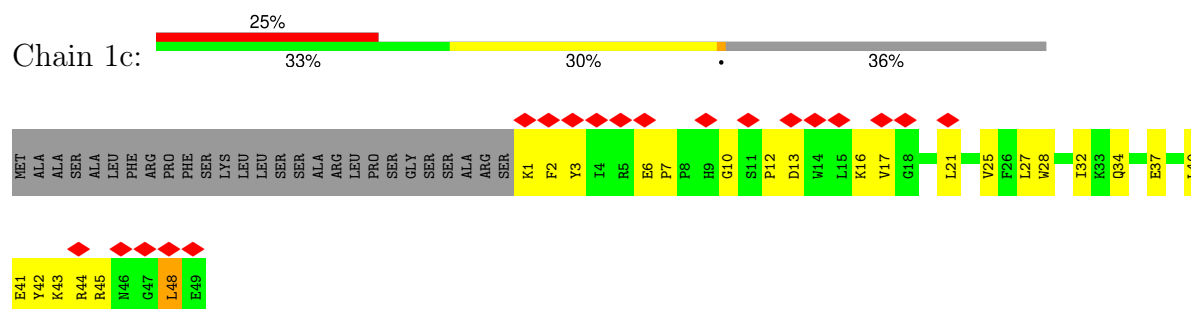
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



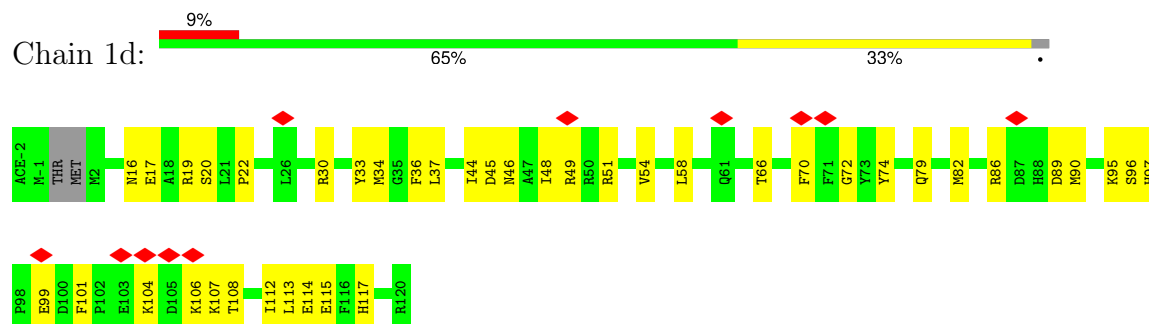
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

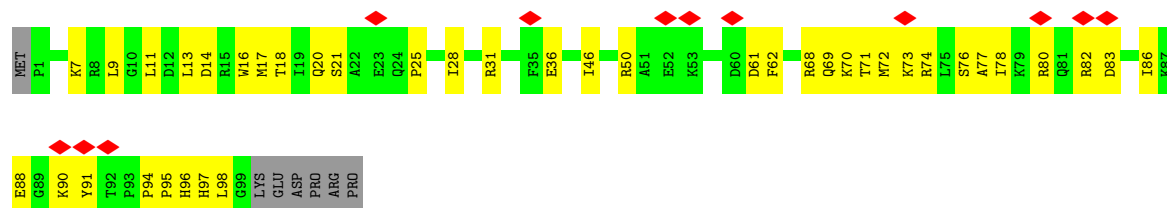


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



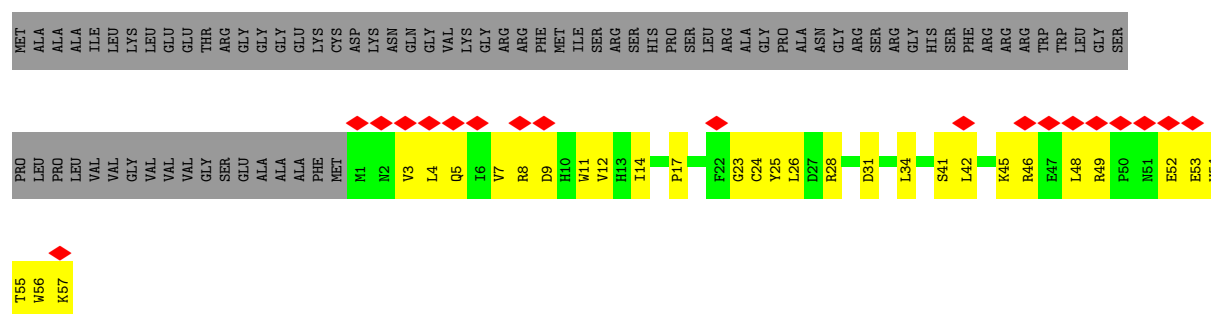
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain 1e: 

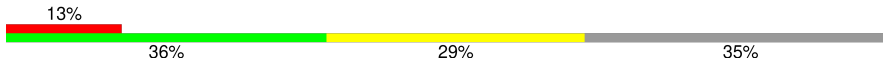


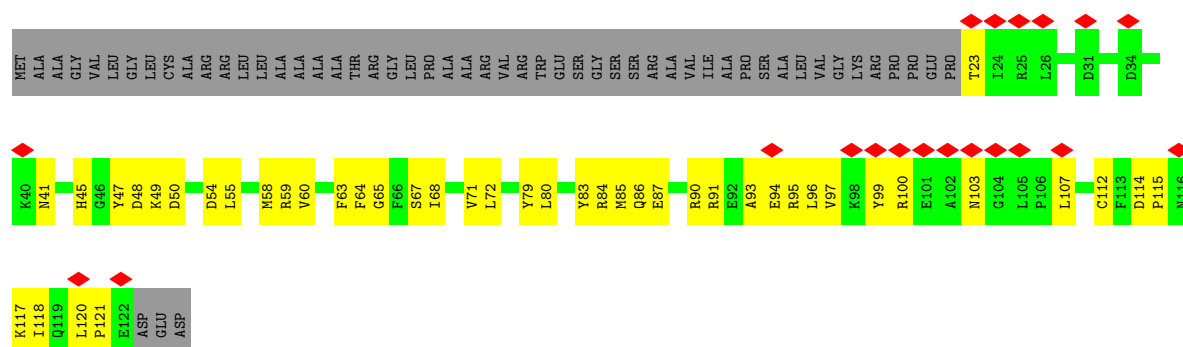
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

Chain 1f: 

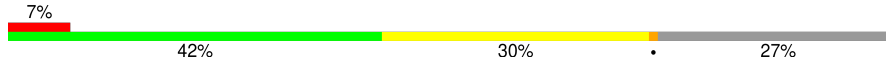


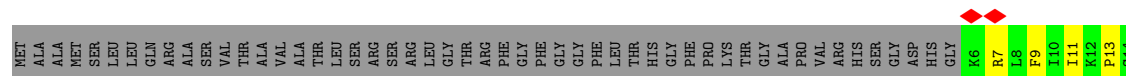
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

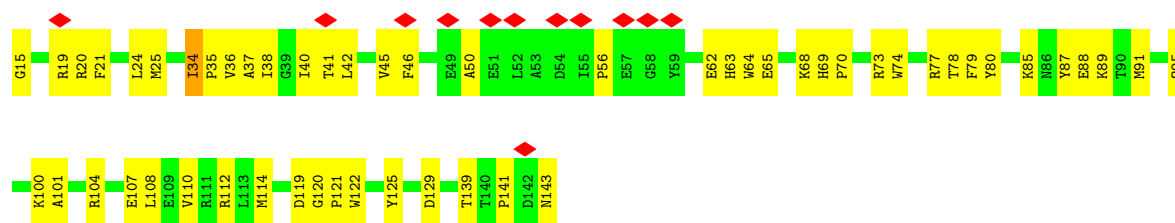
Chain 1g: 



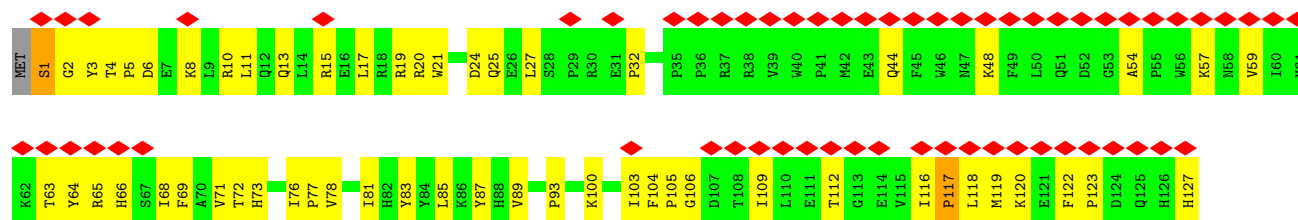
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain 1h: 

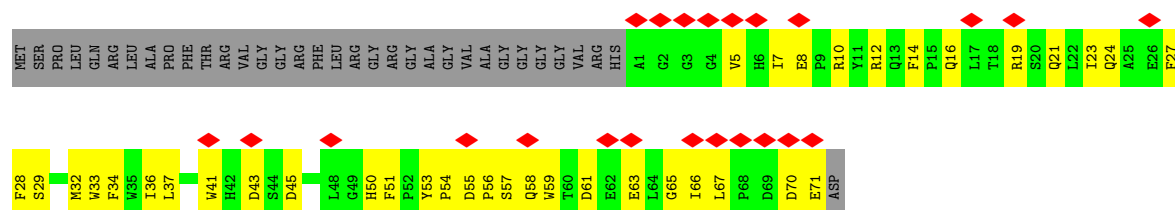




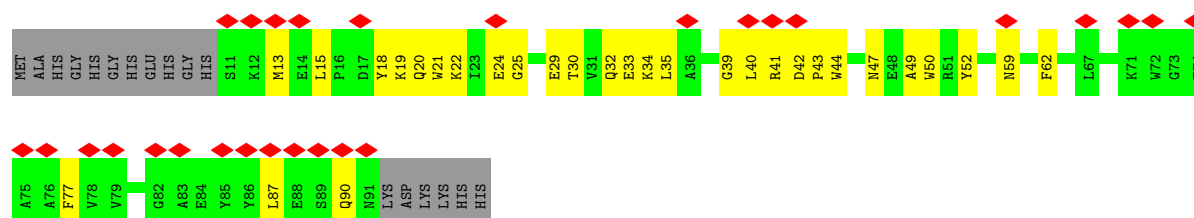
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



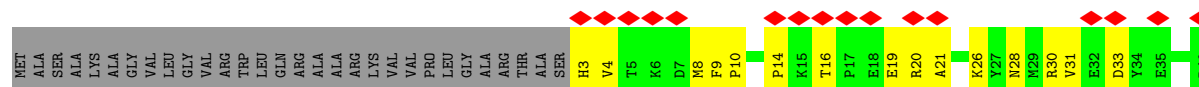
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



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

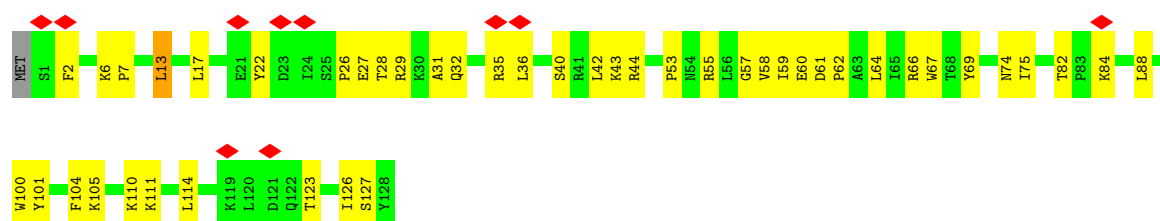


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

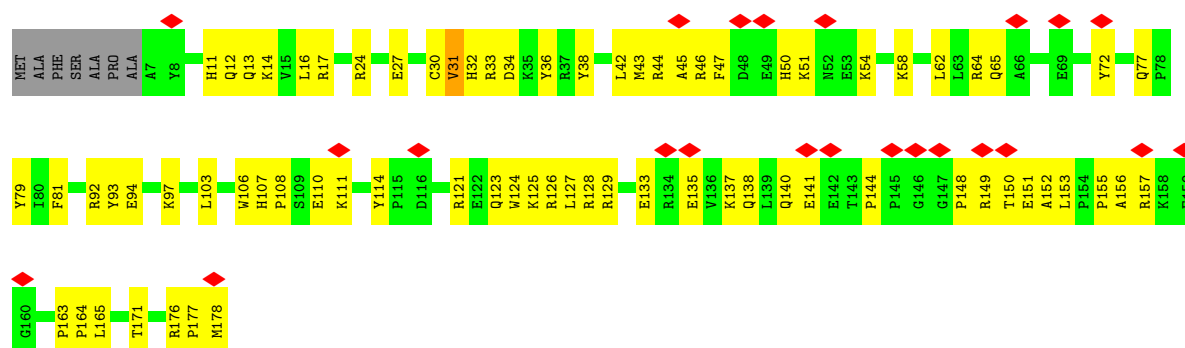




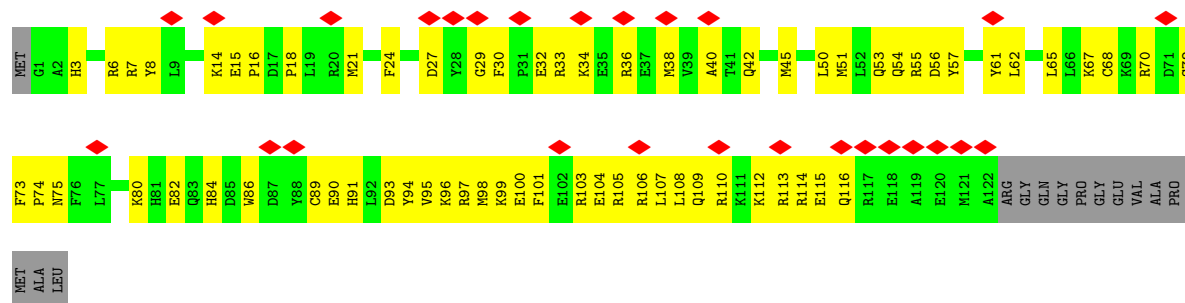
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



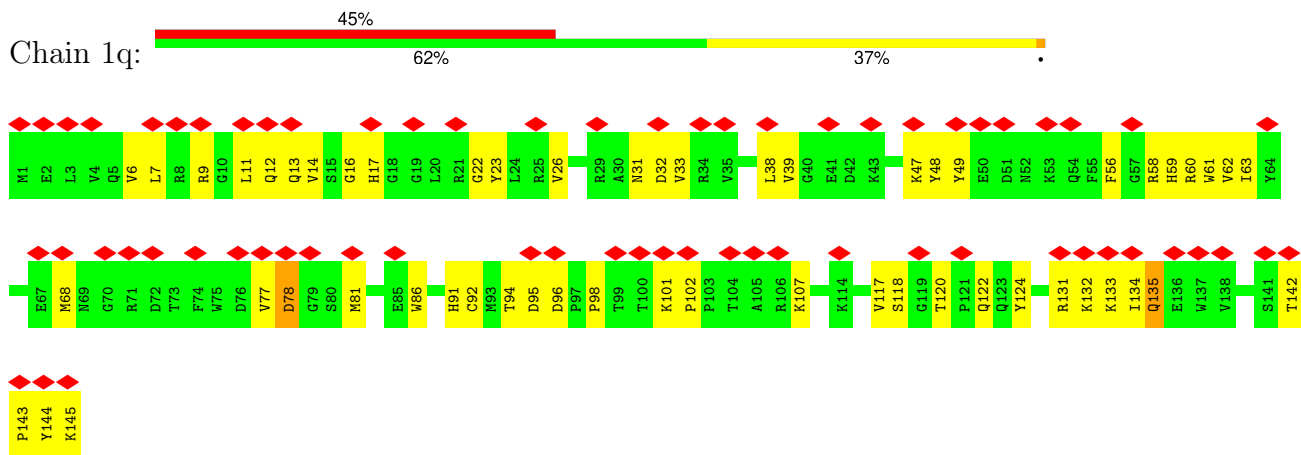
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



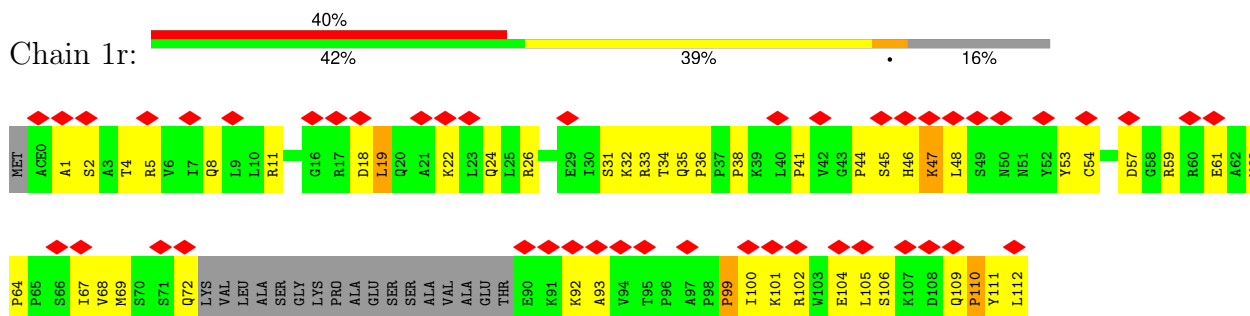
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



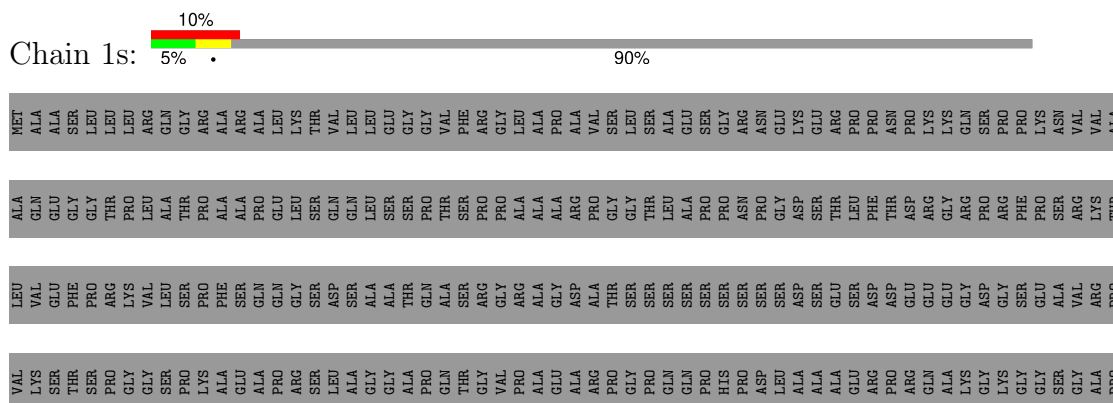
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	29000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	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	0.973	Depositor
Minimum map value	-0.458	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.15	0/713	0.37	0/975
2	1B	0.23	0/1273	0.50	0/1722
3	1C	0.16	0/1791	0.40	0/2439
4	1D	0.17	0/3274	0.37	0/4434
5	1E	0.25	1/1698 (0.1%)	0.45	0/2311
6	1F	0.22	0/3401	0.50	2/4595 (0.0%)
7	1G	0.48	5/5451 (0.1%)	0.63	8/7387 (0.1%)
8	1H	0.28	1/2373 (0.0%)	0.43	0/3244
9	1I	0.21	0/1443	0.50	2/1952 (0.1%)
10	1J	0.24	0/1364	0.39	0/1850
11	1K	0.21	0/751	0.47	0/1018
12	1L	0.15	0/4939	0.39	0/6718
13	1M	0.19	0/3713	0.37	0/5063
14	1N	0.42	2/2765 (0.1%)	0.64	4/3758 (0.1%)
15	1O	0.20	0/2650	0.36	1/3588 (0.0%)
16	1P	0.60	4/2828 (0.1%)	0.76	7/3834 (0.2%)
17	1Q	0.19	0/1070	0.43	0/1446
18	1R	0.21	0/755	0.46	1/1018 (0.1%)
19	1S	0.29	0/711	0.63	1/956 (0.1%)
20	1T	0.20	0/701	0.51	0/946
20	1U	0.25	0/706	0.49	0/954
21	1V	0.31	0/946	0.66	5/1281 (0.4%)
22	1W	0.35	0/995	0.64	1/1340 (0.1%)
23	1X	0.14	0/1436	0.36	0/1938
24	1Y	0.09	0/1037	0.28	0/1404
25	1Z	0.17	0/1199	0.37	0/1617
26	1a	0.13	0/577	0.36	0/777
27	1b	0.17	0/664	0.38	0/912
28	1c	0.11	0/430	0.29	0/581
29	1d	0.13	0/1024	0.31	0/1383
30	1e	0.12	0/836	0.32	0/1118
31	1f	0.14	0/499	0.41	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.17	0/858	0.38	0/1165
33	1h	0.16	0/1184	0.35	0/1603
34	1i	0.22	0/1131	0.58	2/1541 (0.1%)
35	1j	0.15	0/627	0.38	0/858
36	1k	0.14	0/668	0.37	0/903
37	1l	0.22	0/1365	0.38	0/1867
38	1m	0.14	0/1092	0.32	0/1481
39	1n	0.20	0/1549	0.33	0/2098
40	1o	0.19	0/1069	0.42	0/1430
41	1p	0.14	0/1481	0.29	0/1997
42	1q	0.18	0/1253	0.43	0/1704
43	1r	0.36	1/782 (0.1%)	0.71	2/1057 (0.2%)
44	1s	0.28	0/394	0.76	1/533 (0.2%)
All	All	0.27	14/67466 (0.0%)	0.48	37/91469 (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	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1G	628	PRO	CG-CD	-23.83	0.69	1.50
16	1P	48	PRO	CG-CD	-23.00	0.72	1.50
7	1G	628	PRO	CB-CG	16.20	2.30	1.49
16	1P	48	PRO	CB-CG	15.73	2.28	1.49
14	1N	11	MET	CG-SD	-13.35	1.47	1.80
14	1N	11	MET	SD-CE	12.01	2.09	1.79
7	1G	627	SER	C-N	9.72	1.46	1.34
7	1G	628	PRO	CA-CB	-8.05	1.40	1.53
16	1P	47	VAL	C-N	6.18	1.48	1.33
16	1P	48	PRO	N-CD	5.84	1.55	1.47
8	1H	228	TYR	CZ-OH	-5.59	1.26	1.38
7	1G	628	PRO	N-CA	-5.44	1.40	1.47
43	1r	47	LYS	CE-NZ	-5.25	1.33	1.49
5	1E	55	GLN	CD-NE2	-5.24	1.22	1.33

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	1G	628	PRO	CB-CG-CD	-33.13	0.07	106.10
14	1N	11	MET	CG-SD-CE	-27.56	40.27	100.90
16	1P	48	PRO	CB-CG-CD	-23.73	30.18	106.10
16	1P	48	PRO	N-CD-CG	-16.41	78.59	103.20
7	1G	628	PRO	CA-N-CD	-15.75	89.95	112.00
16	1P	48	PRO	CA-N-CD	-14.53	91.66	112.00
34	1i	117	PRO	CA-N-CD	-13.49	93.12	112.00
16	1P	48	PRO	N-CA-CB	-12.14	90.51	103.25
44	1s	64	PRO	CA-N-CD	-10.95	96.67	112.00
16	1P	48	PRO	CA-CB-CG	-10.52	84.51	104.50
6	1F	275	PRO	CA-N-CD	-10.39	97.45	112.00
7	1G	628	PRO	CA-CB-CG	-10.26	85.00	104.50
9	1I	51	PRO	CA-N-CD	-9.74	97.86	111.50
7	1G	628	PRO	N-CA-CB	-9.64	94.50	103.46
21	1V	106	PRO	CA-N-CD	-9.35	98.92	112.00
6	1F	85	PRO	CA-N-CD	-8.98	99.42	112.00
43	1r	110	PRO	CA-N-CD	-8.42	100.21	112.00
15	1O	189	PRO	CA-N-CD	-8.03	100.75	112.00
22	1W	115	PRO	CA-N-CD	-7.03	102.16	112.00
7	1G	54	MET	CG-SD-CE	-6.86	85.81	100.90
14	1N	211	MET	CG-SD-CE	-6.85	85.83	100.90
7	1G	627	SER	C-N-CD	6.72	152.54	125.00
21	1V	19	PRO	CA-N-CD	-6.71	102.61	112.00
16	1P	7	PRO	CA-N-CD	-6.55	102.83	112.00
7	1G	627	SER	CA-C-O	-6.49	111.27	120.16
34	1i	117	PRO	N-CD-CG	-6.49	93.47	103.20
43	1r	99	PRO	CA-N-CD	-6.44	102.99	112.00
7	1G	511	VAL	N-CA-C	-5.86	107.58	113.20
14	1N	11	MET	N-CA-CB	5.73	118.74	110.20
9	1I	47	THR	CA-CB-CG2	-5.56	101.05	110.50
14	1N	259	GLY	N-CA-C	-5.51	107.68	113.58
21	1V	108	ALA	CB-CA-C	-5.28	110.47	116.54
16	1P	47	VAL	N-CA-CB	-5.24	103.88	111.21
18	1R	2	VAL	CA-CB-CG1	-5.13	101.68	110.40
21	1V	105	GLU	CA-C-N	-5.11	115.98	119.66
21	1V	105	GLU	C-N-CA	-5.11	115.98	119.66
19	1S	48	PRO	CA-N-CD	-5.04	104.94	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	207	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	707	0	755	47	0
2	1B	1242	0	1249	99	0
3	1C	1740	0	1691	134	0
4	1D	3189	0	3121	191	0
5	1E	1658	0	1662	118	0
6	1F	3325	0	3288	269	0
7	1G	5362	0	5387	333	0
8	1H	2316	0	2434	179	0
9	1I	1412	0	1364	89	0
10	1J	1339	0	1337	91	0
11	1K	750	0	798	56	0
12	1L	4818	0	4956	234	0
13	1M	3632	0	3836	220	0
14	1N	2712	0	2873	168	0
15	1O	2590	0	2556	124	0
16	1P	2751	0	2776	159	0
17	1Q	1047	0	1042	70	0
18	1R	741	0	704	34	0
19	1S	700	0	719	67	0
20	1T	689	0	687	47	0
20	1U	694	0	691	48	0
21	1V	927	0	972	80	0
22	1W	971	0	975	98	0
23	1X	1398	0	1378	63	0
24	1Y	1016	0	1020	29	0
25	1Z	1168	0	1161	63	0
26	1a	562	0	557	25	0
27	1b	643	0	645	28	0
28	1c	417	0	425	27	0
29	1d	996	0	990	42	0
30	1e	816	0	823	52	0
31	1f	487	0	496	31	0
32	1g	835	0	795	42	0
33	1h	1151	0	1164	70	0
34	1i	1100	0	1106	57	0
35	1j	601	0	546	45	0
36	1k	649	0	626	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	1l	1310	0	1204	70	0
38	1m	1062	0	1075	53	0
39	1n	1495	0	1434	78	0
40	1o	1045	0	1018	74	0
41	1p	1449	0	1416	61	0
42	1q	1212	0	1172	69	0
43	1r	767	0	791	71	0
44	1s	382	0	351	36	0
45	1A	47	0	71	2	0
45	1L	88	0	127	8	0
45	1N	51	0	79	2	0
45	1Y	82	0	118	11	0
46	1A	35	0	42	1	0
46	1I	98	0	147	9	0
46	1L	44	0	65	4	0
46	1f	46	0	69	6	0
47	1B	8	0	0	2	0
47	1F	8	0	0	1	0
47	1G	16	0	0	2	0
47	1I	16	0	0	1	0
48	1E	4	0	0	2	0
48	1G	4	0	0	1	0
49	1F	31	0	19	0	0
50	1G	1	0	0	1	0
51	1M	51	0	78	8	0
52	1N	77	0	98	6	0
52	1q	61	0	66	11	0
53	1O	32	0	12	0	0
54	1O	1	0	0	0	0
55	1P	48	0	26	6	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	66812	0	67110	3413	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 (3413) 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)
52:1N:402:CDL:C14	52:1N:402:CDL:C15	1.79	1.58
7:1G:628:PRO:N	7:1G:628:PRO:CG	1.72	1.42
7:1G:54:MET:HE1	7:1G:94:MET:HB2	1.18	1.18
8:1H:20:LEU:HB3	8:1H:228:TYR:OH	1.50	1.10
7:1G:628:PRO:CG	7:1G:628:PRO:CB	2.30	1.08
16:1P:19:ILE:HD12	16:1P:218:ILE:HG21	1.35	1.08
15:1O:138:MET:HG2	15:1O:144:ILE:HG12	1.36	1.07
14:1N:89:MET:HE2	14:1N:95:MET:HE2	1.34	1.05
6:1F:343:ILE:HD13	6:1F:418:LEU:HD21	1.34	1.02
12:1L:525:MET:HE3	12:1L:528:TYR:HE1	1.20	1.01
7:1G:628:PRO:CD	7:1G:628:PRO:HG3	1.49	0.99
7:1G:628:PRO:CD	7:1G:628:PRO:HG2	1.49	0.99
16:1P:194:ILE:HD11	16:1P:263:TYR:HD2	1.30	0.97
6:1F:82:MET:SD	6:1F:91:LYS:NZ	2.38	0.96
17:1Q:97:GLU:OE1	17:1Q:97:GLU:N	1.99	0.96
14:1N:147:GLN:HB3	33:1h:125:TYR:CE1	2.02	0.94
5:1E:55:GLN:HE22	5:1E:56:ARG:CZ	1.80	0.94
11:1K:62:ILE:HA	11:1K:65:VAL:HG12	1.46	0.93
20:1T:52:MET:HA	20:1T:55:GLU:HG2	1.51	0.93
5:1E:155:GLN:NE2	5:1E:157:ASN:O	2.04	0.91
7:1G:628:PRO:CG	7:1G:628:PRO:HD2	1.40	0.91
21:1V:19:PRO:HD2	21:1V:20:HIS:H	1.35	0.91
7:1G:628:PRO:CG	7:1G:628:PRO:HD3	1.40	0.90
8:1H:17:VAL:HG13	8:1H:228:TYR:HD2	1.37	0.90
2:1B:172:ARG:HD2	2:1B:172:ARG:C	1.95	0.89
7:1G:196:SER:O	7:1G:199:ILE:HG22	1.71	0.89
13:1M:158:LEU:HD12	14:1N:283:ALA:HB1	1.52	0.89
12:1L:525:MET:HE3	12:1L:528:TYR:CE1	2.07	0.89
11:1K:36:MET:HE2	14:1N:68:MET:HE2	1.56	0.88
15:1O:82:PHE:HE1	15:1O:143:PHE:CE2	1.91	0.88
6:1F:200:GLN:NE2	6:1F:202:LYS:HD2	1.89	0.88
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.55	0.87
7:1G:228:ILE:HD13	7:1G:581:GLN:HB2	1.55	0.87
2:1B:81:ARG:HD2	2:1B:81:ARG:O	1.72	0.87
43:1r:110:PRO:HD2	43:1r:111:TYR:H	1.40	0.87
7:1G:243:ARG:HD3	7:1G:244:THR:HG22	1.57	0.86
11:1K:62:ILE:HD11	14:1N:27:LEU:HD21	1.56	0.85
3:1C:131:GLU:OE2	3:1C:145:HIS:NE2	2.10	0.84
15:1O:37:ARG:HH12	15:1O:229:GLU:HA	1.42	0.84
16:1P:19:ILE:HG23	16:1P:43:SER:HB3	1.59	0.84
16:1P:202:LYS:NZ	16:1P:287:VAL:O	2.09	0.84
14:1N:2:ASN:HB3	14:1N:5:ILE:HG13	1.60	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:55:GLN:HE22	5:1E:56:ARG:NH2	1.76	0.83
20:1T:45:LEU:HB3	22:1W:36:TYR:HE2	1.43	0.83
13:1M:282:LEU:HD23	13:1M:342:MET:HE1	1.58	0.83
46:1I:204:PC1:H142	25:1Z:35:MET:HE1	1.59	0.83
17:1Q:79:LEU:HD13	17:1Q:82:LEU:HD12	1.62	0.82
4:1D:161:ILE:HG23	4:1D:238:ARG:HH11	1.42	0.82
19:1S:13:LEU:HA	19:1S:69:ALA:HB3	1.61	0.82
3:1C:40:VAL:HG12	43:1r:69:MET:HE3	1.61	0.82
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.60	0.82
13:1M:325:MET:HE1	13:1M:441:ILE:HG12	1.61	0.82
9:1I:74:GLU:OE1	9:1I:75:GLU:N	2.13	0.81
43:1r:101:LYS:HD3	43:1r:101:LYS:H	1.45	0.81
6:1F:42:TRP:CE3	6:1F:161:LEU:HD22	2.15	0.81
15:1O:138:MET:HG3	15:1O:143:PHE:HB3	1.60	0.81
37:1l:131:LYS:HG3	37:1l:133:TYR:CE1	2.15	0.81
6:1F:153:ILE:HD11	6:1F:175:VAL:HG23	1.62	0.81
16:1P:244:TYR:OH	16:1P:311:GLU:OE1	1.99	0.81
7:1G:628:PRO:CG	7:1G:628:PRO:CA	2.59	0.80
3:1C:22:LEU:HB3	3:1C:48:LEU:HD21	1.63	0.80
4:1D:405:MET:SD	4:1D:421:GLN:NE2	2.54	0.80
19:1S:24:GLN:HA	19:1S:33:ARG:HE	1.47	0.80
22:1W:66:MET:HB3	22:1W:69:LYS:HE3	1.63	0.80
21:1V:39:LYS:HA	21:1V:44:ARG:HD2	1.62	0.80
7:1G:283:MET:HB3	7:1G:560:ILE:HB	1.64	0.80
6:1F:140:GLY:HA2	6:1F:179:ARG:HE	1.46	0.79
20:1U:86:VAL:HG12	20:1U:88:GLU:OE1	1.83	0.79
8:1H:20:LEU:HD12	26:1a:12:MET:HE3	1.65	0.79
38:1m:36:LEU:HD11	39:1n:151:GLU:H	1.47	0.79
3:1C:125:LYS:HE3	4:1D:253:TYR:CE2	2.17	0.79
6:1F:46:LYS:HB2	6:1F:167:CYS:HB3	1.64	0.79
9:1I:111:ILE:HD11	9:1I:131:ILE:HD11	1.64	0.79
22:1W:21:PHE:HB3	22:1W:31:ARG:HH12	1.47	0.79
13:1M:364:LEU:HB3	13:1M:369:LEU:HD22	1.66	0.78
7:1G:43:HIS:HB3	7:1G:46:LEU:HB3	1.63	0.78
22:1W:36:TYR:HE1	22:1W:40:TYR:CZ	2.01	0.78
13:1M:278:ARG:NH1	37:1l:83:MET:SD	2.57	0.78
14:1N:1:FME:HE1	14:1N:9:LEU:HD22	1.65	0.78
15:1O:151:HIS:HA	15:1O:154:GLU:OE2	1.83	0.78
36:1k:40:LEU:HD13	39:1n:45:ALA:HB2	1.64	0.78
7:1G:247:VAL:C	7:1G:248:MET:HE2	2.09	0.78
2:1B:81:ARG:NH1	2:1B:82:GLN:HA	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:42:TRP:CD2	6:1F:161:LEU:HD13	2.19	0.77
7:1G:377:ILE:HG12	7:1G:404:LEU:HD21	1.66	0.77
10:1J:106:TYR:HB3	10:1J:113:VAL:HG21	1.65	0.77
17:1Q:33:ARG:HH21	17:1Q:59:PHE:HB3	1.49	0.77
21:1V:27:TYR:CE2	21:1V:54:LYS:HG3	2.18	0.77
16:1P:92:ILE:HD11	16:1P:218:ILE:HD11	1.65	0.77
22:1W:31:ARG:O	22:1W:34:GLU:HG2	1.85	0.77
21:1V:92:LYS:HA	21:1V:95:ARG:HH12	1.50	0.77
7:1G:350:PRO:HD3	7:1G:458:LEU:HD11	1.65	0.77
43:1r:46:HIS:C	43:1r:47:LYS:HD3	2.10	0.77
42:1q:47:LYS:HE3	42:1q:63:ILE:HD11	1.67	0.77
6:1F:305:PRO:HB3	6:1F:417:GLY:HA3	1.67	0.77
40:1o:112:LYS:HG3	40:1o:116:GLN:NE2	1.99	0.76
4:1D:391:ILE:HB	4:1D:430:ARG:HH12	1.50	0.76
8:1H:80:SER:O	8:1H:84:THR:OG1	2.03	0.76
8:1H:230:ASN:HA	8:1H:233:MET:HE3	1.68	0.76
19:1S:88:ARG:NE	19:1S:88:ARG:O	2.16	0.76
10:1J:120:ASN:HB3	30:1e:73:LYS:HE3	1.68	0.76
18:1R:53:GLY:HA2	18:1R:93:GLN:HE21	1.51	0.76
10:1J:82:VAL:HG13	10:1J:84:VAL:H	1.51	0.76
6:1F:391:SER:HB3	43:1r:48:LEU:HD13	1.67	0.75
6:1F:134:ALA:HB3	6:1F:175:VAL:HG12	1.68	0.75
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	1.67	0.75
7:1G:117:GLN:NE2	47:1G:801:SF4:S3	2.60	0.75
6:1F:43:TYR:HB3	6:1F:236:ARG:HH12	1.52	0.75
7:1G:59:ILE:HD13	7:1G:77:TRP:HD1	1.50	0.75
11:1K:62:ILE:HA	11:1K:65:VAL:CG1	2.16	0.75
20:1U:20:LYS:HG2	36:1k:18:TYR:CD1	2.22	0.75
21:1V:49:GLN:NE2	43:1r:92:LYS:HE2	2.02	0.75
42:1q:6:VAL:O	42:1q:9:ARG:NH1	2.20	0.75
1:1A:69:ILE:HD12	8:1H:148:ILE:HD11	1.68	0.75
6:1F:136:ILE:HD11	6:1F:177:VAL:HG22	1.69	0.75
17:1Q:123:SER:H	17:1Q:129:ARG:HG3	1.51	0.75
42:1q:9:ARG:NH2	52:1q:201:CDL:O1	2.18	0.75
15:1O:82:PHE:CE1	15:1O:143:PHE:CE2	2.75	0.75
8:1H:137:ALA:N	10:1J:70:TYR:OH	2.20	0.75
20:1T:45:LEU:HB3	22:1W:36:TYR:CE2	2.22	0.75
20:1T:51:ILE:HG22	20:1T:55:GLU:OE2	1.86	0.75
2:1B:65:PRO:O	9:1I:47:THR:HG22	1.87	0.74
8:1H:17:VAL:HG13	8:1H:228:TYR:CD2	2.21	0.74
14:1N:103:ALA:HB1	14:1N:108:LEU:HD21	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:329:LEU:O	13:1M:333:ASN:ND2	2.20	0.74
23:1X:141:TYR:OH	33:1h:143:ASN:O	2.05	0.74
14:1N:236:LYS:HG3	14:1N:237:MET:HG3	1.70	0.74
4:1D:287:ILE:HD11	9:1I:2:TYR:HD2	1.52	0.74
13:1M:72:LEU:HD23	13:1M:75:LEU:HD12	1.70	0.74
4:1D:399:LEU:HD22	4:1D:423:ILE:HG21	1.69	0.74
23:1X:18:LYS:HA	26:1a:54:ILE:HD11	1.69	0.74
5:1E:111:ARG:HG3	5:1E:152:PRO:HG3	1.70	0.74
16:1P:186:ARG:HG3	16:1P:187:TRP:HD1	1.53	0.74
12:1L:331:MET:HE2	12:1L:465:GLY:HA2	1.70	0.74
13:1M:244:MET:HE1	13:1M:316:MET:HE1	1.68	0.74
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.70	0.74
6:1F:74:PRO:HB3	6:1F:249:ARG:HH21	1.52	0.73
19:1S:23:CYS:HB2	19:1S:60:VAL:H	1.52	0.73
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	1.69	0.73
12:1L:90:ILE:HD12	12:1L:129:MET:HE1	1.69	0.73
11:1K:91:GLN:OE1	11:1K:91:GLN:N	2.15	0.73
12:1L:526:LEU:HD12	12:1L:530:PRO:HG2	1.70	0.73
13:1M:119:TYR:OH	13:1M:157:SER:O	2.06	0.73
7:1G:36:GLN:HG2	7:1G:39:ARG:HH22	1.52	0.73
16:1P:203:GLN:NE2	16:1P:234:ASN:O	2.22	0.73
16:1P:22:THR:HG23	16:1P:46:ILE:HB	1.70	0.73
22:1W:27:GLU:HA	22:1W:30:ARG:HB2	1.71	0.73
7:1G:504:ASP:OD2	7:1G:629:ASN:ND2	2.22	0.73
23:1X:24:LEU:HB3	25:1Z:71:LEU:HD11	1.71	0.73
34:1i:119:MET:HE3	34:1i:120:LYS:H	1.53	0.73
6:1F:118:LEU:HG	6:1F:225:VAL:HG13	1.71	0.73
7:1G:407:ALA:HB1	7:1G:422:LEU:HD11	1.69	0.73
15:1O:8:PHE:O	15:1O:13:ARG:NH1	2.22	0.73
4:1D:146:ARG:HA	4:1D:370:PRO:HB3	1.71	0.72
8:1H:20:LEU:HD11	8:1H:267:THR:HG21	1.71	0.72
21:1V:92:LYS:HA	21:1V:95:ARG:NH1	2.04	0.72
14:1N:29:ILE:HG13	14:1N:86:ILE:HD11	1.70	0.72
5:1E:55:GLN:NE2	5:1E:56:ARG:CZ	2.52	0.72
22:1W:36:TYR:O	22:1W:40:TYR:HD1	1.72	0.72
20:1T:16:LEU:HD22	20:1T:30:LEU:HD11	1.70	0.72
5:1E:101:GLN:HB3	5:1E:155:GLN:HB3	1.70	0.72
19:1S:64:LEU:O	19:1S:75:ASN:ND2	2.20	0.72
31:1f:53:GLU:N	31:1f:53:GLU:OE2	2.22	0.72
3:1C:183:VAL:O	22:1W:101:THR:OG1	2.06	0.72
7:1G:609:MET:SD	7:1G:609:MET:N	2.62	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:47:GLU:HB3	41:1p:92:ARG:HE	1.53	0.72
7:1G:53:ARG:HH21	7:1G:56:LEU:HD21	1.54	0.72
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.72	0.72
12:1L:42:TYR:HH	34:1i:66:HIS:HD1	1.37	0.72
36:1k:18:TYR:HB2	36:1k:19:LYS:HZ2	1.54	0.72
6:1F:319:PHE:HB2	6:1F:329:LEU:HD23	1.71	0.72
16:1P:40:ARG:NH2	22:1W:110:THR:O	2.22	0.72
27:1b:10:ASN:O	27:1b:14:LYS:NZ	2.22	0.72
7:1G:246:GLU:HG3	7:1G:248:MET:HE1	1.70	0.72
7:1G:366:THR:H	7:1G:491:ASN:HD21	1.35	0.72
34:1i:5:PRO:HA	34:1i:8:LYS:HD2	1.72	0.72
20:1U:9:GLU:OE1	20:1U:9:GLU:N	2.17	0.71
39:1n:92:ARG:HG2	39:1n:93:TYR:CD2	2.25	0.71
4:1D:150:HIS:HB3	4:1D:304:MET:HE2	1.72	0.71
4:1D:379:VAL:HG23	4:1D:387:TYR:HB3	1.72	0.71
7:1G:321:GLY:HA2	7:1G:496:ILE:HD13	1.72	0.71
9:1I:44:GLU:HA	26:1a:1:MET:HE1	1.71	0.71
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.71	0.71
42:1q:107:LYS:H	42:1q:107:LYS:HZ3	1.38	0.71
20:1U:15:VAL:O	20:1U:19:LEU:HD23	1.90	0.71
26:1a:34:LYS:NZ	26:1a:61:HIS:O	2.21	0.71
7:1G:36:GLN:NE2	17:1Q:47:SER:O	2.22	0.71
20:1T:14:ARG:HA	20:1T:17:TYR:HB3	1.72	0.71
39:1n:92:ARG:HG2	39:1n:93:TYR:HD2	1.55	0.71
2:1B:47:PRO:HD3	2:1B:74:VAL:HB	1.71	0.71
2:1B:172:ARG:NH1	2:1B:176:TRP:HB2	2.05	0.71
38:1m:36:LEU:HG	39:1n:149:ARG:O	1.91	0.71
8:1H:92:PRO:HG3	8:1H:256:THR:HG22	1.73	0.71
4:1D:391:ILE:HB	4:1D:430:ARG:HH22	1.56	0.71
3:1C:175:ARG:HD2	16:1P:13:ARG:HD2	1.73	0.70
29:1d:90:MET:HE1	33:1h:107:GLU:HG2	1.71	0.70
7:1G:58:GLU:HB2	7:1G:65:VAL:HG22	1.73	0.70
8:1H:17:VAL:HA	8:1H:228:TYR:CE2	2.25	0.70
12:1L:375:ILE:HG12	35:1j:32:MET:HG3	1.74	0.70
8:1H:107:ALA:HB1	10:1J:57:PHE:HB3	1.72	0.70
5:1E:55:GLN:NE2	5:1E:56:ARG:NH1	2.40	0.70
7:1G:357:ASP:O	19:1S:55:ARG:NH2	2.24	0.70
9:1I:108:ARG:HH22	17:1Q:71:GLY:HA3	1.57	0.70
14:1N:202:ILE:O	14:1N:206:LEU:HD12	1.92	0.70
44:1s:64:PRO:O	44:1s:64:PRO:HD2	1.91	0.70
7:1G:118:ASP:OD1	17:1Q:46:GLN:NE2	2.23	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:41:GLN:HE22	43:1r:67:ILE:HA	1.55	0.70
7:1G:364:LEU:HD22	7:1G:491:ASN:HB3	1.73	0.70
12:1L:482:MET:SD	12:1L:482:MET:N	2.65	0.70
12:1L:577:VAL:HA	45:1Y:201:3PE:H331	1.73	0.70
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.56	0.70
13:1M:300:ALA:O	13:1M:308:SER:OG	2.08	0.70
15:1O:164:LEU:HD21	15:1O:251:GLN:HE21	1.57	0.70
22:1W:115:PRO:O	22:1W:121:LYS:NZ	2.23	0.70
7:1G:257:ASP:HB2	7:1G:369:ALA:HB2	1.71	0.70
13:1M:237:LYS:HD2	13:1M:316:MET:HG2	1.72	0.70
25:1Z:23:ARG:HH21	43:1r:112:LEU:HD11	1.55	0.70
5:1E:137:PHE:CZ	5:1E:173:ILE:HG13	2.27	0.69
8:1H:307:LEU:HA	8:1H:310:MET:HB2	1.74	0.69
13:1M:119:TYR:CE1	13:1M:123:GLU:OE1	2.44	0.69
24:1Y:65:ILE:HD11	24:1Y:100:LEU:HD23	1.74	0.69
37:1l:30:ARG:HH22	38:1m:35:ARG:HD3	1.57	0.69
40:1o:112:LYS:O	40:1o:116:GLN:NE2	2.26	0.69
10:1J:44:VAL:HG12	10:1J:49:GLY:HA3	1.74	0.69
19:1S:67:ARG:HE	19:1S:73:GLU:HB2	1.57	0.69
14:1N:73:ALA:HB2	14:1N:97:MET:HG3	1.74	0.69
1:1A:4:MET:N	1:1A:4:MET:SD	2.65	0.69
2:1B:48:MET:HA	2:1B:48:MET:HE2	1.75	0.69
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.75	0.69
5:1E:55:GLN:HB3	5:1E:61:LEU:HD22	1.75	0.69
7:1G:25:THR:HG22	7:1G:28:GLN:HG2	1.75	0.69
21:1V:50:ILE:HG13	21:1V:54:LYS:NZ	2.07	0.69
6:1F:206:LYS:HA	6:1F:208:PRO:HD2	1.73	0.69
7:1G:42:TYR:HE2	7:1G:48:VAL:HG12	1.58	0.69
12:1L:121:LEU:HD22	12:1L:246:LEU:HD23	1.72	0.69
12:1L:331:MET:HE3	12:1L:387:THR:HG23	1.74	0.69
13:1M:19:LYS:HD2	31:1f:9:ASP:HA	1.74	0.69
16:1P:319:ARG:HA	16:1P:322:ARG:HE	1.55	0.69
7:1G:628:PRO:CG	7:1G:628:PRO:CD	0.69	0.69
22:1W:66:MET:HA	22:1W:69:LYS:HG3	1.73	0.69
1:1A:8:LEU:O	1:1A:12:THR:OG1	2.11	0.69
3:1C:132:ARG:HH21	3:1C:151:ILE:HD13	1.58	0.69
4:1D:34:ASN:HB3	15:1O:158:VAL:HG13	1.75	0.69
13:1M:76:MET:HE3	13:1M:230:VAL:HG11	1.74	0.69
3:1C:130:TYR:OH	4:1D:392:LYS:NZ	2.25	0.69
4:1D:116:GLN:HE22	4:1D:138:ARG:HB3	1.56	0.69
13:1M:367:LEU:HD21	13:1M:404:ALA:HA	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:12:LYS:HZ1	20:1T:32:VAL:HA	1.57	0.69
13:1M:41:LEU:O	13:1M:44:GLN:NE2	2.26	0.69
22:1W:91:GLU:OE1	22:1W:91:GLU:N	2.26	0.69
42:1q:12:GLN:N	42:1q:12:GLN:OE1	2.26	0.69
6:1F:21:ILE:HG21	6:1F:230:VAL:HA	1.74	0.69
8:1H:85:MET:HB3	8:1H:108:MET:SD	2.33	0.69
10:1J:68:PHE:HD1	11:1K:75:LEU:HD21	1.58	0.69
18:1R:18:TYR:HE1	18:1R:24:ARG:HD3	1.57	0.69
20:1T:17:TYR:HA	20:1T:20:LYS:HE3	1.74	0.69
37:1l:82:ASP:O	37:1l:88:ARG:NH1	2.24	0.69
2:1B:57:VAL:HG13	4:1D:189:MET:HE1	1.75	0.68
19:1S:53:LEU:C	19:1S:55:ARG:HE	2.01	0.68
24:1Y:80:ARG:HG3	24:1Y:82:LYS:HG3	1.74	0.68
37:1l:128:VAL:HG21	40:1o:94:TYR:HE1	1.58	0.68
15:1O:167:HIS:HE2	15:1O:248:TRP:CG	2.10	0.68
34:1i:119:MET:HE3	34:1i:120:LYS:N	2.08	0.68
36:1k:33:GLU:N	36:1k:33:GLU:OE2	2.26	0.68
4:1D:237:ASN:HD21	8:1H:284:GLN:HG2	1.58	0.68
12:1L:269:THR:O	12:1L:271:LYS:NZ	2.25	0.68
15:1O:208:LYS:HG3	15:1O:209:THR:HG23	1.74	0.68
13:1M:119:TYR:CE1	13:1M:160:LEU:HD23	2.27	0.68
19:1S:19:ARG:HB2	19:1S:65:TRP:HB2	1.74	0.68
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.27	0.68
13:1M:173:SER:HB2	33:1h:101:ALA:HB2	1.73	0.68
16:1P:71:MET:HE1	18:1R:29:SER:HB2	1.75	0.68
33:1h:21:PHE:CZ	33:1h:25:MET:HE2	2.29	0.68
44:1s:72:SER:H	44:1s:75:HIS:HB2	1.59	0.68
15:1O:314:ASP:OD1	28:1c:1:LYS:NZ	2.26	0.68
38:1m:36:LEU:HD11	39:1n:151:GLU:N	2.08	0.68
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	1.75	0.68
14:1N:344:SER:HB2	29:1d:82:MET:HB2	1.76	0.68
5:1E:192:SER:HB3	6:1F:113:HIS:CE1	2.29	0.68
23:1X:110:VAL:O	23:1X:116:TRP:N	2.19	0.68
34:1i:24:ASP:OD2	39:1n:124:TRP:NE1	2.26	0.68
43:1r:44:PRO:C	43:1r:47:LYS:HZ3	2.02	0.68
21:1V:37:ILE:HD12	21:1V:38:PRO:HD2	1.76	0.68
4:1D:178:PHE:HZ	4:1D:189:MET:HE3	1.59	0.67
7:1G:58:GLU:H	7:1G:86:SER:HB3	1.59	0.67
8:1H:142:TYR:O	8:1H:146:LEU:HD13	1.94	0.67
10:1J:110:GLU:O	30:1e:80:ARG:NH2	2.26	0.67
16:1P:194:ILE:HD11	16:1P:263:TYR:CD2	2.22	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:17:TYR:CE2	36:1k:15:LEU:HD22	2.29	0.67
23:1X:141:TYR:O	25:1Z:115:ARG:NH1	2.26	0.67
6:1F:90:PRO:HB3	6:1F:132:ARG:HD3	1.75	0.67
7:1G:24:THR:HG23	7:1G:28:GLN:HG3	1.74	0.67
7:1G:54:MET:HE1	7:1G:94:MET:CB	2.12	0.67
43:1r:46:HIS:N	43:1r:47:LYS:HZ2	1.91	0.67
6:1F:101:GLU:OE1	6:1F:104:THR:OG1	2.11	0.67
13:1M:17:MET:HE1	29:1d:54:VAL:HG11	1.75	0.67
16:1P:177:ARG:NH2	55:1P:501:NDP:O7N	2.27	0.67
22:1W:36:TYR:HD1	22:1W:40:TYR:CE1	2.13	0.67
32:1g:85:MET:H	32:1g:85:MET:HE2	1.60	0.67
6:1F:145:GLU:OE1	6:1F:148:ASN:ND2	2.28	0.67
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.75	0.67
21:1V:49:GLN:HE21	43:1r:92:LYS:HE2	1.59	0.67
8:1H:42:PRO:O	8:1H:45:LEU:HD23	1.95	0.67
19:1S:53:LEU:HD12	19:1S:55:ARG:HD2	1.76	0.67
42:1q:14:VAL:HA	42:1q:23:TYR:CD2	2.29	0.67
35:1j:57:SER:OG	35:1j:58:GLN:OE1	2.11	0.67
37:1l:131:LYS:CG	37:1l:133:TYR:HE1	2.07	0.67
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	1.76	0.67
19:1S:16:ARG:HD3	19:1S:69:ALA:HB2	1.75	0.67
24:1Y:43:LYS:NZ	45:1Y:201:3PE:O11	2.27	0.67
39:1n:27:GLU:HG2	39:1n:36:TYR:OH	1.94	0.67
2:1B:68:ASP:O	2:1B:71:ARG:HG2	1.94	0.67
7:1G:504:ASP:OD1	19:1S:55:ARG:NH1	2.26	0.67
13:1M:231:LEU:HA	13:1M:235:LEU:HD12	1.75	0.67
5:1E:58:ASN:HD21	5:1E:60:TRP:NE1	1.92	0.67
43:1r:72:GLN:N	43:1r:72:GLN:OE1	2.28	0.67
11:1K:37:MET:HA	11:1K:40:LEU:HB2	1.77	0.66
13:1M:22:MET:O	13:1M:26:ASN:ND2	2.28	0.66
22:1W:36:TYR:HE1	22:1W:40:TYR:HH	1.41	0.66
15:1O:138:MET:CG	15:1O:144:ILE:HG12	2.21	0.66
25:1Z:105:LYS:NZ	25:1Z:106:VAL:O	2.28	0.66
15:1O:45:LYS:HD2	15:1O:235:VAL:HG11	1.76	0.66
22:1W:36:TYR:CE1	22:1W:40:TYR:CZ	2.83	0.66
6:1F:273:SER:HA	6:1F:316:LEU:HB3	1.76	0.66
8:1H:31:MET:HE1	8:1H:272:TRP:HA	1.77	0.66
4:1D:76:CYS:HB2	4:1D:403:ASP:HA	1.77	0.66
4:1D:287:ILE:HD11	9:1I:2:TYR:CD2	2.30	0.66
4:1D:311:ILE:HG22	4:1D:315:LEU:HD23	1.77	0.66
16:1P:190:GLY:HA2	16:1P:254:LEU:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:284:ASP:OD2	43:1r:106:SER:HB2	1.95	0.66
12:1L:294:THR:O	12:1L:524:ASN:ND2	2.28	0.66
12:1L:532:ILE:HD11	37:1l:101:MET:HB3	1.76	0.66
21:1V:106:PRO:HD2	21:1V:106:PRO:O	1.95	0.66
22:1W:36:TYR:O	22:1W:40:TYR:CD1	2.48	0.66
6:1F:351:ILE:HD11	6:1F:372:MET:HB3	1.77	0.66
16:1P:38:LEU:O	16:1P:43:SER:OG	2.14	0.66
4:1D:161:ILE:HG23	4:1D:238:ARG:NH1	2.09	0.66
12:1L:142:ILE:HD13	13:1M:370:PRO:HB2	1.76	0.66
12:1L:437:PHE:HE2	12:1L:441:VAL:HG12	1.61	0.66
13:1M:277:LEU:HD21	13:1M:405:LEU:HB3	1.76	0.66
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.28	0.66
2:1B:172:ARG:HD2	2:1B:172:ARG:O	1.95	0.66
16:1P:144:ARG:HH22	16:1P:148:SER:HB3	1.60	0.66
16:1P:194:ILE:HG12	16:1P:260:HIS:HA	1.77	0.66
19:1S:40:TYR:OH	19:1S:52:ILE:HG12	1.95	0.66
43:1r:63:MET:HE3	43:1r:64:PRO:HD3	1.78	0.66
8:1H:62:ARG:HH12	16:1P:187:TRP:HH2	1.44	0.65
14:1N:318:GLU:OE2	14:1N:319:HIS:N	2.27	0.65
16:1P:135:LEU:HA	16:1P:167:LYS:HE3	1.77	0.65
16:1P:171:ILE:HG22	16:1P:210:VAL:HG21	1.77	0.65
6:1F:150:GLN:O	6:1F:153:ILE:HG22	1.96	0.65
7:1G:255:HIS:HE1	7:1G:258:ILE:HD13	1.61	0.65
7:1G:378:LEU:HB3	7:1G:451:VAL:HG22	1.79	0.65
7:1G:549:HIS:HE1	7:1G:677:ILE:HG13	1.61	0.65
9:1I:54:LYS:HD2	42:1q:91:HIS:CE1	2.31	0.65
13:1M:412:ILE:HD13	13:1M:416:ARG:HD3	1.78	0.65
22:1W:100:ARG:O	22:1W:104:MET:HG2	1.96	0.65
23:1X:12:LEU:HD11	25:1Z:84:LEU:HG	1.78	0.65
37:1l:10:PRO:HD2	38:1m:69:TYR:HD2	1.60	0.65
10:1J:23:LYS:NZ	11:1K:18:GLY:O	2.29	0.65
10:1J:33:LEU:C	10:1J:33:LEU:HD23	2.20	0.65
12:1L:581:LYS:HE3	24:1Y:44:PRO:HD2	1.79	0.65
6:1F:85:PRO:O	6:1F:85:PRO:HD2	1.96	0.65
6:1F:154:ARG:HH12	44:1s:57:GLU:HB3	1.60	0.65
7:1G:361:ASN:HA	7:1G:490:MET:HE1	1.79	0.65
9:1I:169:ILE:HG23	18:1R:66:LEU:HD21	1.78	0.65
13:1M:119:TYR:CZ	13:1M:123:GLU:OE1	2.49	0.65
21:1V:51:THR:HA	21:1V:54:LYS:HZ3	1.60	0.65
6:1F:365:CYS:HB2	47:1F:502:SF4:S2	2.36	0.65
16:1P:91:VAL:HG12	16:1P:126:VAL:HG21	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:36:TYR:HE1	22:1W:40:TYR:OH	1.79	0.65
5:1E:45:ALA:HA	6:1F:198:GLY:HA3	1.79	0.65
13:1M:78:MET:HE1	13:1M:439:LEU:HG	1.78	0.65
21:1V:27:TYR:HE2	21:1V:54:LYS:HG3	1.61	0.65
40:1o:115:GLU:HB3	40:1o:116:GLN:HE22	1.60	0.65
6:1F:215:VAL:HG22	6:1F:220:THR:HG21	1.79	0.65
6:1F:251:SER:C	6:1F:272:MET:HE1	2.21	0.65
7:1G:41:CYS:HB3	7:1G:52:CYS:HB3	1.78	0.65
20:1T:45:LEU:HD12	22:1W:68:MET:HE1	1.78	0.65
40:1o:68:CYS:O	40:1o:72:SER:OG	2.13	0.65
3:1C:101:PHE:CE1	43:1r:99:PRO:HD3	2.32	0.65
4:1D:391:ILE:H	4:1D:430:ARG:HH22	1.42	0.65
8:1H:17:VAL:HA	8:1H:228:TYR:HE2	1.61	0.65
13:1M:13:PRO:HB3	45:1N:401:3PE:H2C1	1.78	0.65
20:1U:87:TYR:C	20:1U:88:GLU:OE2	2.40	0.65
34:1i:54:ALA:HB3	34:1i:57:LYS:HG2	1.79	0.65
42:1q:33:VAL:HG21	52:1q:201:CDL:H112	1.78	0.65
4:1D:165:THR:HG22	8:1H:32:GLN:HG2	1.78	0.65
6:1F:161:LEU:HD23	6:1F:167:CYS:SG	2.37	0.65
20:1T:45:LEU:CB	22:1W:36:TYR:HE2	2.10	0.65
22:1W:21:PHE:HB3	22:1W:31:ARG:NH1	2.11	0.65
41:1p:2:ASP:OD1	41:1p:6:LYS:NZ	2.30	0.65
4:1D:202:ASP:HA	4:1D:323:ILE:HG21	1.78	0.64
4:1D:311:ILE:H	4:1D:311:ILE:HD12	1.62	0.64
12:1L:436:ARG:HG2	39:1n:33:ARG:HD3	1.80	0.64
31:1f:7:VAL:O	31:1f:11:TRP:N	2.30	0.64
3:1C:79:THR:HA	3:1C:134:ILE:HD11	1.79	0.64
6:1F:403:THR:OG1	6:1F:405:CYS:O	2.16	0.64
5:1E:159:ASN:HD21	5:1E:184:PRO:HG3	1.63	0.64
7:1G:632:ARG:HH21	19:1S:60:VAL:HG22	1.62	0.64
13:1M:190:TRP:CD2	24:1Y:126:MET:HE1	2.32	0.64
5:1E:137:PHE:CE2	5:1E:173:ILE:HG13	2.33	0.64
16:1P:133:SER:HA	16:1P:149:LYS:HE3	1.79	0.64
33:1h:42:LEU:O	33:1h:46:PHE:N	2.30	0.64
34:1i:117:PRO:O	34:1i:117:PRO:HD2	1.95	0.64
37:1l:125:TYR:OH	40:1o:7:ARG:NH1	2.30	0.64
40:1o:45:MET:SD	40:1o:45:MET:N	2.69	0.64
3:1C:68:THR:HA	21:1V:82:GLN:NE2	2.12	0.64
3:1C:199:LEU:HD21	4:1D:385:ARG:HD2	1.80	0.64
7:1G:358:LEU:HD23	7:1G:645:ALA:HB2	1.79	0.64
42:1q:47:LYS:NZ	42:1q:49:TYR:CE2	2.65	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:273:ILE:HG22	9:1I:34:LEU:HD11	1.78	0.64
12:1L:162:THR:OG1	37:1I:86:ARG:NH2	2.28	0.64
35:1j:65:GLY:HA3	40:1o:30:PHE:HD2	1.62	0.64
13:1M:431:THR:HG21	32:1g:58:MET:SD	2.38	0.64
17:1Q:33:ARG:NH2	17:1Q:60:ASP:O	2.30	0.64
43:1r:47:LYS:HD3	43:1r:47:LYS:N	2.13	0.64
7:1G:45:ARG:NH1	7:1G:261:GLU:OE1	2.30	0.64
7:1G:46:LEU:HD11	7:1G:161:ARG:HE	1.63	0.64
8:1H:75:PRO:O	8:1H:222:MET:HE2	1.98	0.64
12:1L:478:PRO:HG2	40:1o:90:GLU:HG3	1.80	0.64
14:1N:252:GLY:HA3	14:1N:290:LEU:HD13	1.78	0.64
15:1O:183:ILE:HD12	15:1O:184:GLN:H	1.62	0.64
15:1O:222:GLN:OE1	15:1O:222:GLN:N	2.31	0.64
46:1f:101:PC1:H342	33:1h:79:PHE:CD2	2.32	0.64
42:1q:7:LEU:O	42:1q:11:LEU:HD23	1.97	0.64
7:1G:348:VAL:HA	7:1G:510:GLY:HA2	1.80	0.64
10:1J:127:ILE:HD13	11:1K:2:PRO:HG2	1.79	0.64
15:1O:183:ILE:HD12	15:1O:184:GLN:N	2.13	0.64
22:1W:36:TYR:CD1	22:1W:40:TYR:CE1	2.86	0.64
23:1X:43:MET:HE1	27:1b:52:TYR:CZ	2.33	0.64
23:1X:134:ARG:O	27:1b:57:ARG:NH2	2.31	0.64
37:1I:16:THR:HG23	37:1I:19:GLU:H	1.62	0.64
2:1B:60:MET:HE1	2:1B:76:PHE:HB2	1.80	0.64
6:1F:132:ARG:HH22	44:1s:66:PRO:HD3	1.63	0.64
13:1M:150:LEU:HD21	14:1N:254:LEU:HD21	1.79	0.64
13:1M:410:MET:O	13:1M:414:THR:OG1	2.16	0.64
20:1U:7:THR:OG1	20:1U:9:GLU:OE2	2.16	0.64
31:1f:55:THR:HG22	31:1f:56:TRP:H	1.63	0.64
36:1k:19:LYS:O	36:1k:22:LYS:NZ	2.30	0.64
38:1m:27:GLU:OE2	38:1m:27:GLU:N	2.23	0.64
40:1o:115:GLU:HB3	40:1o:116:GLN:NE2	2.14	0.64
6:1F:102:PRO:HD2	6:1F:302:SER:HB2	1.80	0.63
7:1G:255:HIS:ND1	7:1G:255:HIS:O	2.31	0.63
12:1L:486:MET:HA	12:1L:489:THR:HG23	1.80	0.63
13:1M:457:PRO:HA	32:1g:84:ARG:HH21	1.63	0.63
4:1D:226:GLU:OE1	4:1D:230:THR:OG1	2.15	0.63
7:1G:392:ASN:HA	7:1G:395:ILE:HD12	1.80	0.63
11:1K:5:TYR:HD1	11:1K:43:MET:HE1	1.62	0.63
12:1L:356:ILE:HD11	12:1L:430:ALA:HB2	1.80	0.63
16:1P:263:TYR:CE1	16:1P:284:VAL:HG12	2.33	0.63
24:1Y:43:LYS:NZ	45:1Y:201:3PE:O31	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:131:LYS:CG	37:1l:133:TYR:CE1	2.81	0.63
37:1l:141:GLU:HA	41:1p:122:GLN:HB2	1.80	0.63
12:1L:51:LEU:HG	12:1L:55:MET:HE2	1.80	0.63
12:1L:555:LEU:HD13	38:1m:75:ILE:HG21	1.79	0.63
15:1O:25:ILE:HB	15:1O:123:VAL:HG22	1.81	0.63
16:1P:268:ARG:HB3	16:1P:281:ARG:HD2	1.79	0.63
35:1j:61:ASP:HB3	35:1j:66:ILE:HB	1.80	0.63
6:1F:65:LEU:HD21	6:1F:234:ILE:HG21	1.80	0.63
16:1P:137:ALA:HA	16:1P:146:LEU:HB3	1.80	0.63
21:1V:50:ILE:HG13	21:1V:54:LYS:HZ2	1.64	0.63
40:1o:112:LYS:CG	40:1o:116:GLN:HE21	2.10	0.63
6:1F:25:LEU:O	6:1F:113:HIS:ND1	2.27	0.63
28:1c:40:LEU:HB3	28:1c:44:ARG:NH2	2.14	0.63
21:1V:19:PRO:HD2	21:1V:20:HIS:N	2.04	0.63
1:1A:22:PHE:HA	8:1H:60:PRO:HG3	1.79	0.63
6:1F:205:LEU:HB2	17:1Q:118:TYR:CZ	2.33	0.63
8:1H:133:LEU:O	10:1J:70:TYR:OH	2.12	0.63
15:1O:117:SER:OG	15:1O:260:ARG:NH1	2.31	0.63
16:1P:238:LEU:HA	16:1P:241:LEU:HD12	1.81	0.63
34:1i:106:GLY:HA2	34:1i:118:LEU:HD22	1.80	0.63
3:1C:35:LYS:HE2	21:1V:103:VAL:HG13	1.81	0.63
4:1D:427:GLU:N	4:1D:427:GLU:OE2	2.31	0.63
6:1F:270:GLU:OE1	6:1F:283:HIS:NE2	2.32	0.63
14:1N:251:MET:HB3	14:1N:293:TYR:CE2	2.34	0.63
21:1V:55:LEU:O	21:1V:59:LYS:NZ	2.32	0.63
23:1X:109:CYS:O	23:1X:113:LYS:N	2.26	0.63
23:1X:136:LEU:HD22	23:1X:137:PRO:HD2	1.81	0.63
39:1n:150:THR:HG22	39:1n:152:ALA:H	1.64	0.63
42:1q:17:HIS:NE2	42:1q:33:VAL:O	2.31	0.63
9:1I:153:LYS:O	9:1I:157:ASN:ND2	2.32	0.62
22:1W:61:ASP:HA	22:1W:64:ARG:HB3	1.80	0.62
32:1g:48:ASP:OD1	32:1g:49:LYS:N	2.32	0.62
1:1A:14:ALA:HA	8:1H:79:LEU:HD23	1.81	0.62
7:1G:237:ASN:OD1	7:1G:253:ARG:NH2	2.32	0.62
10:1J:119:PHE:CG	10:1J:120:ASN:N	2.65	0.62
16:1P:29:PHE:HA	16:1P:175:GLU:OE1	1.99	0.62
43:1r:109:GLN:OE1	43:1r:110:PRO:HD2	1.98	0.62
2:1B:67:TYR:CE1	2:1B:154:GLU:HB3	2.34	0.62
8:1H:313:SER:O	25:1Z:54:ASN:ND2	2.30	0.62
12:1L:7:LEU:HD22	12:1L:49:VAL:HG11	1.80	0.62
13:1M:48:ASN:HD21	41:1p:85:PHE:HZ	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:25:MET:N	22:1W:25:MET:SD	2.72	0.62
8:1H:113:VAL:CG2	8:1H:136:VAL:HG13	2.28	0.62
3:1C:18:VAL:HG13	3:1C:22:LEU:HD12	1.80	0.62
7:1G:546:GLN:HG3	7:1G:599:ILE:HD11	1.81	0.62
7:1G:592:LEU:HG	16:1P:6:ILE:HG23	1.82	0.62
13:1M:76:MET:O	13:1M:80:SER:OG	2.14	0.62
15:1O:219:GLU:HG2	15:1O:241:LEU:HD12	1.82	0.62
16:1P:191:VAL:HG23	16:1P:254:LEU:HD12	1.81	0.62
33:1h:114:MET:SD	33:1h:120:GLY:HA3	2.40	0.62
43:1r:46:HIS:N	43:1r:47:LYS:NZ	2.47	0.62
8:1H:89:LEU:HB3	8:1H:91:MET:HG3	1.81	0.62
12:1L:596:MET:O	12:1L:600:THR:OG1	2.15	0.62
13:1M:282:LEU:HD12	13:1M:330:ALA:HB2	1.81	0.62
14:1N:77:ASN:HD21	14:1N:89:MET:HB3	1.64	0.62
2:1B:41:ARG:HD3	2:1B:110:PRO:HG3	1.82	0.62
4:1D:239:THR:OG1	4:1D:293:CYS:SG	2.55	0.62
5:1E:27:ASN:HA	5:1E:30:ARG:HD2	1.81	0.62
7:1G:673:MET:HE1	7:1G:679:ARG:HA	1.82	0.62
25:1Z:23:ARG:NH2	43:1r:112:LEU:HD21	2.14	0.62
28:1c:6:GLU:OE2	28:1c:7:PRO:HD2	2.00	0.62
2:1B:113:VAL:HG23	2:1B:142:VAL:HG22	1.82	0.62
8:1H:104:PHE:O	8:1H:108:MET:HG3	1.99	0.62
3:1C:86:ARG:NH2	21:1V:112:LYS:O	2.33	0.62
3:1C:199:LEU:HD12	4:1D:354:GLU:HA	1.82	0.62
21:1V:22:ARG:O	21:1V:25:ILE:HG13	1.99	0.62
37:1l:98:TRP:HA	37:1l:101:MET:HB2	1.82	0.62
39:1n:92:ARG:HD2	39:1n:93:TYR:HE2	1.63	0.62
4:1D:281:VAL:HG21	4:1D:310:ILE:HG23	1.82	0.62
6:1F:15:LEU:HB2	6:1F:271:GLU:H	1.64	0.62
14:1N:2:ASN:HB3	14:1N:5:ILE:CG1	2.30	0.62
17:1Q:26:PRO:HD2	17:1Q:29:HIS:HB2	1.80	0.62
24:1Y:27:ILE:HG21	45:1Y:202:3PE:H3G1	1.82	0.62
6:1F:399:ILE:HD11	6:1F:412:ALA:HB2	1.82	0.61
12:1L:428:PHE:HA	12:1L:432:LEU:HD12	1.81	0.61
15:1O:275:ILE:HG12	15:1O:277:VAL:HG23	1.83	0.61
22:1W:68:MET:HA	22:1W:68:MET:HE3	1.82	0.61
26:1a:1:MET:HA	26:1a:1:MET:HE3	1.82	0.61
33:1h:88:GLU:HA	33:1h:91:MET:CE	2.29	0.61
37:1l:9:PHE:O	37:1l:26:LYS:NZ	2.33	0.61
2:1B:154:GLU:OE1	2:1B:154:GLU:N	2.32	0.61
10:1J:65:LEU:HD13	10:1J:68:PHE:HD2	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:87:THR:O	14:1N:147:GLN:NE2	2.33	0.61
16:1P:29:PHE:HD1	16:1P:175:GLU:OE1	1.84	0.61
42:1q:9:ARG:NH1	52:1q:201:CDL:HA61	2.15	0.61
3:1C:40:VAL:HG13	43:1r:68:VAL:HB	1.81	0.61
17:1Q:123:SER:HB3	17:1Q:126:LYS:HE2	1.82	0.61
19:1S:88:ARG:HE	19:1S:88:ARG:C	2.07	0.61
14:1N:119:THR:HG21	14:1N:180:ALA:HB2	1.83	0.61
35:1j:54:PRO:HG3	40:1o:95:VAL:HG23	1.81	0.61
39:1n:58:LYS:O	39:1n:62:LEU:N	2.31	0.61
12:1L:95:PHE:HE1	12:1L:456:ARG:HG2	1.66	0.61
16:1P:29:PHE:CE2	16:1P:207:ILE:HD12	2.35	0.61
8:1H:113:VAL:HG21	8:1H:136:VAL:HG13	1.82	0.61
40:1o:112:LYS:C	40:1o:116:GLN:HE21	2.09	0.61
2:1B:153:ALA:O	2:1B:156:LEU:HG	2.01	0.61
6:1F:42:TRP:CE3	6:1F:161:LEU:HD13	2.35	0.61
16:1P:167:LYS:HB2	16:1P:229:ALA:HA	1.83	0.61
17:1Q:129:ARG:HE	44:1s:73:PRO:HB3	1.65	0.61
25:1Z:123:GLU:N	25:1Z:123:GLU:OE2	2.31	0.61
33:1h:69:HIS:ND1	33:1h:70:PRO:HD2	2.14	0.61
6:1F:292:ASP:O	6:1F:339:ARG:NH1	2.26	0.61
7:1G:46:LEU:HD21	7:1G:161:ARG:HB3	1.81	0.61
7:1G:594:ARG:HD2	22:1W:126:HIS:HB3	1.83	0.61
12:1L:237:MET:SD	12:1L:303:ALA:HB2	2.41	0.61
20:1T:60:PHE:HE2	20:1T:62:ILE:HG12	1.63	0.61
22:1W:31:ARG:NH2	22:1W:80:ASP:OD2	2.34	0.61
22:1W:62:LYS:HD3	22:1W:65:GLU:OE1	2.01	0.61
34:1i:103:ILE:HG22	41:1p:17:PRO:HB3	1.81	0.61
39:1n:123:GLN:OE1	39:1n:126:ARG:NH1	2.33	0.61
41:1p:32:LEU:HD13	41:1p:35:ILE:HD11	1.83	0.61
5:1E:15:ASN:HB2	5:1E:60:TRP:HH2	1.65	0.61
6:1F:120:GLU:CD	6:1F:232:PRO:HB3	2.25	0.61
7:1G:59:ILE:HD13	7:1G:77:TRP:CD1	2.32	0.61
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.19	0.61
21:1V:79:VAL:HA	21:1V:82:GLN:HB3	1.82	0.61
35:1j:51:PHE:HB3	40:1o:91:HIS:CE1	2.36	0.61
42:1q:9:ARG:HA	42:1q:12:GLN:HE22	1.66	0.61
4:1D:283:PHE:HA	4:1D:309:ARG:HD3	1.83	0.61
8:1H:79:LEU:HB2	8:1H:222:MET:SD	2.41	0.61
13:1M:78:MET:HA	13:1M:81:GLN:HE22	1.66	0.61
34:1i:106:GLY:H	34:1i:116:ILE:HG23	1.66	0.61
5:1E:184:PRO:HD2	44:1s:44:HIS:CD2	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:28:ARG:NH1	44:1s:37:THR:O	2.33	0.60
6:1F:308:PRO:HD3	6:1F:421:HIS:CE1	2.36	0.60
20:1U:70:LEU:HG	20:1U:76:ILE:HD12	1.83	0.60
22:1W:36:TYR:OH	22:1W:64:ARG:NH2	2.35	0.60
23:1X:121:LEU:HD13	25:1Z:62:ILE:HD11	1.82	0.60
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.01	0.60
2:1B:81:ARG:HD2	2:1B:81:ARG:C	2.25	0.60
12:1L:481:THR:HG1	40:1o:91:HIS:HD1	1.49	0.60
14:1N:240:ILE:HD11	29:1d:48:ILE:HG23	1.82	0.60
17:1Q:58:GLU:OE1	17:1Q:58:GLU:N	2.22	0.60
3:1C:101:PHE:CD1	43:1r:99:PRO:HD3	2.36	0.60
4:1D:110:SER:HB3	4:1D:149:ASN:HB2	1.83	0.60
7:1G:624:GLU:OE1	7:1G:628:PRO:HA	2.02	0.60
9:1I:113:MET:HB2	9:1I:147:LEU:O	2.00	0.60
46:1I:204:PC1:H111	25:1Z:27:ARG:HH22	1.66	0.60
13:1M:286:ILE:HD13	13:1M:326:LEU:HB3	1.84	0.60
17:1Q:19:ILE:HD11	17:1Q:98:LYS:HD3	1.82	0.60
17:1Q:93:VAL:O	17:1Q:97:GLU:OE1	2.19	0.60
32:1g:96:LEU:HD21	32:1g:100:ARG:HH21	1.65	0.60
43:1r:44:PRO:C	43:1r:47:LYS:NZ	2.59	0.60
2:1B:95:LYS:HE3	3:1C:155:TYR:CD1	2.36	0.60
5:1E:13:PRO:O	5:1E:16:ASN:ND2	2.35	0.60
8:1H:152:SER:HA	8:1H:155:LEU:HD23	1.83	0.60
12:1L:502:LEU:O	12:1L:506:ASN:ND2	2.34	0.60
42:1q:14:VAL:HA	42:1q:23:TYR:HD2	1.66	0.60
3:1C:36:TYR:HE2	3:1C:59:PRO:HB2	1.65	0.60
6:1F:306:LEU:HD21	6:1F:418:LEU:HD23	1.83	0.60
24:1Y:123:LEU:HA	24:1Y:126:MET:HB2	1.82	0.60
34:1i:17:LEU:HD23	34:1i:20:ARG:HH21	1.65	0.60
35:1j:29:SER:O	35:1j:32:MET:HE3	2.01	0.60
4:1D:413:ASP:OD1	8:1H:281:ARG:NH1	2.35	0.60
4:1D:421:GLN:HG3	4:1D:423:ILE:HD11	1.82	0.60
5:1E:184:PRO:HD2	44:1s:44:HIS:HD2	1.66	0.60
8:1H:143:GLU:OE2	8:1H:143:GLU:N	2.33	0.60
13:1M:1:FME:HE3	13:1M:111:THR:HG21	1.83	0.60
13:1M:47:GLU:OE1	41:1p:93:ARG:HG2	2.01	0.60
13:1M:336:ARG:HD2	13:1M:426:ILE:HG23	1.84	0.60
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.84	0.60
21:1V:64:VAL:HG22	21:1V:76:ILE:HD11	1.84	0.60
2:1B:68:ASP:OD2	9:1I:47:THR:HG21	2.00	0.60
6:1F:295:LEU:HD22	6:1F:343:ILE:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:42:TYR:O	7:1G:158:ARG:NH2	2.33	0.60
15:1O:113:GLU:OE1	15:1O:266:LYS:NZ	2.33	0.60
34:1i:13:GLN:HE22	39:1n:156:ALA:H	1.49	0.60
3:1C:35:LYS:O	3:1C:35:LYS:NZ	2.27	0.60
6:1F:308:PRO:HD3	6:1F:421:HIS:ND1	2.17	0.60
8:1H:152:SER:HB2	8:1H:301:CYS:HA	1.84	0.60
9:1I:12:MET:HE2	9:1I:12:MET:HA	1.84	0.60
38:1m:101:TYR:OH	38:1m:105:LYS:NZ	2.34	0.60
8:1H:184:MET:HE1	8:1H:293:PHE:CG	2.35	0.60
14:1N:225:THR:HG23	14:1N:226:THR:HG23	1.84	0.60
19:1S:23:CYS:SG	19:1S:24:GLN:N	2.74	0.60
22:1W:21:PHE:HB2	22:1W:31:ARG:HH22	1.67	0.60
40:1o:14:LYS:NZ	40:1o:109:GLN:HA	2.17	0.60
3:1C:125:LYS:CE	4:1D:253:TYR:CE2	2.85	0.60
4:1D:237:ASN:ND2	8:1H:284:GLN:HG2	2.16	0.60
6:1F:165:ASN:HA	6:1F:171:TYR:H	1.67	0.60
13:1M:294:MET:HA	13:1M:294:MET:HE3	1.84	0.60
16:1P:50:ARG:NH1	55:1P:501:NDP:O2B	2.35	0.60
19:1S:73:GLU:C	19:1S:74:LYS:HD3	2.26	0.60
21:1V:64:VAL:HG12	21:1V:65:LYS:HD3	1.83	0.60
40:1o:7:ARG:HG3	40:1o:15:GLU:HB2	1.84	0.60
41:1p:99:GLN:O	41:1p:103:ASN:ND2	2.35	0.60
3:1C:50:ILE:HB	3:1C:107:VAL:HG12	1.83	0.59
13:1M:134:THR:HB	14:1N:302:LEU:HD22	1.83	0.59
13:1M:282:LEU:CD2	13:1M:342:MET:HE1	2.31	0.59
16:1P:141:SER:O	16:1P:147:ARG:NE	2.35	0.59
18:1R:68:HIS:CD2	18:1R:87:CYS:SG	2.94	0.59
20:1T:36:PHE:O	20:1T:42:LEU:N	2.35	0.59
29:1d:104:LYS:NZ	41:1p:77:GLU:OE2	2.35	0.59
2:1B:81:ARG:C	2:1B:81:ARG:HH11	2.10	0.59
16:1P:248:VAL:HG22	16:1P:334:VAL:HG11	1.84	0.59
35:1j:8:GLU:H	35:1j:16:GLN:HE21	1.48	0.59
6:1F:275:PRO:HD2	6:1F:275:PRO:O	2.01	0.59
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.84	0.59
6:1F:433:PHE:O	6:1F:437:HIS:ND1	2.32	0.59
8:1H:293:PHE:O	8:1H:297:THR:OG1	2.18	0.59
12:1L:501:ALA:O	12:1L:505:ASN:ND2	2.33	0.59
13:1M:229:MET:O	13:1M:233:ALA:N	2.34	0.59
13:1M:325:MET:HE1	13:1M:441:ILE:CG1	2.30	0.59
14:1N:268:GLN:HG3	23:1X:167:PHE:HZ	1.68	0.59
15:1O:46:LEU:HB3	15:1O:48:LEU:HD13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:173:ASP:N	15:1O:223:TYR:O	2.31	0.59
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.84	0.59
37:1l:137:ASP:O	37:1l:142:ARG:NH2	2.35	0.59
6:1F:45:THR:HG23	6:1F:236:ARG:NH2	2.17	0.59
7:1G:302:ARG:O	7:1G:306:MET:HG2	2.02	0.59
16:1P:133:SER:OG	16:1P:167:LYS:NZ	2.36	0.59
19:1S:63:LYS:HE3	19:1S:75:ASN:ND2	2.17	0.59
20:1T:25:ILE:HG23	20:1T:40:LEU:HD21	1.83	0.59
2:1B:116:MET:SD	2:1B:156:LEU:HD22	2.42	0.59
3:1C:113:GLU:HG2	3:1C:114:LEU:HD12	1.83	0.59
5:1E:58:ASN:HD21	5:1E:60:TRP:CD1	2.20	0.59
6:1F:99:GLU:CD	6:1F:107:ASP:HB2	2.27	0.59
10:1J:153:LEU:HD21	11:1K:62:ILE:HD13	1.85	0.59
33:1h:34:ILE:O	33:1h:38:ILE:HD12	2.02	0.59
34:1i:10:ARG:HB2	39:1n:155:PRO:HB3	1.82	0.59
3:1C:94:TYR:HB2	3:1C:107:VAL:HG23	1.85	0.59
6:1F:33:LEU:HG	6:1F:37:GLN:HE22	1.67	0.59
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	1.85	0.59
11:1K:36:MET:HE2	14:1N:68:MET:CE	2.32	0.59
16:1P:263:TYR:OH	16:1P:284:VAL:HA	2.02	0.59
19:1S:52:ILE:C	19:1S:52:ILE:HD12	2.27	0.59
20:1U:22:TYR:HD2	20:1U:25:ILE:HD13	1.67	0.59
26:1a:67:GLU:CD	26:1a:67:GLU:H	2.09	0.59
35:1j:63:GLU:OE1	40:1o:99:LYS:NZ	2.35	0.59
1:1A:88:LEU:HD23	8:1H:309:ILE:HD13	1.83	0.59
2:1B:44:SER:O	8:1H:54:LYS:NZ	2.35	0.59
3:1C:73:LYS:HZ1	4:1D:251:LEU:HG	1.68	0.59
4:1D:391:ILE:HB	4:1D:430:ARG:NH1	2.15	0.59
6:1F:391:SER:CB	43:1r:48:LEU:HD13	2.33	0.59
16:1P:30:LEU:HD12	16:1P:94:LEU:HG	1.84	0.59
33:1h:95:GLN:HB2	41:1p:82:LEU:HD11	1.84	0.59
2:1B:144:ILE:HD12	2:1B:162:GLN:HG2	1.85	0.59
9:1I:65:HIS:HA	9:1I:133:GLU:HA	1.85	0.59
16:1P:186:ARG:HG3	16:1P:187:TRP:CD1	2.37	0.59
20:1U:70:LEU:HG	20:1U:76:ILE:CD1	2.33	0.59
40:1o:112:LYS:HG3	40:1o:116:GLN:HE21	1.65	0.59
42:1q:101:LYS:NZ	42:1q:102:PRO:O	2.36	0.59
7:1G:6:SER:OG	7:1G:7:ASN:N	2.35	0.59
9:1I:94:ILE:HG22	9:1I:109:TYR:HA	1.85	0.59
12:1L:81:LYS:HB2	12:1L:135:ASN:HD22	1.67	0.59
15:1O:84:ASP:OD1	15:1O:193:LYS:NZ	2.29	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:38:ILE:HD12	33:1h:38:ILE:H	1.68	0.59
39:1n:65:GLN:OE1	39:1n:65:GLN:N	2.36	0.59
2:1B:82:GLN:HG3	8:1H:220:PHE:CZ	2.38	0.59
13:1M:201:MET:HG2	51:1M:501:PGT:H441	1.82	0.59
14:1N:135:LYS:HZ3	14:1N:187:MET:HE1	1.68	0.59
15:1O:141:GLN:HE21	15:1O:198:TYR:HA	1.67	0.59
22:1W:99:GLN:OE1	22:1W:102:HIS:ND1	2.30	0.59
34:1i:104:PHE:HE1	40:1o:70:ARG:HE	1.51	0.59
37:1l:99:ASN:HB2	38:1m:6:LYS:HE2	1.84	0.59
3:1C:29:VAL:HG13	3:1C:63:PHE:HE2	1.67	0.58
8:1H:85:MET:HG2	8:1H:233:MET:HG3	1.84	0.58
8:1H:222:MET:O	8:1H:225:MET:N	2.35	0.58
11:1K:41:PHE:O	11:1K:45:THR:OG1	2.21	0.58
21:1V:34:LEU:HD12	21:1V:37:ILE:HG21	1.85	0.58
22:1W:61:ASP:OD1	22:1W:61:ASP:N	2.35	0.58
42:1q:13:GLN:HE22	42:1q:33:VAL:C	2.09	0.58
3:1C:192:GLN:HG2	17:1Q:72:TRP:CG	2.38	0.58
4:1D:296:ARG:NE	4:1D:420:THR:OG1	2.36	0.58
6:1F:202:LYS:NZ	6:1F:359:CYS:O	2.36	0.58
8:1H:17:VAL:O	8:1H:228:TYR:CE2	2.55	0.58
12:1L:8:THR:OG1	12:1L:82:MET:HE1	2.03	0.58
6:1F:109:GLU:OE1	6:1F:112:ARG:NH1	2.36	0.58
6:1F:299:PRO:HA	6:1F:334:VAL:HG23	1.86	0.58
7:1G:418:ARG:HD2	44:1s:75:HIS:HA	1.86	0.58
12:1L:126:ILE:HA	12:1L:129:MET:HB2	1.85	0.58
22:1W:75:ASP:HB3	22:1W:78:VAL:HG12	1.84	0.58
3:1C:84:PRO:HB2	17:1Q:86:PHE:HE1	1.68	0.58
7:1G:36:GLN:CD	17:1Q:49:VAL:HG12	2.27	0.58
7:1G:40:PHE:HE1	7:1G:115:ASP:HB3	1.68	0.58
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.37	0.58
12:1L:258:PHE:HA	12:1L:261:ILE:HD12	1.85	0.58
14:1N:209:ILE:O	14:1N:213:LEU:HD12	2.02	0.58
14:1N:326:LEU:HD23	14:1N:330:ILE:HD11	1.85	0.58
15:1O:133:VAL:HG23	15:1O:205:ALA:HB3	1.86	0.58
25:1Z:129:THR:HG22	25:1Z:131:GLU:H	1.68	0.58
35:1j:10:ARG:NH2	35:1j:14:PHE:O	2.32	0.58
1:1A:105:GLU:OE1	1:1A:111:LEU:N	2.37	0.58
2:1B:152:THR:HG23	4:1D:188:ARG:HD2	1.85	0.58
5:1E:101:GLN:NE2	5:1E:142:VAL:HG21	2.18	0.58
5:1E:206:PRO:HB3	6:1F:23:THR:HB	1.83	0.58
8:1H:86:TRP:HE1	8:1H:229:ALA:HB1	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:160:GLY:HA3	39:1n:94:GLU:OE1	2.03	0.58
12:1L:319:ILE:HG21	12:1L:404:THR:HG22	1.85	0.58
12:1L:384:PRO:HA	12:1L:389:PHE:HB2	1.85	0.58
16:1P:210:VAL:HG13	16:1P:230:PHE:HD2	1.68	0.58
28:1c:28:TRP:CD1	29:1d:66:THR:HG1	2.21	0.58
40:1o:50:LEU:O	40:1o:55:ARG:NH1	2.36	0.58
5:1E:9:HIS:NE2	5:1E:63:ILE:HG13	2.19	0.58
5:1E:9:HIS:HB3	7:1G:187:ILE:HA	1.84	0.58
10:1J:83:TRP:HD1	10:1J:84:VAL:HG23	1.68	0.58
12:1L:3:PRO:O	12:1L:7:LEU:HD12	2.04	0.58
13:1M:326:LEU:HA	13:1M:329:LEU:HD23	1.84	0.58
20:1U:43:ASP:O	20:1U:47:GLN:NE2	2.37	0.58
35:1j:21:GLN:HA	35:1j:24:GLN:HE22	1.68	0.58
37:1l:131:LYS:HD2	37:1l:133:TYR:HE1	1.68	0.58
45:1A:201:3PE:H3A1	27:1b:22:PHE:HB3	1.86	0.58
5:1E:121:GLN:HE22	5:1E:128:VAL:HG13	1.69	0.58
6:1F:294:LEU:O	6:1F:309:LYS:NZ	2.33	0.58
14:1N:230:LEU:HD23	14:1N:296:LEU:HD11	1.85	0.58
19:1S:18:ILE:HG22	19:1S:52:ILE:HG22	1.85	0.58
35:1j:65:GLY:HA3	40:1o:30:PHE:CD2	2.39	0.58
4:1D:351:LEU:HA	4:1D:355:GLY:HA2	1.86	0.58
7:1G:60:GLU:O	7:1G:61:LYS:HG3	2.03	0.58
7:1G:127:ARG:NH2	43:1r:45:SER:OG	2.37	0.58
8:1H:306:SER:O	8:1H:310:MET:N	2.33	0.58
16:1P:192:PRO:HB3	16:1P:258:LEU:HD13	1.85	0.58
4:1D:391:ILE:HB	4:1D:430:ARG:NH2	2.19	0.58
6:1F:105:CYS:N	6:1F:257:ASN:OD1	2.37	0.58
6:1F:393:TRP:CZ3	6:1F:416:GLN:HG2	2.38	0.58
22:1W:85:LYS:HA	22:1W:88:MET:HB2	1.85	0.58
30:1e:21:SER:O	30:1e:21:SER:OG	2.22	0.58
32:1g:100:ARG:HA	32:1g:103:ASN:HD21	1.69	0.58
6:1F:66:ARG:NH1	6:1F:72:GLY:O	2.37	0.58
7:1G:376:VAL:HG12	7:1G:405:LYS:HB2	1.86	0.58
10:1J:12:ILE:HG22	10:1J:39:VAL:HG11	1.86	0.58
12:1L:144:TRP:O	12:1L:223:LYS:NZ	2.37	0.58
13:1M:76:MET:HB3	13:1M:226:ALA:HB1	1.85	0.58
14:1N:123:SER:OG	14:1N:125:GLN:OE1	2.22	0.58
18:1R:7:THR:OG1	18:1R:25:ARG:NH1	2.37	0.58
31:1f:46:ARG:HH12	31:1f:55:THR:HG23	1.69	0.58
6:1F:54:ASP:HA	6:1F:57:LEU:HB2	1.85	0.57
6:1F:347:ILE:HG23	6:1F:350:LEU:HB3	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:87:LYS:HB3	43:1r:54:CYS:SG	2.44	0.57
8:1H:158:GLY:HA2	8:1H:315:PRO:HG2	1.86	0.57
20:1U:28:GLU:OE1	20:1U:28:GLU:N	2.29	0.57
29:1d:17:GLU:OE1	29:1d:17:GLU:N	2.23	0.57
3:1C:194:PHE:O	17:1Q:81:ASN:ND2	2.37	0.57
3:1C:206:PHE:CZ	4:1D:360:PRO:HD3	2.39	0.57
6:1F:347:ILE:CG2	6:1F:350:LEU:HB3	2.33	0.57
7:1G:258:ILE:HG13	7:1G:368:ILE:HD13	1.86	0.57
7:1G:316:ALA:HB3	7:1G:519:PRO:HG3	1.86	0.57
8:1H:169:GLN:O	8:1H:171:HIS:N	2.37	0.57
12:1L:135:ASN:ND2	12:1L:199:GLN:OE1	2.32	0.57
12:1L:587:TYR:O	12:1L:590:SER:OG	2.19	0.57
16:1P:206:TYR:CZ	16:1P:208:VAL:HB	2.39	0.57
19:1S:64:LEU:HD23	19:1S:75:ASN:HB2	1.85	0.57
3:1C:210:ARG:HH22	7:1G:35:MET:HG3	1.68	0.57
9:1I:151:LYS:HD2	9:1I:155:LEU:HD23	1.86	0.57
15:1O:155:VAL:O	15:1O:159:THR:OG1	2.15	0.57
4:1D:86:GLY:O	4:1D:90:LEU:HD12	2.04	0.57
19:1S:78:LEU:HD23	19:1S:78:LEU:H	1.68	0.57
20:1U:32:VAL:HA	20:1U:73:PRO:HB2	1.86	0.57
20:1U:46:ASP:OD1	39:1n:44:ARG:NH1	2.36	0.57
21:1V:93:MET:HA	21:1V:96:TRP:CD1	2.39	0.57
22:1W:114:ARG:HB3	22:1W:115:PRO:CD	2.35	0.57
26:1a:65:GLY:N	26:1a:67:GLU:OE1	2.38	0.57
11:1K:98:CYS:O	14:1N:51:ARG:NH2	2.37	0.57
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.68	0.57
14:1N:179:MET:HE3	14:1N:179:MET:HA	1.86	0.57
19:1S:74:LYS:HD3	19:1S:74:LYS:N	2.20	0.57
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.22	0.57
6:1F:25:LEU:HG	6:1F:269:GLU:HG3	1.87	0.57
12:1L:10:THR:HA	12:1L:13:ILE:HG22	1.86	0.57
12:1L:52:LEU:HA	12:1L:55:MET:HE3	1.86	0.57
12:1L:81:LYS:HD3	12:1L:198:LEU:HD12	1.85	0.57
16:1P:57:MET:HE2	16:1P:57:MET:HA	1.86	0.57
34:1i:32:PRO:HB3	39:1n:114:TYR:HE2	1.69	0.57
2:1B:155:ALA:HB2	9:1I:137:PHE:HB2	1.87	0.57
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.86	0.57
6:1F:105:CYS:HB3	6:1F:109:GLU:OE2	2.03	0.57
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.69	0.57
7:1G:26:VAL:HB	7:1G:68:ALA:HB1	1.85	0.57
16:1P:292:MET:N	16:1P:292:MET:SD	2.77	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:77:TRP:HH2	8:1H:100:LEU:HD11	1.70	0.57
2:1B:62:MET:SD	2:1B:156:LEU:HD11	2.44	0.57
4:1D:235:TRP:HB2	8:1H:278:PRO:HG2	1.84	0.57
12:1L:15:LEU:HD22	12:1L:126:ILE:HG23	1.87	0.57
12:1L:433:GLY:O	36:1k:59:ASN:ND2	2.38	0.57
14:1N:272:LYS:HB3	33:1h:108:LEU:HD11	1.86	0.57
30:1e:72:MET:HG2	30:1e:73:LYS:HE2	1.87	0.57
5:1E:9:HIS:CD2	5:1E:63:ILE:HG21	2.39	0.57
6:1F:146:ALA:O	6:1F:149:LEU:HD12	2.04	0.57
6:1F:337:MET:SD	6:1F:337:MET:N	2.77	0.57
9:1I:54:LYS:HD2	42:1q:91:HIS:NE2	2.20	0.57
12:1L:290:LEU:O	12:1L:523:SER:OG	2.22	0.57
15:1O:145:ARG:NH2	15:1O:147:GLN:OE1	2.38	0.57
16:1P:332:GLU:O	16:1P:334:VAL:N	2.38	0.57
21:1V:22:ARG:O	21:1V:26:LEU:HD22	2.04	0.57
21:1V:43:TYR:HB2	21:1V:99:TRP:CZ3	2.40	0.57
27:1b:10:ASN:HA	27:1b:14:LYS:NZ	2.20	0.57
41:1p:70:VAL:O	41:1p:90:GLN:NE2	2.38	0.57
1:1A:25:PRO:HG2	8:1H:60:PRO:HD3	1.86	0.57
5:1E:58:ASN:ND2	5:1E:60:TRP:CD1	2.73	0.57
7:1G:194:GLU:OE2	7:1G:385:ARG:NH1	2.38	0.57
13:1M:131:ILE:HG23	14:1N:302:LEU:HD21	1.86	0.57
52:1q:201:CDL:H741	52:1q:201:CDL:H552	1.87	0.57
5:1E:111:ARG:HD2	5:1E:151:ALA:HA	1.86	0.56
6:1F:376:MET:HA	6:1F:379:PHE:HB2	1.87	0.56
11:1K:71:ALA:O	11:1K:75:LEU:HD12	2.05	0.56
13:1M:114:GLU:HA	13:1M:175:ASN:HA	1.87	0.56
16:1P:90:VAL:HG12	16:1P:128:LYS:HB2	1.87	0.56
20:1U:8:LEU:HD21	20:1U:88:GLU:OE1	2.05	0.56
20:1U:69:LYS:O	34:1i:2:GLY:N	2.38	0.56
35:1j:8:GLU:H	35:1j:16:GLN:NE2	2.03	0.56
40:1o:116:GLN:N	40:1o:116:GLN:CD	2.63	0.56
4:1D:246:THR:HA	21:1V:11:VAL:HG13	1.85	0.56
5:1E:126:ILE:HG12	5:1E:132:THR:HA	1.87	0.56
6:1F:53:PRO:HB3	6:1F:128:ALA:HA	1.87	0.56
7:1G:511:VAL:O	7:1G:514:ILE:HG22	2.05	0.56
9:1I:99:ARG:H	9:1I:104:ARG:HA	1.69	0.56
12:1L:576:MET:SD	45:1Y:201:3PE:H31	2.45	0.56
6:1F:154:ARG:HH22	44:1s:57:GLU:HB3	1.69	0.56
6:1F:343:ILE:O	6:1F:347:ILE:HD12	2.05	0.56
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:52:LEU:HD23	11:1K:45:THR:HG23	1.87	0.56
12:1L:176:ARG:HA	12:1L:179:ASP:HB2	1.87	0.56
12:1L:350:LEU:O	12:1L:350:LEU:HD23	2.05	0.56
14:1N:267:ILE:HD12	14:1N:279:PRO:HB3	1.87	0.56
16:1P:243:GLN:HE22	16:1P:335:LYS:HE3	1.71	0.56
16:1P:293:THR:HG21	16:1P:342:ILE:HD13	1.88	0.56
20:1U:22:TYR:CE1	36:1k:43:PRO:HB2	2.39	0.56
37:1l:77:ILE:HD11	38:1m:67:TRP:CG	2.40	0.56
1:1A:84:LEU:HD21	8:1H:309:ILE:HG12	1.86	0.56
3:1C:158:GLU:OE2	17:1Q:24:GLY:HA2	2.05	0.56
4:1D:148:LEU:HD21	4:1D:174:ARG:HH21	1.70	0.56
7:1G:36:GLN:NE2	7:1G:39:ARG:HH12	2.03	0.56
7:1G:47:SER:OG	7:1G:165:GLU:OE1	2.22	0.56
7:1G:569:LYS:HG3	7:1G:571:ALA:HB2	1.86	0.56
10:1J:129:ASP:HB3	30:1e:31:ARG:HD2	1.87	0.56
10:1J:152:TRP:CE2	30:1e:13:LEU:HD23	2.40	0.56
12:1L:55:MET:SD	12:1L:471:ASN:ND2	2.78	0.56
12:1L:281:GLY:O	12:1L:285:THR:OG1	2.16	0.56
12:1L:500:LEU:HD23	12:1L:500:LEU:H	1.70	0.56
13:1M:216:LEU:HD22	13:1M:220:HIS:NE2	2.20	0.56
13:1M:361:MET:HA	13:1M:364:LEU:HG	1.86	0.56
20:1T:11:ILE:HD11	20:1T:84:LYS:HZ1	1.70	0.56
21:1V:15:VAL:HA	21:1V:77:GLU:HG2	1.86	0.56
23:1X:34:GLN:OE1	23:1X:116:TRP:NE1	2.38	0.56
42:1q:9:ARG:NH2	52:1q:201:CDL:H1O1	2.01	0.56
2:1B:81:ARG:HH11	2:1B:82:GLN:HA	1.70	0.56
2:1B:179:ARG:HG2	16:1P:50:ARG:HH21	1.71	0.56
3:1C:58:ILE:HG13	3:1C:118:GLU:HG3	1.86	0.56
8:1H:222:MET:HE1	8:1H:226:ALA:HB2	1.87	0.56
14:1N:332:LEU:HD23	14:1N:336:VAL:HG11	1.88	0.56
16:1P:38:LEU:HA	16:1P:41:MET:HE1	1.87	0.56
18:1R:28:PHE:HE1	18:1R:33:LYS:HA	1.71	0.56
3:1C:209:TYR:CD2	4:1D:360:PRO:HD2	2.40	0.56
4:1D:233:ARG:HH22	9:1I:24:THR:HA	1.70	0.56
4:1D:249:ASP:O	4:1D:253:TYR:HD2	1.88	0.56
6:1F:109:GLU:HA	6:1F:112:ARG:NH1	2.20	0.56
6:1F:300:GLY:HA3	6:1F:304:THR:HG21	1.88	0.56
7:1G:107:ILE:HA	7:1G:215:PHE:HZ	1.69	0.56
9:1I:52:PHE:HA	42:1q:62:VAL:HG12	1.87	0.56
11:1K:4:VAL:O	11:1K:8:ILE:HD12	2.06	0.56
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:158:TRP:CE2	39:1n:92:ARG:HD3	2.40	0.56
12:1L:560:THR:HA	12:1L:564:LYS:HB2	1.88	0.56
14:1N:338:PRO:HA	23:1X:169:TRP:HZ2	1.70	0.56
15:1O:138:MET:SD	15:1O:144:ILE:HG23	2.46	0.56
20:1T:35:HIS:CD2	20:1T:38:LYS:H	2.24	0.56
3:1C:202:PRO:O	17:1Q:50:ASN:N	2.38	0.56
6:1F:61:LYS:HZ1	6:1F:80:SER:HB3	1.71	0.56
6:1F:272:MET:HB3	6:1F:317:MET:O	2.06	0.56
7:1G:42:TYR:CE2	7:1G:48:VAL:HG12	2.40	0.56
7:1G:372:GLU:O	7:1G:402:ASN:ND2	2.39	0.56
8:1H:31:MET:SD	9:1I:37:THR:OG1	2.63	0.56
8:1H:136:VAL:HB	10:1J:70:TYR:HE1	1.71	0.56
46:1L:702:PC1:H351	33:1h:40:ILE:HG21	1.87	0.56
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.33	0.56
15:1O:37:ARG:NH1	15:1O:229:GLU:OE1	2.39	0.56
7:1G:359:ARG:NH2	7:1G:629:ASN:HD22	2.04	0.56
12:1L:95:PHE:CE1	12:1L:456:ARG:HG2	2.40	0.56
12:1L:298:ILE:HG12	12:1L:356:ILE:HD13	1.88	0.56
14:1N:159:MET:HE2	14:1N:278:MET:SD	2.46	0.56
14:1N:320:THR:HG21	15:1O:265:ASN:HA	1.87	0.56
4:1D:258:VAL:O	4:1D:262:GLY:N	2.33	0.56
6:1F:82:MET:HE1	6:1F:220:THR:C	2.31	0.56
6:1F:139:ARG:HG2	6:1F:141:GLU:H	1.71	0.56
6:1F:402:HIS:O	7:1G:53:ARG:NH1	2.39	0.56
12:1L:156:GLY:O	13:1M:416:ARG:NH2	2.39	0.56
12:1L:486:MET:N	12:1L:486:MET:SD	2.78	0.56
15:1O:80:GLU:HB3	15:1O:190:HIS:CE1	2.41	0.56
20:1T:7:THR:HG23	20:1T:10:ALA:H	1.70	0.56
40:1o:42:GLN:HA	40:1o:45:MET:HE1	1.87	0.56
3:1C:29:VAL:HA	3:1C:32:ILE:HD11	1.88	0.56
4:1D:19:MET:SD	14:1N:295:ARG:NH1	2.79	0.56
4:1D:236:ARG:O	4:1D:240:VAL:HG22	2.05	0.56
5:1E:145:LEU:N	48:1E:301:FES:S1	2.73	0.56
6:1F:127:ARG:HA	6:1F:171:TYR:HE2	1.70	0.56
6:1F:259:SER:HB3	6:1F:335:ILE:HG22	1.88	0.56
8:1H:136:VAL:CG1	10:1J:70:TYR:CE1	2.89	0.56
10:1J:23:LYS:NZ	11:1K:21:MET:O	2.32	0.56
14:1N:318:GLU:CD	14:1N:319:HIS:H	2.14	0.56
17:1Q:11:ILE:HG21	22:1W:23:ARG:HD2	1.88	0.56
1:1A:63:LEU:HD22	10:1J:67:VAL:HG11	1.88	0.55
8:1H:63:PRO:O	8:1H:66:SER:OG	2.17	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:244:MET:HG3	13:1M:301:ILE:HD11	1.88	0.55
16:1P:46:ILE:O	16:1P:48:PRO:HG2	2.06	0.55
32:1g:100:ARG:HD2	32:1g:107:LEU:HA	1.87	0.55
41:1p:27:ASN:HD22	41:1p:30:THR:H	1.54	0.55
42:1q:117:VAL:O	42:1q:120:THR:OG1	2.23	0.55
2:1B:94:ASN:HA	2:1B:97:ALA:HB2	1.88	0.55
3:1C:131:GLU:N	3:1C:131:GLU:OE1	2.39	0.55
5:1E:48:LEU:O	5:1E:90:TYR:OH	2.24	0.55
7:1G:199:ILE:HG12	7:1G:208:LEU:HD12	1.88	0.55
10:1J:160:SER:O	10:1J:164:GLY:N	2.34	0.55
12:1L:560:THR:O	12:1L:565:THR:OG1	2.24	0.55
13:1M:425:ASN:HD22	38:1m:57:GLY:HA2	1.70	0.55
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.86	0.55
14:1N:217:MET:CE	14:1N:323:MET:HA	2.36	0.55
16:1P:106:PHE:CE2	16:1P:145:TYR:HA	2.41	0.55
16:1P:136:ASN:HA	16:1P:292:MET:HE1	1.87	0.55
16:1P:280:THR:O	16:1P:284:VAL:HG13	2.06	0.55
20:1T:45:LEU:HD22	22:1W:36:TYR:CE2	2.41	0.55
33:1h:38:ILE:HG22	33:1h:42:LEU:HG	1.88	0.55
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.88	0.55
8:1H:136:VAL:CG1	10:1J:70:TYR:HE1	2.19	0.55
19:1S:24:GLN:OE1	19:1S:25:ARG:NH1	2.40	0.55
20:1T:16:LEU:HB3	20:1T:30:LEU:HD21	1.89	0.55
28:1c:6:GLU:CD	28:1c:7:PRO:HD2	2.30	0.55
31:1f:53:GLU:HG2	31:1f:54:VAL:HG23	1.88	0.55
38:1m:7:PRO:HG3	38:1m:13:LEU:HD12	1.89	0.55
2:1B:54:CYS:SG	4:1D:190:HIS:NE2	2.74	0.55
4:1D:4:TRP:CG	13:1M:140:THR:HG1	2.25	0.55
6:1F:57:LEU:HD22	6:1F:61:LYS:HZ1	1.72	0.55
7:1G:558:ASP:OD1	7:1G:558:ASP:N	2.38	0.55
7:1G:575:ASN:HD21	7:1G:577:GLU:HB3	1.71	0.55
13:1M:49:SER:HB2	13:1M:59:ASP:HB3	1.89	0.55
28:1c:28:TRP:NE1	29:1d:66:THR:OG1	2.39	0.55
40:1o:104:GLU:O	40:1o:108:LEU:N	2.39	0.55
4:1D:150:HIS:CB	4:1D:304:MET:HE2	2.34	0.55
4:1D:411:LEU:O	4:1D:414:VAL:HG12	2.06	0.55
7:1G:672:TYR:O	7:1G:678:SER:OG	2.17	0.55
16:1P:212:LYS:O	16:1P:216:ASN:ND2	2.38	0.55
23:1X:112:ASP:OD1	23:1X:113:LYS:N	2.40	0.55
40:1o:110:ARG:HD3	40:1o:114:ARG:HD3	1.88	0.55
6:1F:135:TYR:HD1	6:1F:176:PHE:HB2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:19:MET:HE2	7:1G:19:MET:HA	1.87	0.55
9:1I:99:ARG:NH1	9:1I:101:ASP:OD2	2.39	0.55
11:1K:26:LEU:HD22	11:1K:78:LEU:HD13	1.89	0.55
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	1.89	0.55
16:1P:50:ARG:NH1	55:1P:501:NDP:N3A	2.55	0.55
16:1P:126:VAL:HG22	16:1P:128:LYS:H	1.72	0.55
17:1Q:55:TRP:HB2	17:1Q:86:PHE:HB2	1.88	0.55
34:1i:10:ARG:HH12	39:1n:153:LEU:HB2	1.72	0.55
44:1s:42:GLN:CD	44:1s:42:GLN:H	2.15	0.55
4:1D:289:SER:O	4:1D:291:GLY:N	2.38	0.55
6:1F:184:TYR:HB3	6:1F:357:GLU:HB3	1.88	0.55
7:1G:475:GLN:OE1	7:1G:646:ASN:ND2	2.38	0.55
8:1H:287:HIS:CD2	8:1H:291:LYS:HD2	2.41	0.55
9:1I:70:TYR:CD1	9:1I:76:ARG:HG2	2.41	0.55
9:1I:133:GLU:N	9:1I:133:GLU:OE1	2.40	0.55
14:1N:96:THR:O	14:1N:100:MET:HE2	2.07	0.55
16:1P:2:HIS:HB3	16:1P:5:LEU:HD12	1.89	0.55
21:1V:92:LYS:HB3	21:1V:96:TRP:NE1	2.21	0.55
22:1W:33:ARG:NH1	57:1W:201:EHZ:O9	2.40	0.55
22:1W:115:PRO:O	22:1W:115:PRO:HD2	2.07	0.55
1:1A:84:LEU:HB3	27:1b:42:ILE:HG22	1.88	0.55
2:1B:172:ARG:HH12	2:1B:176:TRP:HB2	1.72	0.55
4:1D:239:THR:HG23	4:1D:294:TYR:HB2	1.89	0.55
4:1D:245:VAL:HG13	4:1D:250:ALA:HB2	1.88	0.55
4:1D:342:MET:HE3	7:1G:101:HIS:HB3	1.89	0.55
6:1F:59:GLU:O	6:1F:63:SER:OG	2.21	0.55
7:1G:366:THR:H	7:1G:491:ASN:ND2	2.04	0.55
7:1G:444:LYS:NZ	7:1G:476:ASN:O	2.39	0.55
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.88	0.55
8:1H:137:ALA:HA	8:1H:140:ILE:HG12	1.89	0.55
10:1J:79:TYR:HE1	16:1P:325:ARG:HA	1.71	0.55
12:1L:514:LYS:NZ	45:1L:703:3PE:O12	2.40	0.55
12:1L:542:LEU:HB3	37:1l:83:MET:HG3	1.88	0.55
16:1P:19:ILE:HG23	16:1P:43:SER:CB	2.34	0.55
16:1P:133:SER:O	16:1P:167:LYS:HA	2.07	0.55
16:1P:263:TYR:CZ	16:1P:284:VAL:HA	2.42	0.55
37:1L:158:ILE:HG13	40:1o:96:LYS:HZ3	1.71	0.55
5:1E:101:GLN:OE1	5:1E:101:GLN:HA	2.07	0.55
6:1F:275:PRO:HG2	6:1F:278:GLU:CG	2.36	0.55
7:1G:627:SER:OG	7:1G:629:ASN:OD1	2.17	0.55
7:1G:688:VAL:O	7:1G:692:THR:OG1	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:577:VAL:HG21	14:1N:167:TRP:HB3	1.88	0.55
13:1M:329:LEU:HD22	13:1M:437:MET:HE1	1.89	0.55
15:1O:73:LEU:HD21	15:1O:295:LYS:HG2	1.89	0.55
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	1.89	0.55
25:1Z:30:LEU:HD23	25:1Z:30:LEU:H	1.72	0.55
37:1L:60:PRO:HG3	37:1L:70:ARG:HH12	1.72	0.55
2:1B:86:MET:HB2	2:1B:107:MET:HE1	1.88	0.55
6:1F:312:CYS:O	6:1F:315:VAL:HG23	2.07	0.55
9:1I:84:GLU:HA	9:1I:92:ILE:HB	1.88	0.55
13:1M:36:LEU:HD21	46:1f:101:PC1:H371	1.89	0.55
16:1P:281:ARG:O	16:1P:284:VAL:HG22	2.06	0.55
33:1h:40:ILE:HD12	33:1h:40:ILE:H	1.72	0.55
4:1D:113:CYS:H	4:1D:145:THR:HG21	1.71	0.54
4:1D:258:VAL:HG12	4:1D:296:ARG:HG2	1.89	0.54
6:1F:78:LYS:HD2	6:1F:79:TRP:HD1	1.72	0.54
6:1F:349:ARG:HH11	6:1F:352:GLU:HG3	1.70	0.54
8:1H:153:VAL:HG13	8:1H:174:MET:HE1	1.89	0.54
16:1P:128:LYS:NZ	16:1P:217:ALA:O	2.39	0.54
34:1i:3:TYR:HE1	34:1i:11:LEU:HG	1.71	0.54
40:1o:27:ASP:N	40:1o:27:ASP:OD1	2.38	0.54
41:1p:37:ASP:HA	41:1p:41:ASP:HB3	1.90	0.54
42:1q:94:THR:OG1	42:1q:96:ASP:OD1	2.25	0.54
3:1C:38:GLN:NE2	3:1C:110:TYR:OH	2.40	0.54
3:1C:132:ARG:NH1	3:1C:149:ARG:H	2.05	0.54
5:1E:123:LYS:HG3	5:1E:124:LEU:N	2.22	0.54
7:1G:343:LEU:O	7:1G:508:LYS:N	2.40	0.54
10:1J:135:PHE:HD1	25:1Z:68:ARG:HH11	1.55	0.54
12:1L:42:TYR:OH	34:1i:66:HIS:ND1	2.26	0.54
12:1L:237:MET:HA	12:1L:237:MET:CE	2.33	0.54
12:1L:331:MET:CE	12:1L:387:THR:HG23	2.38	0.54
37:1L:128:VAL:HG21	40:1o:94:TYR:CE1	2.41	0.54
39:1n:43:MET:HE1	39:1n:46:ARG:HH21	1.71	0.54
40:1o:109:GLN:O	40:1o:113:ARG:HG2	2.08	0.54
4:1D:349:PHE:CD2	7:1G:105:CYS:HB3	2.42	0.54
5:1E:34:ILE:HD13	5:1E:49:PRO:HB2	1.88	0.54
6:1F:150:GLN:HE21	44:1s:51:PHE:HE1	1.54	0.54
6:1F:302:SER:O	6:1F:414:PRO:HG3	2.07	0.54
8:1H:81:LEU:HD12	8:1H:82:ALA:N	2.22	0.54
9:1I:142:GLU:OE1	42:1q:118:SER:OG	2.20	0.54
10:1J:49:GLY:HA2	10:1J:139:GLU:OE1	2.08	0.54
13:1M:329:LEU:HG	13:1M:359:TRP:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:1:ALA:H2	21:1V:64:VAL:HB	1.71	0.54
43:1r:105:LEU:HD12	43:1r:110:PRO:CB	2.37	0.54
2:1B:109:GLU:N	8:1H:59:GLU:OE2	2.40	0.54
4:1D:391:ILE:H	4:1D:430:ARG:NH2	2.05	0.54
12:1L:83:ASP:OD1	12:1L:85:PHE:N	2.38	0.54
12:1L:448:PRO:O	12:1L:452:ASN:ND2	2.37	0.54
37:1l:21:ALA:HA	37:1l:31:VAL:HG12	1.89	0.54
42:1q:92:CYS:O	43:1r:33:ARG:NH1	2.40	0.54
6:1F:43:TYR:HB3	6:1F:236:ARG:NH1	2.21	0.54
6:1F:276:LEU:HD23	6:1F:312:CYS:HB3	1.90	0.54
8:1H:130:ILE:O	8:1H:134:ARG:HG2	2.08	0.54
8:1H:296:LEU:HA	27:1b:21:SER:HB3	1.90	0.54
11:1K:22:TYR:HB2	12:1L:585:LYS:HG2	1.88	0.54
12:1L:35:TYR:OH	34:1i:73:HIS:NE2	2.29	0.54
3:1C:136:ASP:OD2	3:1C:137:MET:N	2.41	0.54
4:1D:173:GLU:HA	4:1D:176:LYS:HZ3	1.73	0.54
5:1E:23:PHE:HB2	5:1E:28:TYR:CE2	2.42	0.54
5:1E:123:LYS:HD3	5:1E:173:ILE:HG21	1.89	0.54
6:1F:24:ASN:O	6:1F:113:HIS:HB3	2.07	0.54
7:1G:55:CYS:SG	7:1G:68:ALA:N	2.81	0.54
13:1M:78:MET:HB3	13:1M:436:LEU:HD12	1.90	0.54
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.42	0.54
14:1N:36:ASN:OD1	14:1N:134:GLN:NE2	2.41	0.54
30:1e:31:ARG:HH21	30:1e:68:ARG:HH21	1.56	0.54
37:1l:123:PRO:HG2	37:1l:125:TYR:HE2	1.72	0.54
4:1D:284:ASP:N	4:1D:306:GLN:OE1	2.38	0.54
6:1F:257:ASN:HB2	6:1F:333:ALA:HA	1.89	0.54
45:1L:701:3PE:H3A2	45:1L:701:3PE:H2G1	1.90	0.54
34:1i:21:TRP:CD1	34:1i:25:GLN:HE22	2.26	0.54
35:1j:32:MET:O	35:1j:36:ILE:HG12	2.08	0.54
36:1k:35:LEU:HB2	36:1k:40:LEU:HG	1.89	0.54
38:1m:36:LEU:HD21	39:1n:150:THR:HA	1.89	0.54
43:1r:63:MET:HE3	43:1r:63:MET:HA	1.89	0.54
2:1B:38:ASN:HA	2:1B:41:ARG:HB2	1.90	0.54
3:1C:41:GLN:HB2	3:1C:51:PHE:HE1	1.73	0.54
3:1C:68:THR:HA	21:1V:82:GLN:HE21	1.73	0.54
4:1D:130:PRO:HG3	4:1D:138:ARG:HH22	1.72	0.54
6:1F:112:ARG:HD2	6:1F:145:GLU:OE2	2.08	0.54
15:1O:210:PHE:HD2	15:1O:211:LEU:HD13	1.72	0.54
21:1V:76:ILE:HA	21:1V:79:VAL:HG12	1.89	0.54
34:1i:68:ILE:HA	34:1i:71:VAL:HG12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:131:LYS:CD	37:1l:133:TYR:HE1	2.21	0.54
38:1m:36:LEU:HD12	38:1m:36:LEU:O	2.08	0.54
38:1m:82:THR:HG23	38:1m:84:LYS:H	1.72	0.54
43:1r:8:GLN:O	43:1r:11:ARG:HG2	2.08	0.54
4:1D:233:ARG:HG2	9:1I:30:LEU:HD21	1.88	0.54
4:1D:414:VAL:O	4:1D:418:ILE:HD12	2.07	0.54
6:1F:65:LEU:HD23	6:1F:242:PHE:CE1	2.42	0.54
6:1F:110:ILE:HD12	6:1F:225:VAL:HG12	1.89	0.54
6:1F:116:HIS:HA	6:1F:119:VAL:HG22	1.90	0.54
9:1I:62:ARG:NH1	9:1I:119:CYS:O	2.41	0.54
11:1K:43:MET:HG3	14:1N:75:ILE:HG21	1.89	0.54
22:1W:31:ARG:HA	22:1W:34:GLU:CD	2.33	0.54
16:1P:197:GLY:O	16:1P:239:PHE:HB2	2.08	0.54
19:1S:42:GLU:OE2	19:1S:42:GLU:N	2.32	0.54
20:1T:31:SER:N	20:1T:34:SER:OG	2.41	0.54
22:1W:52:LEU:HD11	22:1W:104:MET:SD	2.47	0.54
26:1a:12:MET:HA	26:1a:15:CYS:HB2	1.90	0.54
1:1A:98:LEU:HD22	8:1H:298:LEU:HD11	1.89	0.53
3:1C:53:HIS:HE1	17:1Q:6:GLN:HE21	1.54	0.53
6:1F:132:ARG:HH21	44:1s:63:MET:HE1	1.71	0.53
7:1G:305:GLY:C	7:1G:306:MET:HE2	2.33	0.53
7:1G:418:ARG:HE	44:1s:74:ARG:HG3	1.73	0.53
8:1H:283:ASP:OD1	8:1H:283:ASP:N	2.40	0.53
10:1J:68:PHE:CD1	11:1K:75:LEU:HD21	2.42	0.53
12:1L:358:LYS:HE3	39:1n:79:TYR:HE2	1.73	0.53
14:1N:7:THR:HG23	52:1N:402:CDL:H111	1.90	0.53
15:1O:65:ASP:HB2	28:1c:2:PHE:CE1	2.43	0.53
26:1a:2:TRP:NE1	52:1q:201:CDL:OB5	2.41	0.53
28:1c:28:TRP:O	28:1c:32:ILE:HD12	2.08	0.53
31:1f:49:ARG:HG3	31:1f:52:GLU:HB3	1.89	0.53
39:1n:27:GLU:HA	39:1n:36:TYR:CE2	2.44	0.53
41:1p:162:MET:HA	41:1p:165:GLU:HG3	1.89	0.53
2:1B:47:PRO:HA	2:1B:85:VAL:O	2.08	0.53
3:1C:145:HIS:CD2	3:1C:148:LEU:HD21	2.43	0.53
4:1D:284:ASP:CG	43:1r:106:SER:HB2	2.34	0.53
4:1D:417:ILE:O	4:1D:421:GLN:N	2.30	0.53
6:1F:143:TYR:HE1	44:1s:51:PHE:HB2	1.72	0.53
12:1L:76:LEU:HD21	12:1L:196:TRP:HE3	1.72	0.53
14:1N:128:LEU:O	14:1N:132:THR:OG1	2.18	0.53
16:1P:116:ALA:HA	16:1P:119:GLN:HE22	1.73	0.53
36:1k:21:TRP:HB3	36:1k:49:ALA:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:32:ASP:OD2	42:1q:33:VAL:N	2.42	0.53
43:1r:19:LEU:H	43:1r:19:LEU:HD12	1.73	0.53
3:1C:175:ARG:HH12	16:1P:40:ARG:HG2	1.73	0.53
7:1G:257:ASP:HA	7:1G:394:ARG:HH12	1.72	0.53
7:1G:514:ILE:HD11	7:1G:522:LEU:HD13	1.90	0.53
12:1L:51:LEU:HD11	12:1L:88:MET:HE2	1.91	0.53
12:1L:286:LEU:HD21	45:1L:703:3PE:H2D1	1.90	0.53
13:1M:44:GLN:HB2	32:1g:83:TYR:HE1	1.74	0.53
16:1P:244:TYR:HE2	16:1P:310:LEU:HD21	1.73	0.53
20:1T:36:PHE:HA	20:1T:40:LEU:HB3	1.91	0.53
20:1U:36:PHE:O	20:1U:40:LEU:N	2.41	0.53
28:1c:28:TRP:NE1	29:1d:66:THR:HG1	2.06	0.53
33:1h:34:ILE:O	33:1h:37:ALA:N	2.41	0.53
1:1A:98:LEU:O	1:1A:101:SER:OG	2.27	0.53
6:1F:125:GLY:O	6:1F:129:MET:HG2	2.08	0.53
6:1F:182:GLY:O	7:1G:177:ARG:NH2	2.41	0.53
46:1L:702:PC1:H241	13:1M:450:ASN:HB2	1.89	0.53
13:1M:47:GLU:N	13:1M:47:GLU:OE2	2.42	0.53
7:1G:385:ARG:HB2	7:1G:415:LEU:HD13	1.90	0.53
13:1M:102:LEU:HD13	13:1M:128:PRO:HG2	1.91	0.53
13:1M:168:GLN:HE22	33:1h:104:ARG:HD3	1.72	0.53
15:1O:270:LEU:HD23	15:1O:270:LEU:H	1.72	0.53
39:1n:24:ARG:NH1	39:1n:27:GLU:OE2	2.42	0.53
43:1r:57:ASP:O	43:1r:61:GLU:HG2	2.07	0.53
3:1C:30:ALA:HA	3:1C:37:VAL:HG11	1.90	0.53
6:1F:91:LYS:HG3	6:1F:131:ALA:HA	1.90	0.53
7:1G:255:HIS:CE1	7:1G:258:ILE:HB	2.44	0.53
7:1G:439:PHE:O	7:1G:443:LEU:HD12	2.09	0.53
8:1H:143:GLU:HA	8:1H:146:LEU:HB2	1.90	0.53
13:1M:73:LEU:HA	13:1M:76:MET:SD	2.48	0.53
21:1V:85:ASN:HA	21:1V:88:SER:HB3	1.90	0.53
22:1W:24:ASP:OD1	22:1W:27:GLU:N	2.26	0.53
22:1W:65:GLU:HA	22:1W:68:MET:HG2	1.89	0.53
37:1l:158:ILE:HG13	40:1o:96:LYS:NZ	2.24	0.53
43:1r:110:PRO:HD2	43:1r:111:TYR:N	2.13	0.53
11:1K:6:MET:HA	11:1K:9:ILE:HB	1.91	0.53
15:1O:13:ARG:HB2	15:1O:16:ARG:HD3	1.90	0.53
17:1Q:40:PRO:O	17:1Q:52:THR:HG22	2.09	0.53
41:1p:72:ASP:OD1	41:1p:74:THR:HG22	2.08	0.53
7:1G:35:MET:HE1	7:1G:81:THR:HB	1.91	0.53
12:1L:511:LEU:HD11	39:1n:38:TYR:CD2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:9:LEU:HD21	14:1N:42:PRO:HG2	1.90	0.53
16:1P:185:MET:N	16:1P:185:MET:SD	2.82	0.53
20:1T:35:HIS:CE1	20:1T:38:LYS:HD3	2.44	0.53
28:1c:41:GLU:OE2	28:1c:45:ARG:NH2	2.41	0.53
37:1l:135:TYR:OH	40:1o:40:ALA:O	2.27	0.53
3:1C:210:ARG:HH12	7:1G:35:MET:HG3	1.73	0.53
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.44	0.53
4:1D:391:ILE:CB	4:1D:430:ARG:HH12	2.22	0.53
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.90	0.53
7:1G:41:CYS:SG	7:1G:51:ASN:N	2.81	0.53
7:1G:122:MET:HA	7:1G:122:MET:HE3	1.90	0.53
9:1I:146:GLU:HA	42:1q:124:TYR:HD2	1.74	0.53
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.09	0.53
19:1S:44:LYS:O	19:1S:48:PRO:HD3	2.09	0.53
20:1T:45:LEU:HD22	22:1W:36:TYR:CD2	2.44	0.53
28:1c:34:GLN:NE2	28:1c:37:GLU:OE1	2.41	0.53
2:1B:79:SER:O	2:1B:83:SER:OG	2.22	0.53
3:1C:11:ILE:HD12	3:1C:14:ARG:HH22	1.74	0.53
4:1D:307:SER:O	4:1D:311:ILE:HD12	2.09	0.53
6:1F:342:ASP:OD1	6:1F:429:ARG:NH2	2.42	0.53
7:1G:136:ALA:HB1	18:1R:74:ASN:HB2	1.90	0.53
7:1G:180:ASP:OD1	7:1G:180:ASP:N	2.40	0.53
13:1M:268:GLY:O	13:1M:272:THR:OG1	2.24	0.53
14:1N:239:VAL:O	14:1N:243:LEU:HD12	2.08	0.53
4:1D:224:GLU:HG2	9:1I:36:MET:SD	2.48	0.52
4:1D:224:GLU:OE1	9:1I:40:TYR:OH	2.28	0.52
6:1F:322:LEU:HB3	6:1F:327:THR:HG23	1.90	0.52
8:1H:162:LEU:HA	8:1H:165:LEU:HD23	1.92	0.52
8:1H:183:MET:HE1	46:1I:204:PC1:H272	1.90	0.52
9:1I:64:GLU:O	9:1I:134:GLY:N	2.38	0.52
12:1L:316:THR:HB	12:1L:395:ILE:HG23	1.92	0.52
13:1M:359:TRP:HB2	13:1M:415:GLN:HE21	1.73	0.52
14:1N:2:ASN:HB3	14:1N:5:ILE:CD1	2.39	0.52
15:1O:135:LEU:HD21	15:1O:149:VAL:HA	1.90	0.52
18:1R:34:GLU:OE1	42:1q:124:TYR:HA	2.09	0.52
22:1W:90:LEU:HD12	22:1W:91:GLU:N	2.25	0.52
34:1i:83:TYR:HE1	41:1p:48:ARG:HD3	1.75	0.52
7:1G:177:ARG:HA	7:1G:181:MET:HE1	1.91	0.52
9:1I:97:GLU:OE1	42:1q:131:ARG:NH2	2.42	0.52
13:1M:216:LEU:HD12	13:1M:291:VAL:HG22	1.91	0.52
15:1O:171:TYR:HE2	15:1O:211:LEU:HD21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:86:GLU:OE1	18:1R:25:ARG:NH2	2.42	0.52
16:1P:118:ALA:HB2	16:1P:156:VAL:HG23	1.90	0.52
16:1P:169:SER:HB3	16:1P:231:VAL:HG12	1.92	0.52
16:1P:179:LEU:HD13	16:1P:317:VAL:HG11	1.92	0.52
22:1W:99:GLN:OE1	22:1W:99:GLN:N	2.38	0.52
25:1Z:109:SER:OG	25:1Z:111:PHE:O	2.26	0.52
35:1j:67:LEU:O	40:1o:110:ARG:NH2	2.40	0.52
40:1o:72:SER:O	40:1o:75:ASN:HB3	2.09	0.52
2:1B:67:TYR:HE1	2:1B:154:GLU:HB3	1.74	0.52
4:1D:183:ARG:HH11	4:1D:207:LEU:HD23	1.75	0.52
6:1F:19:ASP:OD2	6:1F:245:PHE:CE2	2.62	0.52
8:1H:179:TRP:NE1	25:1Z:43:LEU:HG	2.25	0.52
16:1P:278:TRP:CD1	16:1P:278:TRP:H	2.27	0.52
21:1V:48:GLU:OE1	21:1V:49:GLN:N	2.42	0.52
4:1D:19:MET:O	4:1D:21:PRO:HD3	2.09	0.52
6:1F:224:ASN:O	6:1F:228:VAL:HG23	2.10	0.52
6:1F:342:ASP:O	6:1F:346:ALA:N	2.40	0.52
10:1J:43:ILE:HG22	11:1K:46:LEU:HD11	1.90	0.52
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.91	0.52
16:1P:271:GLU:HA	16:1P:277:PRO:HB3	1.92	0.52
22:1W:35:LEU:HD11	22:1W:39:TRP:CE3	2.44	0.52
33:1h:70:PRO:HD3	41:1p:60:TYR:OH	2.10	0.52
33:1h:114:MET:HG2	33:1h:122:TRP:CD1	2.43	0.52
34:1i:71:VAL:O	34:1i:76:ILE:HG13	2.09	0.52
45:1A:201:3PE:H271	8:1H:295:PRO:HB3	1.91	0.52
6:1F:49:LEU:HG	6:1F:127:ARG:HB2	1.91	0.52
7:1G:246:GLU:HG3	7:1G:248:MET:CE	2.39	0.52
8:1H:124:ASN:C	8:1H:124:ASN:HD22	2.17	0.52
13:1M:46:GLY:O	32:1g:84:ARG:NH1	2.42	0.52
16:1P:266:VAL:HA	16:1P:269:LEU:HD12	1.92	0.52
21:1V:1:ALA:N	21:1V:63:ASP:OD1	2.41	0.52
32:1g:112:CYS:HB3	41:1p:141:ARG:HD2	1.91	0.52
42:1q:9:ARG:HA	42:1q:12:GLN:NE2	2.24	0.52
1:1A:79:SER:HA	1:1A:87:MET:HE3	1.92	0.52
4:1D:147:LEU:HA	4:1D:304:MET:HE1	1.91	0.52
6:1F:258:ILE:HA	6:1F:334:VAL:HG13	1.91	0.52
7:1G:66:VAL:HB	7:1G:71:MET:HG2	1.92	0.52
7:1G:584:LYS:HG3	17:1Q:36:ARG:NE	2.25	0.52
10:1J:35:VAL:O	10:1J:39:VAL:HG12	2.09	0.52
10:1J:174:GLY:HA2	14:1N:48:PHE:HE2	1.75	0.52
12:1L:393:ASP:OD1	12:1L:393:ASP:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:302:MET:HA	13:1M:302:MET:HE3	1.91	0.52
15:1O:27:VAL:HG21	15:1O:39:ALA:HB2	1.92	0.52
41:1p:158:GLN:O	41:1p:161:ARG:N	2.36	0.52
2:1B:62:MET:HG2	2:1B:69:MET:HB3	1.92	0.52
2:1B:158:TYR:HE2	42:1q:78:ASP:HB2	1.74	0.52
5:1E:93:LYS:HD3	5:1E:94:PRO:HD2	1.90	0.52
8:1H:85:MET:HG3	8:1H:233:MET:HE2	1.92	0.52
10:1J:173:ARG:NH1	14:1N:1:FME:O1	2.43	0.52
12:1L:153:LEU:HD21	13:1M:360:LEU:HD11	1.91	0.52
18:1R:28:PHE:CE1	18:1R:33:LYS:HA	2.45	0.52
20:1U:27:PRO:HA	20:1U:30:LEU:HD12	1.90	0.52
39:1n:92:ARG:HD2	39:1n:93:TYR:CE2	2.43	0.52
1:1A:73:LEU:HD12	10:1J:55:MET:SD	2.50	0.52
3:1C:39:GLN:HE22	43:1r:67:ILE:HD11	1.74	0.52
4:1D:147:LEU:HD22	4:1D:218:PHE:HE2	1.74	0.52
7:1G:640:ASN:HD21	19:1S:24:GLN:HG3	1.75	0.52
10:1J:18:VAL:HG22	11:1K:14:ILE:HG21	1.91	0.52
13:1M:124:ALA:HB1	14:1N:256:PRO:HD3	1.90	0.52
14:1N:91:ASN:OD1	14:1N:94:ALA:N	2.36	0.52
16:1P:50:ARG:HB3	16:1P:73:TRP:NE1	2.24	0.52
25:1Z:127:LEU:O	30:1e:97:HIS:ND1	2.43	0.52
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.91	0.52
12:1L:144:TRP:CE2	12:1L:223:LYS:HE2	2.45	0.52
14:1N:153:LEU:O	14:1N:156:THR:OG1	2.26	0.52
14:1N:175:LEU:HD13	14:1N:219:LEU:HD21	1.91	0.52
19:1S:55:ARG:H	19:1S:55:ARG:CZ	2.23	0.52
23:1X:73:ILE:HD12	23:1X:74:LYS:N	2.24	0.52
23:1X:107:ASP:N	23:1X:107:ASP:OD1	2.39	0.52
32:1g:64:PHE:HA	32:1g:68:ILE:HB	1.92	0.52
34:1i:100:LYS:NZ	41:1p:116:GLU:OE1	2.37	0.52
39:1n:30:CYS:O	39:1n:32:HIS:N	2.43	0.52
4:1D:163:ALA:O	4:1D:166:PRO:HD2	2.10	0.52
4:1D:352:TYR:CD2	9:1I:86:VAL:HG21	2.45	0.52
7:1G:554:ALA:HA	7:1G:560:ILE:HD11	1.92	0.52
9:1I:7:MET:HA	9:1I:7:MET:HE3	1.93	0.52
13:1M:19:LYS:HB2	13:1M:22:MET:HG2	1.91	0.52
13:1M:130:LEU:HG	13:1M:150:LEU:HD12	1.92	0.52
14:1N:341:PRO:HB2	29:1d:79:GLN:NE2	2.24	0.52
18:1R:18:TYR:CE1	18:1R:24:ARG:HB2	2.45	0.52
20:1T:58:PHE:CD1	20:1T:60:PHE:HD1	2.27	0.52
20:1T:72:CYS:N	20:1T:75:GLU:OE1	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.26	0.52
30:1e:16:TRP:CE3	30:1e:17:MET:HB3	2.45	0.52
30:1e:86:ILE:HG22	30:1e:91:TYR:O	2.10	0.52
46:1f:101:PC1:H342	33:1h:79:PHE:CE2	2.45	0.52
36:1k:40:LEU:HD23	36:1k:40:LEU:H	1.74	0.52
7:1G:59:ILE:HG21	7:1G:77:TRP:HE1	1.75	0.51
7:1G:283:MET:SD	7:1G:291:LEU:HB3	2.50	0.51
8:1H:264:LEU:HD11	26:1a:12:MET:SD	2.50	0.51
13:1M:434:ASN:HB3	33:1h:21:PHE:CE2	2.45	0.51
17:1Q:127:ARG:HG2	44:1s:70:ARG:HH12	1.75	0.51
20:1U:6:LEU:HD23	20:1U:6:LEU:H	1.75	0.51
29:1d:33:TYR:O	29:1d:36:PHE:HB3	2.10	0.51
33:1h:36:VAL:O	33:1h:40:ILE:HD12	2.10	0.51
6:1F:137:TYR:HB2	6:1F:196:ILE:HD11	1.92	0.51
6:1F:275:PRO:HD3	6:1F:278:GLU:OE2	2.10	0.51
13:1M:30:HIS:HA	13:1M:33:LEU:HD12	1.91	0.51
15:1O:179:ILE:HD12	15:1O:180:GLN:N	2.25	0.51
16:1P:29:PHE:HD1	16:1P:175:GLU:CD	2.18	0.51
43:1r:101:LYS:HD3	43:1r:101:LYS:N	2.20	0.51
5:1E:142:VAL:HG23	5:1E:143:GLU:O	2.10	0.51
7:1G:162:PHE:HZ	7:1G:198:ASN:HD22	1.57	0.51
7:1G:319:ALA:HB3	7:1G:345:THR:HA	1.91	0.51
10:1J:33:LEU:HD22	10:1J:65:LEU:HG	1.91	0.51
12:1L:71:LEU:HD11	13:1M:380:PHE:CZ	2.45	0.51
12:1L:312:LEU:HD12	12:1L:328:HIS:CD2	2.44	0.51
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.92	0.51
20:1U:22:TYR:CD2	20:1U:25:ILE:HD13	2.45	0.51
20:1U:64:ASP:OD2	39:1n:17:ARG:NE	2.43	0.51
32:1g:85:MET:HE2	32:1g:85:MET:N	2.24	0.51
2:1B:137:ASP:HB2	2:1B:145:TYR:OH	2.10	0.51
3:1C:32:ILE:HD13	3:1C:33:LEU:HD23	1.93	0.51
3:1C:155:TYR:HB2	22:1W:102:HIS:CE1	2.46	0.51
7:1G:166:ILE:HG12	7:1G:262:TRP:CH2	2.45	0.51
8:1H:126:LYS:O	8:1H:130:ILE:HG12	2.10	0.51
8:1H:167:THR:HG22	23:1X:97:ARG:HH22	1.76	0.51
14:1N:215:MET:HE1	14:1N:244:MET:SD	2.50	0.51
20:1U:37:MET:N	20:1U:37:MET:SD	2.83	0.51
21:1V:19:PRO:CD	21:1V:20:HIS:N	2.72	0.51
22:1W:22:SER:OG	22:1W:27:GLU:OE2	2.23	0.51
29:1d:101:PHE:HZ	33:1h:110:VAL:HG22	1.76	0.51
33:1h:9:PHE:HE2	33:1h:11:ILE:HG12	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:13:GLN:NE2	39:1n:156:ALA:H	2.09	0.51
41:1p:139:GLN:O	41:1p:143:SER:OG	2.29	0.51
3:1C:61:LEU:HD21	3:1C:107:VAL:HG21	1.92	0.51
5:1E:205:PRO:O	5:1E:207:LYS:NZ	2.39	0.51
7:1G:545:TYR:HB3	7:1G:560:ILE:HD13	1.91	0.51
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.46	0.51
13:1M:269:MET:HE1	13:1M:296:LEU:HG	1.93	0.51
14:1N:292:PHE:HA	14:1N:295:ARG:HB2	1.91	0.51
16:1P:86:GLU:OE1	16:1P:87:HIS:ND1	2.43	0.51
16:1P:97:ARG:HH22	55:1P:501:NDP:H2B	1.74	0.51
19:1S:39:ARG:NH1	19:1S:87:THR:OG1	2.44	0.51
28:1c:45:ARG:NH1	29:1d:20:SER:OG	2.41	0.51
35:1j:56:PRO:HA	35:1j:59:TRP:CD2	2.46	0.51
7:1G:59:ILE:HG12	7:1G:60:GLU:O	2.10	0.51
7:1G:349:PHE:HB3	7:1G:509:PRO:HB2	1.93	0.51
7:1G:599:ILE:HG13	7:1G:600:ILE:N	2.26	0.51
7:1G:620:ARG:NE	7:1G:633:TYR:OH	2.44	0.51
8:1H:193:THR:O	8:1H:193:THR:OG1	2.28	0.51
8:1H:281:ARG:NE	8:1H:284:GLN:OE1	2.40	0.51
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.11	0.51
12:1L:366:MET:HB3	12:1L:369:THR:HB	1.93	0.51
13:1M:139:GLN:HG3	13:1M:140:THR:H	1.76	0.51
14:1N:108:LEU:HD12	14:1N:191:THR:HG21	1.93	0.51
29:1d:95:LYS:H	29:1d:95:LYS:HD2	1.74	0.51
31:1f:48:LEU:HD21	31:1f:53:GLU:HA	1.92	0.51
39:1n:153:LEU:HG	39:1n:165:LEU:HD12	1.91	0.51
3:1C:11:ILE:O	4:1D:129:GLN:HG2	2.11	0.51
4:1D:141:PHE:HA	4:1D:144:ILE:HG22	1.92	0.51
5:1E:147:ALA:HB2	6:1F:108:ARG:NE	2.25	0.51
8:1H:17:VAL:CG1	8:1H:228:TYR:HD2	2.18	0.51
8:1H:181:LEU:HA	8:1H:184:MET:HB2	1.92	0.51
13:1M:134:THR:O	13:1M:142:ARG:NE	2.43	0.51
13:1M:278:ARG:NH1	37:1l:82:ASP:OD1	2.42	0.51
13:1M:447:LEU:HD21	13:1M:454:ILE:HD12	1.93	0.51
17:1Q:34:LYS:NZ	17:1Q:103:PHE:O	2.44	0.51
17:1Q:81:ASN:O	17:1Q:82:LEU:HD23	2.11	0.51
20:1T:54:MET:HA	20:1T:54:MET:HE3	1.91	0.51
20:1U:69:LYS:HB3	34:1i:3:TYR:CE2	2.45	0.51
22:1W:35:LEU:HD11	22:1W:39:TRP:HE3	1.75	0.51
30:1e:46:ILE:HG22	30:1e:50:ARG:HB3	1.93	0.51
32:1g:79:TYR:HE1	33:1h:69:HIS:CD2	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:90:GLU:HA	40:1o:93:ASP:OD2	2.10	0.51
2:1B:142:VAL:HG11	2:1B:145:TYR:CE2	2.45	0.51
4:1D:227:GLU:HA	25:1Z:25:LEU:HD11	1.91	0.51
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.91	0.51
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.93	0.51
14:1N:77:ASN:ND2	14:1N:89:MET:HB3	2.25	0.51
14:1N:211:MET:HE1	14:1N:251:MET:HA	1.93	0.51
19:1S:79:ASN:OD1	19:1S:80:ASN:ND2	2.44	0.51
21:1V:7:THR:HG22	21:1V:9:GLY:H	1.75	0.51
35:1j:61:ASP:OD1	40:1o:106:ARG:NH1	2.44	0.51
42:1q:56:PHE:HA	42:1q:59:HIS:HD2	1.76	0.51
8:1H:17:VAL:HA	8:1H:228:TYR:CD2	2.45	0.51
9:1I:175:TYR:CE1	43:1r:38:PRO:HG3	2.46	0.51
12:1L:378:LEU:HD22	12:1L:383:MET:HE3	1.92	0.51
13:1M:243:MET:HB3	13:1M:301:ILE:HG21	1.92	0.51
13:1M:244:MET:HG3	13:1M:301:ILE:CD1	2.41	0.51
15:1O:168:VAL:HG22	15:1O:219:GLU:HB2	1.93	0.51
4:1D:29:LYS:HG2	4:1D:30:PRO:HD2	1.92	0.51
4:1D:241:ASP:OD2	4:1D:290:ARG:NH2	2.43	0.51
5:1E:55:GLN:NE2	5:1E:56:ARG:NH2	2.55	0.51
6:1F:68:ARG:HB3	6:1F:106:LYS:NZ	2.26	0.51
14:1N:2:ASN:HB2	15:1O:254:ARG:HD3	1.92	0.51
25:1Z:38:VAL:O	25:1Z:42:THR:HG23	2.10	0.51
32:1g:97:VAL:HG13	32:1g:107:LEU:HD12	1.93	0.51
39:1n:125:LYS:O	39:1n:129:ARG:HG3	2.11	0.51
5:1E:149:VAL:HG11	6:1F:267:THR:HG23	1.92	0.50
6:1F:409:ASP:HB3	6:1F:413:TRP:CZ2	2.47	0.50
7:1G:194:GLU:HG2	7:1G:195:LEU:HD23	1.92	0.50
9:1I:70:TYR:CE1	9:1I:76:ARG:HG2	2.46	0.50
15:1O:312:VAL:HG11	28:1c:2:PHE:HB2	1.92	0.50
21:1V:19:PRO:CD	21:1V:20:HIS:H	2.16	0.50
23:1X:14:VAL:HG22	23:1X:60:LYS:HD3	1.93	0.50
25:1Z:140:PHE:HB2	26:1a:45:TRP:CG	2.45	0.50
27:1b:14:LYS:HD3	27:1b:14:LYS:N	2.25	0.50
30:1e:77:ALA:HA	30:1e:80:ARG:HB2	1.93	0.50
37:1l:131:LYS:HE2	40:1o:97:ARG:NH1	2.26	0.50
2:1B:112:TYR:CZ	2:1B:167:ILE:HD11	2.46	0.50
3:1C:78:LEU:HA	3:1C:93:VAL:O	2.11	0.50
6:1F:45:THR:O	6:1F:49:LEU:HD13	2.11	0.50
6:1F:347:ILE:HD12	6:1F:347:ILE:H	1.75	0.50
7:1G:106:PRO:HB2	9:1I:78:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:380:VAL:HA	7:1G:409:ILE:HD11	1.93	0.50
9:1I:112:ASP:CG	9:1I:115:LYS:HB2	2.36	0.50
12:1L:199:GLN:HA	41:1p:113:GLN:HG2	1.93	0.50
12:1L:213:LEU:HB3	12:1L:273:VAL:HG21	1.94	0.50
12:1L:593:ILE:O	12:1L:597:ILE:HG23	2.11	0.50
13:1M:105:PHE:O	13:1M:109:THR:OG1	2.26	0.50
13:1M:325:MET:CE	13:1M:441:ILE:HG12	2.37	0.50
16:1P:112:LYS:O	16:1P:115:HIS:ND1	2.43	0.50
29:1d:112:ILE:O	41:1p:159:LYS:NZ	2.37	0.50
7:1G:53:ARG:NH2	7:1G:56:LEU:HD21	2.23	0.50
8:1H:186:PHE:O	8:1H:189:THR:OG1	2.28	0.50
12:1L:15:LEU:HD21	12:1L:125:LEU:HD23	1.93	0.50
12:1L:323:HIS:NE2	40:1o:51:MET:HE1	2.26	0.50
12:1L:600:THR:HG22	12:1L:601:LEU:H	1.76	0.50
14:1N:77:ASN:ND2	14:1N:89:MET:SD	2.85	0.50
16:1P:20:VAL:HB	16:1P:89:ASN:H	1.75	0.50
21:1V:27:TYR:HB3	21:1V:55:LEU:HG	1.93	0.50
21:1V:52:ASN:OD1	21:1V:53:GLU:N	2.45	0.50
24:1Y:46:ALA:HB3	24:1Y:50:GLU:HG3	1.92	0.50
31:1f:28:ARG:HH12	46:1f:101:PC1:H112	1.75	0.50
32:1g:55:LEU:HD11	32:1g:59:ARG:HE	1.75	0.50
39:1n:93:TYR:HD1	39:1n:176:ARG:CD	2.24	0.50
6:1F:101:GLU:OE2	6:1F:302:SER:N	2.37	0.50
9:1I:114:THR:HG21	9:1I:144:HIS:HE1	1.76	0.50
12:1L:216:LEU:HD22	12:1L:259:LEU:HD11	1.93	0.50
13:1M:341:THR:HG21	38:1m:64:LEU:HD21	1.92	0.50
19:1S:30:GLN:HA	19:1S:33:ARG:HH11	1.75	0.50
19:1S:73:GLU:H	19:1S:74:LYS:HZ3	1.59	0.50
23:1X:39:ASN:HD22	25:1Z:73:PRO:HB2	1.77	0.50
23:1X:74:LYS:NZ	26:1a:66:LEU:O	2.34	0.50
32:1g:95:ARG:HH22	41:1p:64:HIS:CD2	2.29	0.50
1:1A:59:ALA:HB1	10:1J:67:VAL:HG23	1.92	0.50
3:1C:132:ARG:HH22	3:1C:149:ARG:HB2	1.76	0.50
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.76	0.50
8:1H:184:MET:HE1	8:1H:293:PHE:CD2	2.46	0.50
10:1J:163:ILE:HA	10:1J:166:VAL:HG12	1.94	0.50
51:1M:501:PGT:H242	14:1N:284:MET:HG3	1.93	0.50
18:1R:89:LEU:HB3	18:1R:91:PHE:HE1	1.77	0.50
21:1V:29:LYS:O	21:1V:33:VAL:HG23	2.11	0.50
23:1X:64:GLN:HA	23:1X:67:LEU:HD12	1.93	0.50
28:1c:17:VAL:O	28:1c:21:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:10:ASN:HD21	8:1H:83:LEU:HB3	1.76	0.50
1:1A:75:LEU:HD13	8:1H:305:ILE:HD12	1.94	0.50
2:1B:92:LEU:HD11	2:1B:100:LEU:HD13	1.93	0.50
3:1C:137:MET:HE3	3:1C:152:LEU:HB3	1.94	0.50
4:1D:335:ARG:NH2	9:1I:126:CYS:O	2.37	0.50
7:1G:27:LEU:HA	7:1G:37:ILE:HD13	1.93	0.50
8:1H:162:LEU:HD21	8:1H:237:PHE:HE1	1.77	0.50
9:1I:26:LEU:HD12	9:1I:26:LEU:O	2.12	0.50
13:1M:399:ASN:O	13:1M:403:THR:OG1	2.25	0.50
18:1R:37:GLU:OE1	18:1R:37:GLU:N	2.30	0.50
23:1X:45:CYS:HB2	23:1X:134:ARG:NH2	2.26	0.50
31:1f:41:SER:HB3	33:1h:91:MET:HE1	1.92	0.50
40:1o:65:LEU:HD22	40:1o:82:GLU:HB3	1.93	0.50
42:1q:48:TYR:HD1	42:1q:62:VAL:HG23	1.77	0.50
43:1r:105:LEU:HD12	43:1r:110:PRO:HB2	1.92	0.50
3:1C:184:VAL:HG21	22:1W:110:THR:HB	1.94	0.50
4:1D:399:LEU:HD23	4:1D:428:VAL:HG21	1.94	0.50
6:1F:343:ILE:CD1	6:1F:418:LEU:HD21	2.25	0.50
7:1G:127:ARG:HH21	43:1r:45:SER:HG	1.60	0.50
7:1G:432:ILE:H	7:1G:432:ILE:HD12	1.75	0.50
13:1M:263:MET:HE2	38:1m:100:TRP:C	2.36	0.50
21:1V:18:THR:O	21:1V:18:THR:OG1	2.27	0.50
22:1W:62:LYS:HZ3	22:1W:106:PHE:C	2.18	0.50
25:1Z:94:GLU:HG3	25:1Z:106:VAL:HG12	1.94	0.50
4:1D:180:PHE:O	4:1D:184:VAL:HG22	2.11	0.50
10:1J:68:PHE:HE1	11:1K:75:LEU:HD11	1.76	0.50
12:1L:254:VAL:HG21	12:1L:329:ILE:HG23	1.93	0.50
15:1O:244:ASP:OD1	15:1O:245:LYS:NZ	2.45	0.50
16:1P:244:TYR:O	16:1P:248:VAL:HG23	2.12	0.50
17:1Q:12:ALA:HA	22:1W:16:SER:HA	1.92	0.50
20:1T:35:HIS:HD2	20:1T:37:MET:H	1.58	0.50
27:1b:12:TRP:HD1	27:1b:19:VAL:HG11	1.76	0.50
2:1B:71:ARG:O	8:1H:37:PRO:HA	2.11	0.50
2:1B:71:ARG:NH1	9:1I:49:ASN:OD1	2.42	0.50
4:1D:106:LEU:HD11	4:1D:391:ILE:HG12	1.94	0.50
4:1D:225:LEU:O	4:1D:229:LEU:HB2	2.12	0.50
4:1D:301:VAL:O	4:1D:304:MET:HB2	2.11	0.50
5:1E:156:ILE:HG12	5:1E:161:TYR:HE2	1.77	0.50
7:1G:56:LEU:HD22	7:1G:65:VAL:HG12	1.94	0.50
12:1L:166:THR:HG21	45:1L:701:3PE:H112	1.94	0.50
15:1O:48:LEU:HD23	15:1O:123:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:118:THR:OG1	15:1O:120:GLN:HG3	2.11	0.50
17:1Q:67:ASN:OD1	17:1Q:72:TRP:N	2.45	0.50
23:1X:78:ALA:O	23:1X:82:THR:HG23	2.12	0.50
24:1Y:35:VAL:HG21	45:1Y:202:3PE:H252	1.94	0.50
25:1Z:110:VAL:HG11	30:1e:71:THR:HB	1.93	0.50
35:1j:27:PHE:CD1	35:1j:27:PHE:C	2.90	0.50
36:1k:18:TYR:HB2	36:1k:19:LYS:NZ	2.26	0.50
4:1D:170:MET:HE1	4:1D:218:PHE:HE1	1.77	0.49
7:1G:100:ASN:HD21	7:1G:179:ASN:HD21	1.58	0.49
7:1G:588:THR:HG22	22:1W:126:HIS:CE1	2.47	0.49
10:1J:78:MET:HE2	10:1J:78:MET:HA	1.94	0.49
11:1K:24:SER:O	11:1K:89:TYR:HD1	1.95	0.49
15:1O:261:MET:SD	15:1O:264:GLN:NE2	2.85	0.49
16:1P:209:ASP:HA	16:1P:212:LYS:HE2	1.93	0.49
32:1g:114:ASP:HB3	32:1g:117:LYS:HG3	1.94	0.49
34:1i:1:SAC:C	34:1i:1:SAC:H2A1	2.42	0.49
37:1l:3:HIS:CG	37:1l:4:VAL:H	2.28	0.49
38:1m:60:GLU:OE2	38:1m:60:GLU:N	2.41	0.49
42:1q:48:TYR:HE2	42:1q:86:TRP:CD2	2.30	0.49
2:1B:54:CYS:HA	4:1D:108:TYR:HB2	1.93	0.49
4:1D:233:ARG:NH2	9:1I:24:THR:HA	2.27	0.49
6:1F:145:GLU:OE1	6:1F:145:GLU:HA	2.12	0.49
6:1F:394:GLU:HB2	7:1G:129:ARG:HH22	1.77	0.49
7:1G:59:ILE:HA	7:1G:80:LEU:HB2	1.94	0.49
7:1G:379:LEU:HD12	7:1G:408:LEU:HB3	1.95	0.49
8:1H:32:GLN:OE1	8:1H:34:ARG:NH2	2.34	0.49
13:1M:233:ALA:C	13:1M:237:LYS:HZ3	2.20	0.49
13:1M:332:THR:HG22	13:1M:433:GLU:HG2	1.93	0.49
14:1N:147:GLN:HB3	33:1h:125:TYR:CD1	2.45	0.49
16:1P:46:ILE:HD12	18:1R:26:VAL:HG21	1.93	0.49
25:1Z:112:HIS:N	30:1e:61:ASP:OD2	2.45	0.49
38:1m:2:PHE:HB2	39:1n:72:TYR:CG	2.47	0.49
39:1n:47:PHE:HA	39:1n:50:HIS:CE1	2.47	0.49
3:1C:125:LYS:NZ	4:1D:253:TYR:CE2	2.79	0.49
6:1F:26:TYR:HB3	6:1F:28:ARG:CZ	2.41	0.49
7:1G:372:GLU:HA	7:1G:398:SER:OG	2.12	0.49
7:1G:399:TRP:HH2	44:1s:74:ARG:NE	2.10	0.49
7:1G:567:THR:HG22	7:1G:586:ALA:HB3	1.93	0.49
7:1G:579:ARG:O	7:1G:581:GLN:NE2	2.45	0.49
12:1L:137:LEU:HB2	12:1L:196:TRP:HB3	1.94	0.49
13:1M:35:SER:O	13:1M:39:LEU:HD12	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:127:VAL:O	13:1M:131:ILE:HG13	2.12	0.49
15:1O:23:LYS:HA	15:1O:167:HIS:ND1	2.26	0.49
15:1O:188:ASN:HB2	15:1O:191:GLU:HG3	1.94	0.49
16:1P:270:PHE:HD2	16:1P:278:TRP:HB2	1.78	0.49
16:1P:323:THR:HG23	16:1P:325:ARG:H	1.77	0.49
22:1W:20:ILE:HG12	22:1W:77:ARG:HG2	1.94	0.49
22:1W:39:TRP:HH2	22:1W:89:GLU:HB2	1.77	0.49
24:1Y:87:LEU:HD12	24:1Y:90:PHE:HB3	1.95	0.49
34:1i:68:ILE:HD12	34:1i:69:PHE:N	2.27	0.49
35:1j:32:MET:HE1	35:1j:33:TRP:CD1	2.46	0.49
38:1m:53:PRO:HG3	39:1n:128:ARG:HD3	1.94	0.49
40:1o:56:ASP:OD1	40:1o:57:TYR:N	2.45	0.49
3:1C:184:VAL:HG11	22:1W:110:THR:HG21	1.94	0.49
9:1I:27:TRP:NE1	46:1I:203:PC1:O21	2.45	0.49
13:1M:72:LEU:HD11	13:1M:233:ALA:HB3	1.95	0.49
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.94	0.49
13:1M:247:THR:HA	13:1M:250:LEU:HD12	1.95	0.49
19:1S:82:SER:OG	19:1S:83:ALA:N	2.43	0.49
21:1V:30:ILE:HD12	21:1V:31:LEU:N	2.28	0.49
35:1j:24:GLN:OE1	35:1j:24:GLN:N	2.44	0.49
2:1B:156:LEU:C	2:1B:156:LEU:HD12	2.38	0.49
5:1E:21:PHE:CZ	5:1E:23:PHE:HE2	2.30	0.49
5:1E:202:LEU:O	44:1s:35:ASN:ND2	2.39	0.49
6:1F:105:CYS:O	6:1F:109:GLU:HG2	2.13	0.49
7:1G:194:GLU:HG2	7:1G:195:LEU:CD2	2.42	0.49
7:1G:534:ARG:NH2	7:1G:556:MET:O	2.44	0.49
10:1J:33:LEU:HD22	10:1J:65:LEU:CD1	2.42	0.49
36:1k:25:GLY:N	36:1k:29:GLU:OE2	2.40	0.49
36:1k:35:LEU:HD11	36:1k:41:ARG:C	2.37	0.49
3:1C:167:PRO:HA	17:1Q:82:LEU:HD21	1.93	0.49
4:1D:171:PHE:CD1	4:1D:174:ARG:HD3	2.48	0.49
6:1F:28:ARG:HB3	44:1s:33:PHE:O	2.13	0.49
6:1F:343:ILE:HD12	6:1F:343:ILE:C	2.38	0.49
6:1F:412:ALA:HB1	6:1F:416:GLN:NE2	2.27	0.49
12:1L:83:ASP:N	12:1L:86:SER:OG	2.37	0.49
13:1M:313:THR:HA	13:1M:316:MET:HE3	1.95	0.49
15:1O:242:LYS:HG3	15:1O:244:ASP:HB3	1.94	0.49
16:1P:332:GLU:CD	16:1P:333:ASP:H	2.20	0.49
29:1d:46:ASN:HB2	29:1d:51:ARG:HB2	1.92	0.49
35:1j:8:GLU:O	35:1j:16:GLN:NE2	2.39	0.49
3:1C:36:TYR:CZ	3:1C:56:GLY:HA3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.94	0.49
3:1C:206:PHE:HZ	4:1D:360:PRO:HD3	1.75	0.49
7:1G:13:VAL:HG23	7:1G:13:VAL:O	2.13	0.49
7:1G:306:MET:HE2	7:1G:306:MET:N	2.28	0.49
8:1H:142:TYR:CD2	8:1H:289:LEU:HD22	2.48	0.49
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.47	0.49
12:1L:542:LEU:HD21	37:1I:88:ARG:HD2	1.95	0.49
13:1M:54:LEU:HD11	31:1f:34:LEU:HD11	1.94	0.49
16:1P:173:GLY:N	16:1P:176:ASP:HB3	2.27	0.49
34:1i:10:ARG:HD3	39:1n:155:PRO:HA	1.94	0.49
3:1C:36:TYR:CE2	3:1C:56:GLY:HA3	2.48	0.49
3:1C:79:THR:OG1	4:1D:390:LYS:HE3	2.13	0.49
6:1F:145:GLU:HA	6:1F:148:ASN:HD22	1.77	0.49
7:1G:161:ARG:O	7:1G:165:GLU:HG3	2.12	0.49
8:1H:134:ARG:HD2	8:1H:282:TYR:CE2	2.47	0.49
8:1H:136:VAL:CB	10:1J:70:TYR:HE1	2.25	0.49
8:1H:287:HIS:HE1	46:1I:203:PC1:H141	1.77	0.49
10:1J:33:LEU:HD22	10:1J:65:LEU:HD11	1.95	0.49
10:1J:111:GLU:HB2	30:1e:80:ARG:HH22	1.78	0.49
12:1L:149:ILE:HG12	13:1M:364:LEU:HD22	1.94	0.49
13:1M:90:THR:HG21	45:1N:401:3PE:O21	2.11	0.49
13:1M:141:GLU:HG3	13:1M:141:GLU:O	2.12	0.49
13:1M:201:MET:HE1	13:1M:261:PHE:CZ	2.48	0.49
15:1O:281:GLU:OE1	15:1O:281:GLU:N	2.42	0.49
21:1V:33:VAL:HA	21:1V:36:GLN:HE22	1.78	0.49
23:1X:7:PRO:HD2	25:1Z:84:LEU:HD11	1.94	0.49
23:1X:43:MET:HE1	27:1b:52:TYR:CE1	2.48	0.49
23:1X:69:PHE:HA	23:1X:72:GLN:HE22	1.78	0.49
25:1Z:129:THR:OG1	30:1e:98:LEU:O	2.29	0.49
30:1e:25:PRO:O	30:1e:28:ILE:HG13	2.13	0.49
38:1m:40:SER:HA	38:1m:43:LYS:HB2	1.94	0.49
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.94	0.49
10:1J:115:ILE:O	10:1J:117:PHE:N	2.46	0.49
11:1K:1:FME:HCN	30:1e:69:GLN:OE1	2.12	0.49
11:1K:94:ASN:HB3	12:1L:583:LEU:HD13	1.94	0.49
13:1M:269:MET:O	13:1M:273:SER:OG	2.23	0.49
15:1O:89:ASN:O	32:1g:23:THR:N	2.45	0.49
15:1O:190:HIS:HA	15:1O:193:LYS:NZ	2.28	0.49
38:1m:62:PRO:HB2	38:1m:66:ARG:HH12	1.78	0.49
41:1p:118:GLU:OE1	41:1p:118:GLU:N	2.44	0.49
42:1q:117:VAL:HB	42:1q:122:GLN:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:141:PRO:HB3	16:1P:61:PRO:HD3	1.94	0.49
7:1G:598:LYS:HG3	22:1W:118:PHE:HZ	1.78	0.49
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.76	0.49
10:1J:122:LEU:HD11	30:1e:76:SER:HA	1.94	0.49
12:1L:237:MET:HE1	12:1L:244:SER:HB2	1.95	0.49
12:1L:331:MET:N	12:1L:331:MET:SD	2.85	0.49
16:1P:177:ARG:HH22	55:1P:501:NDP:PA	2.36	0.49
22:1W:40:TYR:CD1	22:1W:40:TYR:N	2.81	0.49
23:1X:50:LYS:NZ	33:1h:141:PRO:O	2.45	0.49
40:1o:107:LEU:HA	40:1o:110:ARG:HB3	1.94	0.49
42:1q:48:TYR:HE2	42:1q:86:TRP:CG	2.31	0.49
2:1B:93:THR:HA	2:1B:132:VAL:HA	1.95	0.48
3:1C:66:ASP:HB2	21:1V:89:LEU:HB2	1.94	0.48
4:1D:151:ILE:O	4:1D:155:THR:OG1	2.29	0.48
7:1G:94:MET:HE3	7:1G:120:SER:HA	1.95	0.48
8:1H:85:MET:HB3	8:1H:108:MET:CE	2.42	0.48
12:1L:159:HIS:NE2	13:1M:416:ARG:HA	2.27	0.48
13:1M:387:SER:O	38:1m:111:LYS:NZ	2.33	0.48
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.12	0.48
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.46	0.48
21:1V:34:LEU:HD11	21:1V:44:ARG:HA	1.95	0.48
23:1X:79:GLU:HB2	23:1X:80:PRO:HD3	1.95	0.48
23:1X:101:LYS:O	23:1X:105:LYS:HG2	2.13	0.48
25:1Z:23:ARG:HH22	43:1r:112:LEU:HD21	1.75	0.48
28:1c:43:LYS:NZ	28:1c:48:LEU:HB2	2.28	0.48
30:1e:94:PRO:HB2	30:1e:96:HIS:CE1	2.48	0.48
37:1l:129:GLY:HA3	40:1o:100:GLU:OE2	2.13	0.48
39:1n:97:LYS:HB3	39:1n:177:PRO:HG3	1.95	0.48
39:1n:138:GLN:NE2	39:1n:155:PRO:O	2.46	0.48
43:1r:1:ALA:N	43:1r:2:SER:OG	2.36	0.48
6:1F:65:LEU:O	6:1F:75:THR:N	2.46	0.48
9:1I:40:TYR:HE1	43:1r:24:GLN:HE22	1.61	0.48
11:1K:43:MET:HE2	11:1K:43:MET:HA	1.94	0.48
51:1M:501:PGT:H2	14:1N:276:ILE:HD12	1.94	0.48
14:1N:95:MET:O	14:1N:99:THR:OG1	2.22	0.48
16:1P:138:ASP:H	16:1P:146:LEU:HB3	1.77	0.48
32:1g:115:PRO:O	32:1g:118:ILE:HG22	2.14	0.48
37:1l:90:ASP:OD1	37:1l:90:ASP:N	2.45	0.48
43:1r:31:SER:OG	43:1r:35:GLN:OE1	2.31	0.48
2:1B:85:VAL:HA	2:1B:112:TYR:O	2.14	0.48
4:1D:256:SER:OG	4:1D:257:GLY:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:386:PRO:HA	6:1F:430:MET:HE1	1.95	0.48
7:1G:382:THR:HB	7:1G:454:GLY:HA3	1.94	0.48
12:1L:357:ARG:HB3	39:1n:31:VAL:HG13	1.95	0.48
12:1L:483:PRO:HG3	35:1j:53:TYR:CE2	2.48	0.48
46:1L:702:PC1:H372	32:1g:79:TYR:OH	2.12	0.48
13:1M:43:ASN:HB3	33:1h:80:TYR:OH	2.14	0.48
13:1M:317:ILE:HB	13:1M:454:ILE:HD11	1.94	0.48
51:1M:501:PGT:H181	51:1M:501:PGT:H152	1.55	0.48
14:1N:95:MET:HE3	14:1N:148:SER:OG	2.13	0.48
14:1N:230:LEU:HD21	14:1N:244:MET:CE	2.43	0.48
15:1O:29:GLY:O	15:1O:126:ARG:NH2	2.43	0.48
17:1Q:126:LYS:HB3	17:1Q:128:THR:HG22	1.95	0.48
20:1U:21:LEU:HD12	36:1k:47:ASN:HA	1.95	0.48
20:1U:78:ASP:HB3	34:1i:15:ARG:NE	2.28	0.48
31:1f:28:ARG:O	31:1f:57:LYS:NZ	2.46	0.48
32:1g:94:GLU:HB3	41:1p:8:VAL:HG21	1.94	0.48
40:1o:24:PHE:HD1	40:1o:107:LEU:HD13	1.79	0.48
41:1p:26:PRO:HB3	41:1p:31:TYR:HE2	1.78	0.48
1:1A:68:GLU:HB3	1:1A:98:LEU:HD12	1.94	0.48
2:1B:90:GLY:HA2	47:1B:201:SF4:S2	2.53	0.48
3:1C:56:GLY:C	3:1C:59:PRO:HD2	2.39	0.48
6:1F:24:ASN:HB2	6:1F:39:ARG:HD3	1.94	0.48
6:1F:143:TYR:CE1	44:1s:51:PHE:HB2	2.48	0.48
6:1F:226:GLU:OE2	6:1F:255:LEU:N	2.40	0.48
7:1G:613:TYR:CE2	7:1G:622:ARG:HG2	2.48	0.48
10:1J:64:MET:O	10:1J:67:VAL:HG12	2.14	0.48
13:1M:263:MET:CE	38:1m:100:TRP:HB3	2.43	0.48
13:1M:329:LEU:HD22	13:1M:437:MET:CE	2.43	0.48
14:1N:325:LEU:HG	52:1N:402:CDL:H732	1.95	0.48
16:1P:9:GLY:C	16:1P:10:LYS:HE2	2.38	0.48
18:1R:18:TYR:OH	18:1R:27:ARG:NH2	2.46	0.48
21:1V:49:GLN:HE22	43:1r:92:LYS:HA	1.78	0.48
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.48	0.48
32:1g:99:TYR:C	32:1g:99:TYR:CD1	2.91	0.48
3:1C:179:GLU:HG3	16:1P:33:TYR:CD2	2.48	0.48
4:1D:19:MET:HE1	14:1N:295:ARG:CZ	2.43	0.48
4:1D:350:LYS:HG3	7:1G:121:MET:HG3	1.95	0.48
5:1E:15:ASN:OD1	5:1E:63:ILE:HG12	2.13	0.48
5:1E:104:THR:O	6:1F:349:ARG:HG2	2.13	0.48
6:1F:68:ARG:HH12	6:1F:230:VAL:HG11	1.77	0.48
6:1F:97:ALA:HA	6:1F:107:ASP:OD1	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:248:LEU:HA	14:1N:251:MET:HE3	1.96	0.48
20:1T:60:PHE:HB2	20:1T:83:LYS:HE2	1.95	0.48
21:1V:91:ARG:HB3	21:1V:95:ARG:HH22	1.78	0.48
32:1g:45:HIS:HB3	32:1g:58:MET:SD	2.53	0.48
37:1l:46:ASP:OD1	37:1l:46:ASP:N	2.45	0.48
39:1n:51:LYS:HD2	39:1n:51:LYS:O	2.13	0.48
41:1p:29:VAL:O	41:1p:33:THR:HG23	2.13	0.48
42:1q:48:TYR:CD1	42:1q:62:VAL:HG23	2.48	0.48
44:1s:34:ASP:OD1	44:1s:37:THR:OG1	2.31	0.48
5:1E:33:ALA:HA	5:1E:36:LYS:HG2	1.95	0.48
6:1F:87:ASP:OD1	6:1F:89:ARG:NE	2.39	0.48
6:1F:376:MET:C	6:1F:376:MET:SD	2.97	0.48
6:1F:398:GLN:CD	7:1G:92:GLY:HA3	2.39	0.48
6:1F:417:GLY:O	6:1F:421:HIS:HB2	2.14	0.48
8:1H:85:MET:HB2	8:1H:105:MET:SD	2.53	0.48
8:1H:137:ALA:HB3	8:1H:282:TYR:OH	2.14	0.48
9:1I:12:MET:O	27:1b:9:LYS:NZ	2.41	0.48
10:1J:45:LEU:HD23	10:1J:50:SER:HA	1.95	0.48
12:1L:49:VAL:HG13	12:1L:50:PRO:HD3	1.96	0.48
15:1O:189:PRO:HD2	15:1O:190:HIS:N	2.29	0.48
15:1O:204:ASN:OD1	15:1O:204:ASN:N	2.45	0.48
16:1P:250:TYR:CD1	16:1P:326:TRP:HB2	2.49	0.48
17:1Q:112:LYS:HG2	17:1Q:114:LYS:HZ2	1.78	0.48
19:1S:66:ALA:N	19:1S:73:GLU:OE1	2.47	0.48
23:1X:101:LYS:H	23:1X:101:LYS:HZ3	1.59	0.48
25:1Z:108:GLU:HB2	30:1e:74:ARG:HH21	1.78	0.48
26:1a:6:LEU:HD21	52:1q:201:CDL:H732	1.96	0.48
35:1j:41:TRP:HB2	36:1k:77:PHE:HZ	1.79	0.48
3:1C:137:MET:HE1	3:1C:153:THR:HB	1.95	0.48
3:1C:209:TYR:HD2	4:1D:360:PRO:HD2	1.77	0.48
4:1D:220:PHE:HB2	43:1r:22:LYS:HD2	1.96	0.48
4:1D:295:ASP:O	4:1D:299:CYS:N	2.43	0.48
5:1E:77:PRO:O	5:1E:81:TYR:HD2	1.95	0.48
6:1F:149:LEU:HD11	6:1F:177:VAL:HG11	1.96	0.48
7:1G:163:ALA:HA	7:1G:167:ALA:HB3	1.95	0.48
7:1G:275:LYS:HA	42:1q:134:ILE:HD13	1.96	0.48
8:1H:281:ARG:HH21	8:1H:284:GLN:CD	2.22	0.48
10:1J:33:LEU:HD22	10:1J:65:LEU:CG	2.43	0.48
12:1L:313:MET:O	12:1L:317:ILE:HG22	2.14	0.48
13:1M:276:CYS:HB3	13:1M:406:TYR:CD1	2.49	0.48
13:1M:452:LYS:HE2	32:1g:86:GLN:HE22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:230:ASP:OD1	15:1O:230:ASP:N	2.45	0.48
16:1P:128:LYS:HE2	16:1P:130:ILE:HD11	1.95	0.48
20:1U:60:PHE:CE1	20:1U:80:ILE:HD12	2.49	0.48
21:1V:87:LEU:HD13	21:1V:91:ARG:HE	1.78	0.48
27:1b:15:GLU:OE1	27:1b:18:LEU:N	2.42	0.48
27:1b:27:LEU:HB3	27:1b:31:LEU:HD13	1.96	0.48
37:1l:85:ILE:HG12	37:1l:86:ARG:H	1.78	0.48
3:1C:64:LEU:HD12	3:1C:72:PHE:HB2	1.94	0.48
4:1D:392:LYS:HZ1	4:1D:397:ALA:HB2	1.79	0.48
5:1E:155:GLN:C	5:1E:156:ILE:HD13	2.38	0.48
7:1G:362:TYR:O	7:1G:363:LEU:HD23	2.14	0.48
10:1J:82:VAL:HB	16:1P:325:ARG:HH22	1.78	0.48
12:1L:21:MET:HA	12:1L:21:MET:HE2	1.96	0.48
13:1M:263:MET:HE3	38:1m:100:TRP:HB3	1.95	0.48
16:1P:34:VAL:O	16:1P:38:LEU:HG	2.13	0.48
19:1S:62:PRO:HG2	19:1S:79:ASN:HA	1.95	0.48
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.47	0.48
37:1l:138:LEU:HB3	37:1l:141:GLU:HG2	1.95	0.48
39:1n:178:MET:N	39:1n:178:MET:SD	2.87	0.48
42:1q:56:PHE:HD1	43:1r:26:ARG:HE	1.61	0.48
1:1A:11:VAL:O	1:1A:15:SER:N	2.44	0.48
3:1C:111:THR:OG1	3:1C:117:ILE:HD11	2.14	0.48
4:1D:146:ARG:HH22	4:1D:270:ARG:HD3	1.79	0.48
5:1E:57:GLN:OE1	44:1s:49:TYR:OH	2.26	0.48
5:1E:154:VAL:H	5:1E:164:LEU:HD11	1.79	0.48
6:1F:98:ASP:HA	6:1F:139:ARG:HB2	1.96	0.48
6:1F:186:CYS:O	6:1F:192:LEU:HB2	2.14	0.48
6:1F:419:ILE:O	6:1F:423:ARG:HB2	2.14	0.48
7:1G:508:LYS:HD3	7:1G:509:PRO:HD2	1.96	0.48
8:1H:281:ARG:HB3	8:1H:284:GLN:OE1	2.13	0.48
12:1L:224:SER:O	12:1L:226:GLN:NE2	2.47	0.48
13:1M:208:PRO:HG3	13:1M:216:LEU:HG	1.96	0.48
14:1N:89:MET:HE2	14:1N:95:MET:CE	2.24	0.48
17:1Q:55:TRP:NE1	17:1Q:108:ARG:HH22	2.11	0.48
21:1V:36:GLN:OE1	21:1V:36:GLN:N	2.40	0.48
23:1X:45:CYS:SG	23:1X:49:GLU:HG3	2.54	0.48
34:1i:59:VAL:O	34:1i:63:THR:OG1	2.25	0.48
34:1i:122:PHE:CD1	34:1i:123:PRO:HD2	2.49	0.48
39:1n:12:GLN:O	39:1n:16:LEU:HG	2.13	0.48
44:1s:47:SER:O	44:1s:50:THR:OG1	2.26	0.48
3:1C:197:PHE:CD1	7:1G:220:TRP:HD1	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:349:PHE:HD1	9:1I:82:LEU:HD11	1.78	0.48
5:1E:163:ASP:HB3	5:1E:188:SER:H	1.79	0.48
6:1F:393:TRP:O	6:1F:397:LYS:HG2	2.14	0.48
9:1I:73:GLY:HA3	18:1R:43:LEU:HD23	1.96	0.48
16:1P:211:SER:O	16:1P:215:ILE:HG22	2.14	0.48
16:1P:331:MET:SD	16:1P:332:GLU:N	2.87	0.48
29:1d:115:GLU:OE1	29:1d:115:GLU:N	2.45	0.48
46:1f:101:PC1:H31	46:1f:101:PC1:H322	1.52	0.48
33:1h:129:ASP:N	33:1h:129:ASP:OD1	2.43	0.48
37:1l:58:ARG:NH1	37:1l:70:ARG:O	2.47	0.48
40:1o:7:ARG:HD3	40:1o:8:TYR:CE1	2.49	0.48
43:1r:100:ILE:HG23	43:1r:102:ARG:HH12	1.78	0.48
1:1A:72:LEU:HA	10:1J:147:TYR:OH	2.14	0.47
1:1A:82:ASN:HD21	27:1b:46:ARG:HG3	1.77	0.47
2:1B:68:ASP:OD1	8:1H:34:ARG:HG2	2.12	0.47
3:1C:193:GLU:OE1	3:1C:193:GLU:N	2.31	0.47
5:1E:42:HIS:CE1	6:1F:216:PHE:HB3	2.49	0.47
7:1G:43:HIS:NE2	7:1G:261:GLU:OE2	2.41	0.47
7:1G:503:LEU:HD21	7:1G:509:PRO:HB3	1.94	0.47
7:1G:574:VAL:HG21	7:1G:630:LEU:HD22	1.96	0.47
9:1I:116:CYS:SG	9:1I:117:ILE:N	2.87	0.47
14:1N:112:HIS:NE2	14:1N:164:ILE:HG12	2.28	0.47
15:1O:133:VAL:HG23	15:1O:205:ALA:CB	2.44	0.47
20:1T:55:GLU:HB2	22:1W:41:ARG:NH2	2.29	0.47
33:1h:114:MET:HE3	33:1h:122:TRP:CE2	2.49	0.47
36:1k:35:LEU:HD12	36:1k:40:LEU:HG	1.96	0.47
39:1n:33:ARG:NH1	39:1n:36:TYR:CD2	2.82	0.47
40:1o:100:GLU:HA	40:1o:103:ARG:HB3	1.96	0.47
4:1D:399:LEU:HD13	4:1D:423:ILE:HG13	1.96	0.47
5:1E:81:TYR:CD1	7:1G:186:TYR:HD2	2.32	0.47
7:1G:343:LEU:HD12	7:1G:507:TYR:CZ	2.50	0.47
12:1L:122:VAL:O	12:1L:126:ILE:HG12	2.14	0.47
13:1M:272:THR:O	13:1M:275:ILE:HB	2.14	0.47
26:1a:3:PHE:HZ	52:1q:201:CDL:HA4	1.79	0.47
4:1D:119:SER:O	4:1D:123:GLU:HG2	2.14	0.47
5:1E:108:CYS:SG	5:1E:152:PRO:HA	2.54	0.47
5:1E:168:ASP:HA	5:1E:171:GLU:HG2	1.96	0.47
7:1G:399:TRP:HH2	44:1s:74:ARG:HE	1.62	0.47
7:1G:673:MET:HG2	7:1G:688:VAL:HG21	1.95	0.47
12:1L:69:MET:HE1	13:1M:451:PRO:HG2	1.97	0.47
12:1L:407:TRP:O	12:1L:411:MET:HE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:570:GLN:OE1	14:1N:167:TRP:NE1	2.48	0.47
16:1P:206:TYR:OH	16:1P:208:VAL:HB	2.14	0.47
19:1S:24:GLN:HB3	19:1S:25:ARG:CZ	2.43	0.47
19:1S:40:TYR:OH	19:1S:52:ILE:CG1	2.61	0.47
22:1W:87:LYS:HA	22:1W:90:LEU:HG	1.96	0.47
28:1c:21:LEU:O	28:1c:25:VAL:HG22	2.14	0.47
36:1k:52:TYR:OH	39:1n:34:ASP:N	2.47	0.47
42:1q:56:PHE:HZ	43:1r:33:ARG:HD3	1.79	0.47
6:1F:246:GLY:HA3	6:1F:251:SER:HA	1.95	0.47
6:1F:363:THR:HG21	7:1G:97:LEU:HD21	1.96	0.47
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.54	0.47
7:1G:194:GLU:H	7:1G:194:GLU:CD	2.20	0.47
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.15	0.47
12:1L:202:PHE:O	41:1p:121:ARG:NH2	2.48	0.47
12:1L:556:ILE:O	12:1L:560:THR:OG1	2.26	0.47
13:1M:337:VAL:HG11	13:1M:345:ALA:HB2	1.95	0.47
14:1N:112:HIS:CE1	14:1N:164:ILE:HG12	2.50	0.47
15:1O:82:PHE:HE1	15:1O:143:PHE:CD2	2.30	0.47
19:1S:44:LYS:NZ	19:1S:52:ILE:HG23	2.30	0.47
20:1U:46:ASP:O	20:1U:49:GLU:HG3	2.14	0.47
21:1V:21:GLU:O	21:1V:25:ILE:HG23	2.15	0.47
23:1X:101:LYS:H	23:1X:101:LYS:NZ	2.12	0.47
45:1Y:201:3PE:H2	45:1Y:201:3PE:H221	1.50	0.47
41:1p:69:ARG:HA	41:1p:69:ARG:HD2	1.66	0.47
2:1B:30:VAL:HG22	2:1B:173:LEU:HB3	1.95	0.47
5:1E:9:HIS:CD2	7:1G:187:ILE:HD13	2.50	0.47
5:1E:143:GLU:CD	6:1F:349:ARG:HH22	2.23	0.47
5:1E:154:VAL:HG22	5:1E:164:LEU:CD1	2.45	0.47
6:1F:205:LEU:HB2	17:1Q:118:TYR:CE2	2.49	0.47
7:1G:218:ARG:O	7:1G:221:GLU:HG2	2.15	0.47
10:1J:10:SER:HB2	11:1K:7:ASN:HD22	1.78	0.47
19:1S:13:LEU:HG	19:1S:98:ALA:HA	1.97	0.47
22:1W:32:VAL:O	22:1W:36:TYR:HB2	2.14	0.47
33:1h:119:ASP:OD1	33:1h:119:ASP:N	2.43	0.47
42:1q:56:PHE:CZ	43:1r:33:ARG:HD3	2.50	0.47
3:1C:178:ASP:H	16:1P:36:ASN:HD21	1.61	0.47
5:1E:78:MET:O	5:1E:82:GLU:HG2	2.14	0.47
5:1E:147:ALA:O	5:1E:153:MET:HE2	2.15	0.47
6:1F:43:TYR:CB	6:1F:236:ARG:HH12	2.23	0.47
6:1F:56:ILE:HD12	6:1F:59:GLU:HB2	1.96	0.47
6:1F:293:ASN:O	6:1F:339:ARG:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:617:ASP:OD1	7:1G:618:GLN:N	2.47	0.47
12:1L:434:LYS:HG3	36:1k:52:TYR:CD1	2.49	0.47
13:1M:14:MET:O	13:1M:18:SER:OG	2.31	0.47
19:1S:20:ILE:HA	19:1S:64:LEU:HA	1.96	0.47
21:1V:111:TRP:O	21:1V:112:LYS:HB3	2.15	0.47
29:1d:106:LYS:HB3	41:1p:77:GLU:HG3	1.97	0.47
29:1d:114:GLU:OE1	29:1d:114:GLU:N	2.47	0.47
36:1k:22:LYS:HB2	36:1k:24:GLU:OE1	2.15	0.47
39:1n:27:GLU:OE1	39:1n:36:TYR:CE2	2.67	0.47
41:1p:162:MET:O	41:1p:166:ARG:HB2	2.15	0.47
4:1D:205:LEU:HD11	43:1r:38:PRO:HB3	1.97	0.47
5:1E:12:THR:HG1	5:1E:15:ASN:H	1.62	0.47
6:1F:65:LEU:HA	6:1F:242:PHE:CZ	2.50	0.47
6:1F:232:PRO:O	6:1F:236:ARG:HG3	2.15	0.47
6:1F:258:ILE:HD12	6:1F:265:PRO:HA	1.96	0.47
7:1G:36:GLN:OE1	17:1Q:48:GLY:HA2	2.15	0.47
7:1G:126:ASP:OD1	7:1G:126:ASP:N	2.46	0.47
7:1G:226:GLU:HB3	7:1G:253:ARG:CZ	2.45	0.47
7:1G:364:LEU:HD13	7:1G:491:ASN:HD22	1.79	0.47
7:1G:385:ARG:HA	7:1G:392:ASN:ND2	2.30	0.47
8:1H:106:LEU:HD21	8:1H:150:LEU:HD12	1.96	0.47
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.39	0.47
13:1M:59:ASP:OD1	13:1M:245:ARG:NH2	2.46	0.47
13:1M:68:LEU:HD22	13:1M:317:ILE:HG23	1.97	0.47
14:1N:25:HIS:N	30:1e:14:ASP:OD2	2.36	0.47
14:1N:30:TRP:HD1	14:1N:70:LEU:HD23	1.80	0.47
14:1N:197:ASN:ND2	14:1N:269:GLU:OE2	2.35	0.47
15:1O:65:ASP:HB2	28:1c:2:PHE:CD1	2.50	0.47
15:1O:82:PHE:HZ	15:1O:138:MET:HE2	1.79	0.47
15:1O:101:TYR:HE2	15:1O:155:VAL:HG12	1.80	0.47
15:1O:188:ASN:O	15:1O:192:MET:HG3	2.15	0.47
16:1P:12:GLY:O	16:1P:15:SER:OG	2.33	0.47
16:1P:29:PHE:CE2	16:1P:171:ILE:HD13	2.49	0.47
17:1Q:35:VAL:HG11	17:1Q:57:MET:SD	2.55	0.47
20:1T:52:MET:HE2	22:1W:37:ARG:HB3	1.97	0.47
21:1V:98:PRO:HD2	21:1V:99:TRP:CE2	2.49	0.47
22:1W:41:ARG:HD2	22:1W:41:ARG:HA	1.63	0.47
23:1X:13:LYS:HA	23:1X:13:LYS:HE2	1.96	0.47
23:1X:152:GLU:OE2	23:1X:153:ALA:N	2.48	0.47
25:1Z:23:ARG:HG3	25:1Z:25:LEU:HD23	1.97	0.47
25:1Z:86:MET:HG2	25:1Z:124:LEU:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:15:GLY:O	33:1h:19:ARG:N	2.36	0.47
34:1i:13:GLN:HG3	39:1n:163:PRO:HG3	1.97	0.47
37:1l:156:TYR:CD1	40:1o:33:ARG:HB2	2.50	0.47
39:1n:11:HIS:HA	39:1n:14:LYS:HE2	1.96	0.47
40:1o:16:PRO:HG2	40:1o:101:PHE:CE1	2.50	0.47
3:1C:67:HIS:HB3	3:1C:70:ALA:HB3	1.95	0.47
5:1E:51:LEU:HB3	5:1E:90:TYR:CZ	2.49	0.47
5:1E:55:GLN:HE21	5:1E:56:ARG:NH1	2.13	0.47
6:1F:370:ASP:O	6:1F:374:LYS:HG2	2.14	0.47
8:1H:105:MET:HE2	8:1H:105:MET:HB2	1.78	0.47
13:1M:79:ALA:HB2	13:1M:436:LEU:HD11	1.97	0.47
13:1M:257:MET:HE2	13:1M:257:MET:HA	1.95	0.47
33:1h:21:PHE:CE2	33:1h:25:MET:HE2	2.50	0.47
2:1B:125:TYR:CE1	9:1I:88:PRO:HB2	2.49	0.47
4:1D:93:TYR:O	4:1D:385:ARG:NH1	2.47	0.47
6:1F:129:MET:HG3	6:1F:221:THR:HG21	1.97	0.47
7:1G:384:PRO:HA	7:1G:387:GLU:HB2	1.95	0.47
10:1J:51:PHE:CD1	10:1J:143:ILE:HD13	2.50	0.47
10:1J:60:TYR:HE2	11:1K:38:LEU:HD22	1.80	0.47
12:1L:10:THR:HG21	34:1i:78:VAL:HG23	1.97	0.47
12:1L:367:PRO:O	12:1L:371:THR:OG1	2.27	0.47
15:1O:141:GLN:NE2	15:1O:198:TYR:HA	2.29	0.47
15:1O:175:PRO:HB2	15:1O:177:PRO:HD2	1.96	0.47
20:1T:14:ARG:HD2	20:1T:57:GLU:OE2	2.15	0.47
21:1V:49:GLN:HE22	43:1r:93:ALA:N	2.12	0.47
22:1W:39:TRP:O	22:1W:43:VAL:HG23	2.15	0.47
22:1W:106:PHE:O	22:1W:108:HIS:ND1	2.44	0.47
25:1Z:34:SER:O	25:1Z:38:VAL:HG12	2.15	0.47
36:1k:35:LEU:HD11	36:1k:42:ASP:N	2.30	0.47
2:1B:94:ASN:HB3	3:1C:174:LEU:HD13	1.97	0.47
5:1E:69:VAL:HA	5:1E:72:ILE:HG22	1.98	0.47
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.97	0.47
6:1F:83:ASN:HD21	6:1F:128:ALA:HB1	1.80	0.47
7:1G:229:ASP:OD1	7:1G:230:VAL:N	2.48	0.47
7:1G:462:ASP:HB2	7:1G:465:ALA:HB3	1.96	0.47
9:1I:54:LYS:HD2	42:1q:91:HIS:CD2	2.50	0.47
9:1I:120:GLY:HA2	9:1I:133:GLU:OE2	2.14	0.47
12:1L:373:LEU:HG	12:1L:431:PHE:CE2	2.50	0.47
12:1L:507:THR:O	12:1L:510:TYR:HB2	2.15	0.47
14:1N:211:MET:HE1	14:1N:250:SER:C	2.39	0.47
14:1N:243:LEU:O	14:1N:246:VAL:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:81:ALA:HA	20:1T:84:LYS:NZ	2.30	0.47
23:1X:110:VAL:HB	23:1X:116:TRP:HB2	1.97	0.47
31:1f:57:LYS:O	33:1h:85:LYS:NZ	2.30	0.47
39:1n:13:GLN:HB3	39:1n:17:ARG:HH22	1.80	0.47
42:1q:9:ARG:HG3	42:1q:9:ARG:HH11	1.80	0.47
6:1F:138:ILE:HG23	6:1F:179:ARG:HA	1.97	0.46
6:1F:194:GLU:HA	6:1F:197:GLU:HB2	1.97	0.46
7:1G:200:ILE:HG22	17:1Q:45:MET:HE1	1.96	0.46
8:1H:114:TYR:OH	10:1J:61:LEU:O	2.22	0.46
10:1J:64:MET:HG2	10:1J:68:PHE:CE2	2.51	0.46
12:1L:14:ILE:HD11	12:1L:43:ALA:HA	1.96	0.46
12:1L:88:MET:HE2	12:1L:88:MET:HA	1.97	0.46
12:1L:187:ALA:HA	13:1M:383:THR:HG22	1.96	0.46
13:1M:148:TYR:O	13:1M:152:TYR:HB2	2.16	0.46
14:1N:195:PRO:HB2	24:1Y:138:PRO:HG3	1.98	0.46
14:1N:270:MET:HE1	14:1N:282:MET:SD	2.55	0.46
15:1O:164:LEU:HD11	15:1O:259:LEU:HD22	1.96	0.46
19:1S:36:ILE:HD12	19:1S:40:TYR:CD2	2.50	0.46
20:1T:81:ALA:HA	20:1T:84:LYS:HZ3	1.80	0.46
25:1Z:36:PHE:O	25:1Z:40:ILE:HG12	2.15	0.46
27:1b:15:GLU:OE1	27:1b:17:VAL:N	2.48	0.46
43:1r:4:THR:OG1	43:1r:5:ARG:N	2.48	0.46
6:1F:143:TYR:OH	44:1s:50:THR:N	2.48	0.46
6:1F:274:VAL:O	6:1F:317:MET:HE2	2.15	0.46
7:1G:206:GLY:N	47:1G:801:SF4:S1	2.84	0.46
15:1O:317:ILE:HA	15:1O:320:LYS:HD3	1.97	0.46
21:1V:67:LEU:HD11	21:1V:76:ILE:HG21	1.98	0.46
21:1V:112:LYS:NZ	21:1V:113:TRP:O	2.41	0.46
30:1e:95:PRO:HA	30:1e:98:LEU:HD12	1.97	0.46
32:1g:72:LEU:H	32:1g:72:LEU:HD12	1.81	0.46
32:1g:93:ALA:HB2	41:1p:100:GLU:HB3	1.97	0.46
35:1j:16:GLN:H	35:1j:16:GLN:CD	2.24	0.46
40:1o:6:ARG:HH22	40:1o:105:ARG:HH12	1.62	0.46
1:1A:1:FME:O1	1:1A:2:ASN:N	2.43	0.46
1:1A:13:LEU:HD13	8:1H:10:ILE:HG21	1.97	0.46
1:1A:106:TRP:CZ2	8:1H:291:LYS:HB3	2.50	0.46
6:1F:68:ARG:HB3	6:1F:106:LYS:HZ2	1.81	0.46
7:1G:255:HIS:CE1	7:1G:258:ILE:HD13	2.45	0.46
7:1G:286:ASN:N	7:1G:290:LEU:O	2.42	0.46
7:1G:647:GLU:HA	7:1G:650:LYS:HE2	1.97	0.46
8:1H:11:ILE:O	8:1H:15:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.97	0.46
45:1L:701:3PE:H112	45:1L:701:3PE:H11	1.97	0.46
14:1N:85:THR:HG22	30:1e:18:THR:OG1	2.15	0.46
14:1N:278:MET:HB3	14:1N:279:PRO:HD3	1.96	0.46
15:1O:70:ASP:HB3	15:1O:73:LEU:HD23	1.96	0.46
16:1P:29:PHE:CZ	16:1P:207:ILE:HD12	2.50	0.46
16:1P:234:ASN:C	16:1P:234:ASN:OD1	2.58	0.46
16:1P:235:ARG:HG3	16:1P:340:VAL:HG23	1.96	0.46
17:1Q:56:LYS:HB2	17:1Q:58:GLU:OE1	2.16	0.46
22:1W:21:PHE:HB2	22:1W:31:ARG:NH2	2.29	0.46
25:1Z:6:VAL:HG11	43:1r:41:PRO:HB3	1.98	0.46
33:1h:78:THR:HG23	33:1h:79:PHE:CD1	2.50	0.46
39:1n:43:MET:HE1	39:1n:46:ARG:NH2	2.30	0.46
2:1B:116:MET:HA	2:1B:146:VAL:HG13	1.97	0.46
5:1E:149:VAL:HG13	5:1E:150:ASN:OD1	2.14	0.46
6:1F:138:ILE:HG21	6:1F:146:ALA:HB2	1.97	0.46
6:1F:296:ALA:HB2	6:1F:422:PHE:CZ	2.49	0.46
6:1F:391:SER:O	6:1F:395:ILE:HG13	2.15	0.46
6:1F:398:GLN:O	6:1F:402:HIS:ND1	2.49	0.46
7:1G:404:LEU:HD13	7:1G:405:LYS:C	2.41	0.46
8:1H:136:VAL:HB	10:1J:70:TYR:CE1	2.49	0.46
8:1H:272:TRP:O	8:1H:276:SER:OG	2.21	0.46
11:1K:54:THR:HG21	30:1e:28:ILE:HD12	1.97	0.46
13:1M:276:CYS:HB3	13:1M:406:TYR:CG	2.50	0.46
13:1M:281:ASP:OD1	13:1M:340:ARG:HB3	2.15	0.46
13:1M:286:ILE:O	13:1M:289:SER:OG	2.24	0.46
14:1N:25:HIS:ND1	14:1N:27:LEU:HB3	2.31	0.46
14:1N:186:HIS:O	14:1N:190:MET:HG2	2.15	0.46
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.15	0.46
29:1d:34:MET:SD	29:1d:72:GLY:HA3	2.55	0.46
34:1i:10:ARG:HA	34:1i:13:GLN:HE21	1.80	0.46
1:1A:80:GLN:HA	27:1b:45:ASN:HD21	1.79	0.46
3:1C:33:LEU:O	3:1C:37:VAL:HG12	2.15	0.46
3:1C:137:MET:HG3	3:1C:162:PHE:CD1	2.51	0.46
6:1F:19:ASP:OD2	6:1F:245:PHE:HE2	1.99	0.46
6:1F:138:ILE:O	6:1F:180:GLY:N	2.48	0.46
6:1F:258:ILE:HG13	6:1F:266:CYS:O	2.16	0.46
7:1G:438:PRO:O	7:1G:442:ILE:HD13	2.14	0.46
7:1G:684:MET:N	7:1G:684:MET:SD	2.87	0.46
9:1I:14:MET:HE2	9:1I:14:MET:HA	1.98	0.46
9:1I:145:GLU:H	9:1I:145:GLU:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:150:MET:HE3	12:1L:153:LEU:HD13	1.96	0.46
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.96	0.46
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.51	0.46
13:1M:30:HIS:O	13:1M:34:ILE:HG12	2.16	0.46
13:1M:422:HIS:O	38:1m:55:ARG:NH1	2.41	0.46
14:1N:243:LEU:HD21	29:1d:44:ILE:HG23	1.98	0.46
14:1N:324:LYS:HA	14:1N:324:LYS:HD2	1.65	0.46
15:1O:82:PHE:HZ	15:1O:138:MET:CE	2.29	0.46
16:1P:251:ARG:HB3	16:1P:251:ARG:HH11	1.80	0.46
18:1R:2:VAL:HG13	18:1R:10:LYS:NZ	2.30	0.46
22:1W:45:ASN:OD1	22:1W:46:THR:N	2.48	0.46
23:1X:42:PHE:HD1	23:1X:58:GLU:HB2	1.80	0.46
23:1X:162:HIS:HB3	33:1h:100:LYS:NZ	2.30	0.46
24:1Y:69:PHE:HE2	45:1Y:202:3PE:H3F1	1.80	0.46
38:1m:123:THR:O	41:1p:135:SER:OG	2.28	0.46
41:1p:27:ASN:ND2	41:1p:30:THR:H	2.12	0.46
2:1B:62:MET:CG	2:1B:69:MET:HB3	2.46	0.46
2:1B:81:ARG:HD3	8:1H:61:LEU:HD21	1.97	0.46
4:1D:4:TRP:CD1	13:1M:140:THR:HA	2.50	0.46
7:1G:429:LEU:O	7:1G:473:ILE:HD11	2.16	0.46
9:1I:136:ASN:HD22	9:1I:161:TRP:HZ2	1.62	0.46
10:1J:55:MET:O	10:1J:59:ILE:HG12	2.15	0.46
10:1J:146:LEU:HA	11:1K:58:MET:CE	2.45	0.46
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.51	0.46
12:1L:466:PHE:O	12:1L:470:ASN:ND2	2.48	0.46
19:1S:95:SER:OG	19:1S:96:GLY:N	2.49	0.46
32:1g:121:PRO:O	41:1p:166:ARG:NH2	2.49	0.46
1:1A:111:LEU:HD21	8:1H:290:TRP:HB3	1.98	0.46
3:1C:25:PHE:O	3:1C:29:VAL:HG23	2.16	0.46
3:1C:185:ALA:HB2	22:1W:105:ARG:HH21	1.81	0.46
4:1D:267:TRP:CE3	4:1D:272:THR:HG21	2.51	0.46
5:1E:192:SER:HB3	6:1F:113:HIS:HE1	1.80	0.46
7:1G:82:ASN:OD1	7:1G:87:LYS:NZ	2.33	0.46
12:1L:511:LEU:O	12:1L:511:LEU:HD13	2.16	0.46
46:1L:702:PC1:C24	13:1M:450:ASN:HB2	2.45	0.46
13:1M:25:ILE:HG23	32:1g:60:VAL:HG11	1.98	0.46
16:1P:141:SER:OG	16:1P:146:LEU:HB2	2.16	0.46
20:1U:26:ASP:HB3	20:1U:29:LYS:HB2	1.98	0.46
25:1Z:30:LEU:HD12	25:1Z:34:SER:HB3	1.97	0.46
3:1C:39:GLN:HB3	3:1C:51:PHE:HB2	1.98	0.46
8:1H:87:VAL:HG12	8:1H:88:PRO:HD3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:25:HIS:ND1	11:1K:88:ASP:OD2	2.43	0.46
12:1L:600:THR:O	12:1L:602:PHE:N	2.48	0.46
13:1M:21:ASN:OD1	13:1M:21:ASN:N	2.48	0.46
13:1M:209:LEU:HD21	13:1M:264:LEU:HD13	1.98	0.46
14:1N:211:MET:SD	14:1N:251:MET:HG3	2.56	0.46
14:1N:217:MET:HE3	14:1N:323:MET:HA	1.96	0.46
17:1Q:127:ARG:HG2	44:1s:70:ARG:NH1	2.30	0.46
19:1S:90:LEU:HA	19:1S:93:VAL:HG23	1.98	0.46
29:1d:82:MET:O	29:1d:86:ARG:N	2.36	0.46
29:1d:99:GLU:OE1	29:1d:99:GLU:N	2.32	0.46
32:1g:47:TYR:HB2	32:1g:54:ASP:OD1	2.16	0.46
33:1h:70:PRO:HA	33:1h:73:ARG:HD3	1.98	0.46
3:1C:93:VAL:HG13	3:1C:108:LYS:HG2	1.98	0.46
5:1E:162:GLU:O	5:1E:186:PRO:HA	2.15	0.46
7:1G:244:THR:OG1	17:1Q:73:SER:OG	2.25	0.46
7:1G:584:LYS:HD2	7:1G:584:LYS:HA	1.81	0.46
7:1G:704:CYS:SG	9:1I:104:ARG:HB2	2.56	0.46
46:1I:204:PC1:H153	25:1Z:35:MET:SD	2.56	0.46
12:1L:428:PHE:CD2	12:1L:505:ASN:HB3	2.51	0.46
13:1M:367:LEU:HD23	13:1M:367:LEU:HA	1.66	0.46
15:1O:86:PRO:HA	15:1O:143:PHE:CE2	2.51	0.46
16:1P:145:TYR:HB2	16:1P:282:ASP:OD2	2.16	0.46
22:1W:33:ARG:O	22:1W:37:ARG:N	2.47	0.46
1:1A:104:TYR:CE2	10:1J:166:VAL:HG23	2.51	0.46
2:1B:48:MET:HE3	2:1B:79:SER:C	2.41	0.46
2:1B:81:ARG:O	2:1B:81:ARG:NH1	2.39	0.46
3:1C:178:ASP:OD1	3:1C:181:LYS:NZ	2.40	0.46
4:1D:157:HIS:CD2	4:1D:419:GLY:HA3	2.50	0.46
4:1D:342:MET:HG2	7:1G:98:LEU:HD21	1.98	0.46
6:1F:275:PRO:HG2	6:1F:278:GLU:HG3	1.97	0.46
7:1G:588:THR:OG1	17:1Q:62:ARG:O	2.33	0.46
8:1H:91:MET:HE2	8:1H:91:MET:HB3	1.77	0.46
11:1K:85:TYR:HB3	11:1K:92:ASN:ND2	2.31	0.46
12:1L:3:PRO:HB3	41:1p:36:PHE:CD1	2.51	0.46
12:1L:42:TYR:HH	34:1i:66:HIS:CE1	2.33	0.46
12:1L:154:LEU:HD23	12:1L:154:LEU:HA	1.75	0.46
13:1M:88:THR:O	13:1M:92:LYS:HG3	2.16	0.46
14:1N:230:LEU:HD21	14:1N:244:MET:HE2	1.96	0.46
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.50	0.46
15:1O:13:ARG:HA	15:1O:13:ARG:HD3	1.77	0.46
15:1O:164:LEU:H	15:1O:164:LEU:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:162:GLU:HB3	16:1P:224:LYS:HB3	1.98	0.46
18:1R:10:LYS:H	18:1R:33:LYS:HD2	1.81	0.46
25:1Z:68:ARG:HD3	25:1Z:69:ILE:HD12	1.97	0.46
25:1Z:110:VAL:HG13	30:1e:70:LYS:HD2	1.98	0.46
28:1c:1:LYS:HZ1	28:1c:3:TYR:HE2	1.60	0.46
39:1n:27:GLU:HA	39:1n:36:TYR:HE2	1.81	0.46
5:1E:78:MET:HA	5:1E:81:TYR:HB2	1.98	0.45
7:1G:503:LEU:HD23	7:1G:503:LEU:HA	1.80	0.45
10:1J:111:GLU:OE1	30:1e:80:ARG:NH2	2.49	0.45
10:1J:129:ASP:OD2	10:1J:129:ASP:C	2.59	0.45
12:1L:362:LEU:HD12	12:1L:366:MET:HE2	1.97	0.45
14:1N:25:HIS:HB3	14:1N:28:LEU:HD23	1.98	0.45
16:1P:2:HIS:CE1	16:1P:4:ALA:HB3	2.51	0.45
16:1P:46:ILE:HG23	18:1R:26:VAL:HG21	1.98	0.45
22:1W:42:GLU:O	22:1W:46:THR:HG23	2.15	0.45
24:1Y:119:LEU:HD23	24:1Y:119:LEU:HA	1.81	0.45
38:1m:22:TYR:CE2	39:1n:64:ARG:HA	2.51	0.45
40:1o:70:ARG:HG2	40:1o:70:ARG:HH11	1.80	0.45
1:1A:3:ILE:O	1:1A:6:THR:OG1	2.25	0.45
1:1A:65:PHE:HZ	1:1A:102:LEU:HB2	1.81	0.45
4:1D:123:GLU:HB2	4:1D:128:ILE:O	2.17	0.45
4:1D:123:GLU:OE1	4:1D:130:PRO:HD3	2.16	0.45
5:1E:106:THR:O	5:1E:110:LEU:HG	2.17	0.45
6:1F:298:ILE:O	6:1F:334:VAL:HA	2.15	0.45
7:1G:575:ASN:ND2	7:1G:579:ARG:HB3	2.31	0.45
11:1K:26:LEU:HD22	11:1K:78:LEU:HB2	1.98	0.45
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.98	0.45
14:1N:37:LEU:HD12	14:1N:63:GLN:HB3	1.98	0.45
16:1P:83:LYS:HB3	16:1P:83:LYS:HE2	1.71	0.45
16:1P:134:HIS:CE1	16:1P:136:ASN:HB3	2.51	0.45
20:1T:36:PHE:HB2	20:1T:71:MET:SD	2.56	0.45
23:1X:125:SER:N	25:1Z:66:GLU:OE1	2.49	0.45
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	1.98	0.45
30:1e:72:MET:HE3	30:1e:72:MET:HB2	1.86	0.45
30:1e:82:ARG:O	30:1e:86:ILE:HG12	2.16	0.45
33:1h:68:LYS:HG2	41:1p:62:TYR:CE1	2.51	0.45
35:1j:5:VAL:HG23	35:1j:7:ILE:O	2.17	0.45
36:1k:35:LEU:O	36:1k:39:GLY:N	2.42	0.45
42:1q:94:THR:OG1	42:1q:95:ASP:N	2.49	0.45
2:1B:38:ASN:HB3	2:1B:170:GLU:OE2	2.16	0.45
2:1B:41:ARG:HH22	8:1H:57:THR:HB	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:158:TYR:CD1	9:1I:138:GLU:HB3	2.52	0.45
4:1D:172:GLU:OE2	4:1D:176:LYS:NZ	2.49	0.45
5:1E:9:HIS:CE1	5:1E:63:ILE:HG13	2.51	0.45
6:1F:114:ASP:N	6:1F:114:ASP:OD1	2.48	0.45
6:1F:120:GLU:OE2	6:1F:236:ARG:NE	2.50	0.45
7:1G:437:HIS:CD2	7:1G:438:PRO:HD2	2.51	0.45
7:1G:595:GLU:OE1	7:1G:595:GLU:N	2.44	0.45
10:1J:65:LEU:HA	10:1J:68:PHE:CD2	2.52	0.45
13:1M:81:GLN:O	13:1M:85:SER:OG	2.34	0.45
13:1M:350:THR:O	33:1h:13:PRO:HG3	2.15	0.45
14:1N:159:MET:HE1	14:1N:278:MET:HG3	1.98	0.45
15:1O:19:THR:OG1	15:1O:20:GLU:N	2.49	0.45
15:1O:171:TYR:CE2	15:1O:211:LEU:HD21	2.52	0.45
17:1Q:69:LEU:O	17:1Q:71:GLY:N	2.50	0.45
18:1R:54:SER:HB3	18:1R:57:ILE:HD11	1.99	0.45
20:1U:20:LYS:HG2	36:1k:18:TYR:CE1	2.50	0.45
45:1Y:201:3PE:H32	45:1Y:201:3PE:H321	1.30	0.45
27:1b:51:ASN:HB3	33:1h:139:THR:HG22	1.98	0.45
34:1i:71:VAL:HG13	34:1i:72:THR:HG23	1.97	0.45
35:1j:34:PHE:CD1	35:1j:34:PHE:C	2.94	0.45
43:1r:110:PRO:CD	43:1r:111:TYR:H	2.20	0.45
1:1A:83:ASN:O	1:1A:86:THR:HG22	2.16	0.45
2:1B:44:SER:O	2:1B:44:SER:OG	2.32	0.45
2:1B:118:SER:N	47:1B:201:SF4:S1	2.90	0.45
4:1D:132:PRO:HA	4:1D:135:GLN:HG3	1.98	0.45
5:1E:60:TRP:CG	5:1E:94:PRO:HA	2.51	0.45
5:1E:148:CYS:HB3	6:1F:103:GLY:H	1.81	0.45
6:1F:276:LEU:HD21	6:1F:297:VAL:HG21	1.97	0.45
7:1G:515:ARG:HH12	7:1G:516:LYS:HE3	1.82	0.45
7:1G:628:PRO:N	7:1G:628:PRO:HG3	1.96	0.45
8:1H:28:LEU:HD23	8:1H:34:ARG:NH2	2.31	0.45
11:1K:48:ILE:HG23	11:1K:53:PHE:HB3	1.98	0.45
12:1L:243:VAL:O	12:1L:247:LEU:HD12	2.16	0.45
14:1N:176:ARG:NH1	14:1N:225:THR:OG1	2.48	0.45
27:1b:10:ASN:HA	27:1b:14:LYS:HZ3	1.80	0.45
34:1i:44:GLN:OE1	34:1i:48:LYS:NZ	2.49	0.45
35:1j:70:ASP:OD2	35:1j:71:GLU:N	2.49	0.45
39:1n:107:HIS:CD2	39:1n:108:PRO:HD2	2.51	0.45
39:1n:140:GLN:NE2	39:1n:141:GLU:HG3	2.30	0.45
4:1D:284:ASP:HB2	4:1D:306:GLN:NE2	2.32	0.45
6:1F:250:ASN:HD22	6:1F:319:PHE:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:375:VAL:O	6:1F:378:ARG:HG2	2.16	0.45
7:1G:141:ASN:OD1	7:1G:141:ASN:N	2.49	0.45
7:1G:237:ASN:HB3	7:1G:253:ARG:HB3	1.97	0.45
7:1G:397:LYS:HG3	7:1G:401:HIS:CE1	2.52	0.45
8:1H:26:LYS:HG2	8:1H:36:GLY:HA3	1.99	0.45
12:1L:79:SER:HB2	12:1L:135:ASN:HB3	1.99	0.45
12:1L:357:ARG:NH1	39:1n:77:GLN:O	2.33	0.45
12:1L:511:LEU:HD11	39:1n:38:TYR:HD2	1.82	0.45
13:1M:278:ARG:NH2	37:1l:83:MET:HE1	2.32	0.45
16:1P:263:TYR:CZ	16:1P:284:VAL:HG12	2.52	0.45
18:1R:19:ASP:O	18:1R:25:ARG:HD3	2.17	0.45
20:1U:8:LEU:CD2	20:1U:88:GLU:OE1	2.65	0.45
24:1Y:8:TYR:HE1	24:1Y:24:SER:HB3	1.81	0.45
40:1o:95:VAL:HA	40:1o:98:MET:SD	2.57	0.45
43:1r:109:GLN:OE1	43:1r:111:TYR:O	2.34	0.45
5:1E:100:ILE:HD12	5:1E:156:ILE:HG23	1.97	0.45
6:1F:224:ASN:O	6:1F:227:THR:OG1	2.33	0.45
11:1K:55:LEU:O	11:1K:58:MET:HG3	2.16	0.45
11:1K:62:ILE:CA	11:1K:65:VAL:HG12	2.33	0.45
11:1K:78:LEU:HA	11:1K:81:VAL:HG12	1.97	0.45
12:1L:69:MET:HG3	12:1L:71:LEU:HG	1.98	0.45
16:1P:294:LEU:HD12	16:1P:296:HIS:CE1	2.52	0.45
19:1S:63:LYS:HE3	19:1S:75:ASN:CG	2.42	0.45
21:1V:49:GLN:HE21	43:1r:92:LYS:CE	2.29	0.45
22:1W:102:HIS:HA	22:1W:105:ARG:NH1	2.31	0.45
23:1X:129:LYS:HB2	27:1b:58:ASP:HB2	1.97	0.45
25:1Z:76:GLN:O	25:1Z:80:ASP:HB2	2.17	0.45
37:1l:85:ILE:HG22	37:1l:88:ARG:HB2	1.99	0.45
39:1n:108:PRO:HA	39:1n:111:LYS:HB2	1.98	0.45
42:1q:12:GLN:O	42:1q:16:GLY:N	2.49	0.45
42:1q:86:TRP:CE3	42:1q:98:PRO:HD2	2.51	0.45
1:1A:106:TRP:CH2	8:1H:291:LYS:HB3	2.52	0.45
4:1D:178:PHE:CZ	4:1D:189:MET:HE3	2.46	0.45
5:1E:48:LEU:HB3	5:1E:49:PRO:HD3	1.98	0.45
5:1E:51:LEU:HD21	5:1E:84:ALA:HB2	1.98	0.45
7:1G:203:CYS:HB3	50:1G:804:K:K	2.10	0.45
7:1G:549:HIS:CE1	7:1G:677:ILE:HA	2.50	0.45
9:1I:51:PRO:HD2	9:1I:52:PHE:N	2.30	0.45
13:1M:190:TRP:CE3	24:1Y:126:MET:HE1	2.51	0.45
14:1N:105:LYS:HB3	14:1N:105:LYS:HE2	1.82	0.45
14:1N:129:LEU:HD13	52:1N:402:CDL:H532	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:121:MET:HE3	25:1Z:137:THR:HA	1.98	0.45
40:1o:73:PHE:CD1	40:1o:74:PRO:HA	2.52	0.45
41:1p:94:ASP:HA	41:1p:97:VAL:HG12	1.99	0.45
3:1C:87:GLN:H	3:1C:87:GLN:CD	2.24	0.45
3:1C:210:ARG:NH2	7:1G:35:MET:HG3	2.31	0.45
4:1D:151:ILE:HG23	4:1D:170:MET:HB3	1.99	0.45
4:1D:192:ALA:O	4:1D:195:ARG:NH1	2.49	0.45
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.49	0.45
6:1F:109:GLU:HA	6:1F:112:ARG:HH11	1.82	0.45
6:1F:255:LEU:HD22	6:1F:269:GLU:HG2	1.99	0.45
6:1F:326:GLN:HG3	6:1F:420:ARG:NH2	2.32	0.45
7:1G:56:LEU:HB3	7:1G:65:VAL:HG11	1.99	0.45
7:1G:98:LEU:O	7:1G:98:LEU:HD13	2.17	0.45
7:1G:193:SER:HB2	7:1G:196:SER:HB2	1.98	0.45
7:1G:533:THR:HG23	7:1G:535:GLN:HG3	1.98	0.45
7:1G:681:SER:HB3	7:1G:684:MET:HG2	1.99	0.45
8:1H:86:TRP:HH2	8:1H:232:ILE:HG22	1.82	0.45
8:1H:157:ASN:HA	8:1H:168:THR:HG21	1.98	0.45
8:1H:219:PRO:HB2	8:1H:220:PHE:H	1.67	0.45
12:1L:324:LEU:H	12:1L:324:LEU:HD12	1.81	0.45
13:1M:275:ILE:HG21	13:1M:288:TYR:CD1	2.52	0.45
51:1M:501:PGT:O4P	51:1M:501:PGT:O6	2.28	0.45
14:1N:234:TRP:CE2	14:1N:304:MET:HB3	2.52	0.45
16:1P:264:ARG:HB3	16:1P:281:ARG:HH21	1.81	0.45
21:1V:51:THR:HA	21:1V:54:LYS:NZ	2.30	0.45
22:1W:36:TYR:CE1	22:1W:40:TYR:OH	2.55	0.45
27:1b:31:LEU:N	27:1b:32:PRO:HD2	2.32	0.45
39:1n:92:ARG:CD	39:1n:93:TYR:HE2	2.29	0.45
40:1o:34:LYS:HA	40:1o:34:LYS:HD3	1.73	0.45
43:1r:100:ILE:O	43:1r:102:ARG:NH1	2.48	0.45
2:1B:142:VAL:HG11	2:1B:145:TYR:CD2	2.51	0.45
2:1B:146:VAL:HG21	2:1B:156:LEU:HA	1.99	0.45
3:1C:51:PHE:HD2	21:1V:111:TRP:CD2	2.34	0.45
4:1D:312:SER:O	4:1D:316:ASN:HB2	2.17	0.45
6:1F:65:LEU:HD11	6:1F:234:ILE:HD13	1.97	0.45
6:1F:143:TYR:HA	6:1F:179:ARG:HD3	1.98	0.45
6:1F:343:ILE:HD12	6:1F:344:VAL:N	2.32	0.45
7:1G:162:PHE:CZ	7:1G:198:ASN:HB2	2.52	0.45
7:1G:432:ILE:HA	7:1G:440:SER:HB3	1.99	0.45
8:1H:235:ASN:HD21	8:1H:270:PHE:HD2	1.65	0.45
12:1L:155:ILE:HD11	12:1L:248:HIS:NE2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:554:ASP:C	12:1L:554:ASP:OD2	2.59	0.45
16:1P:208:VAL:HA	16:1P:211:SER:OG	2.17	0.45
21:1V:59:LYS:HE2	21:1V:59:LYS:HB2	1.74	0.45
22:1W:57:LYS:HE2	22:1W:57:LYS:HA	1.99	0.45
23:1X:72:GLN:OE1	23:1X:72:GLN:N	2.36	0.45
32:1g:41:ASN:OD1	32:1g:41:ASN:N	2.49	0.45
37:1l:14:PRO:HA	37:1l:19:GLU:CD	2.42	0.45
42:1q:13:GLN:NE2	42:1q:33:VAL:O	2.33	0.45
3:1C:83:VAL:HB	3:1C:86:ARG:HD2	1.99	0.45
4:1D:169:TRP:NE1	8:1H:32:GLN:HA	2.32	0.45
4:1D:417:ILE:O	4:1D:421:GLN:HB2	2.17	0.45
6:1F:31:TRP:O	6:1F:115:PRO:HD2	2.16	0.45
6:1F:307:ILE:HA	6:1F:421:HIS:ND1	2.32	0.45
11:1K:89:TYR:HB3	11:1K:91:GLN:CD	2.42	0.45
12:1L:10:THR:O	12:1L:14:ILE:HG23	2.17	0.45
12:1L:97:THR:HG21	12:1L:125:LEU:HD22	1.98	0.45
12:1L:283:ILE:HD13	37:1l:112:MET:HG3	1.99	0.45
14:1N:266:ILE:HG22	14:1N:270:MET:HE2	1.98	0.45
16:1P:144:ARG:NH2	16:1P:148:SER:HB3	2.28	0.45
17:1Q:56:LYS:HD2	17:1Q:84:LEU:O	2.17	0.45
19:1S:18:ILE:HD12	19:1S:18:ILE:HA	1.81	0.45
24:1Y:61:THR:HG22	24:1Y:103:ARG:HB3	1.99	0.45
28:1c:45:ARG:HH22	29:1d:19:ARG:HB2	1.82	0.45
29:1d:90:MET:CE	33:1h:107:GLU:HA	2.47	0.45
43:1r:22:LYS:HE2	43:1r:22:LYS:HB3	1.79	0.45
2:1B:158:TYR:CE2	42:1q:78:ASP:HB2	2.51	0.44
2:1B:175:ILE:HG22	2:1B:179:ARG:HD2	1.99	0.44
3:1C:41:GLN:NE2	43:1r:67:ILE:HD12	2.31	0.44
3:1C:118:GLU:OE1	3:1C:118:GLU:N	2.37	0.44
4:1D:171:PHE:CE1	4:1D:174:ARG:HD3	2.52	0.44
4:1D:183:ARG:HD3	4:1D:207:LEU:HD23	1.99	0.44
4:1D:421:GLN:CG	4:1D:423:ILE:HD11	2.46	0.44
6:1F:74:PRO:HB3	6:1F:249:ARG:NH2	2.25	0.44
6:1F:287:VAL:HG11	6:1F:294:LEU:HB2	1.98	0.44
8:1H:272:TRP:HE1	9:1I:37:THR:HG23	1.81	0.44
10:1J:138:GLU:HG2	30:1e:28:ILE:HG21	1.99	0.44
12:1L:7:LEU:HD12	12:1L:7:LEU:H	1.82	0.44
12:1L:528:TYR:CB	37:1l:101:MET:HE1	2.47	0.44
13:1M:14:MET:HE1	13:1M:26:ASN:C	2.42	0.44
13:1M:378:GLU:O	13:1M:382:ILE:HG12	2.16	0.44
14:1N:89:MET:SD	14:1N:98:MET:HE3	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:40:ARG:HH22	15:1O:52:PRO:HB3	1.82	0.44
15:1O:45:LYS:HD2	15:1O:235:VAL:HG21	2.00	0.44
15:1O:238:ILE:C	15:1O:238:ILE:HD12	2.42	0.44
20:1T:12:LYS:NZ	20:1T:32:VAL:HA	2.31	0.44
23:1X:100:ARG:HA	23:1X:100:ARG:HD3	1.75	0.44
25:1Z:27:ARG:NH2	25:1Z:28:ARG:O	2.50	0.44
30:1e:36:GLU:HB2	30:1e:62:PHE:CE1	2.51	0.44
31:1f:41:SER:HB2	41:1p:86:GLU:OE2	2.17	0.44
42:1q:7:LEU:O	42:1q:7:LEU:HD23	2.17	0.44
4:1D:169:TRP:CD1	8:1H:33:LEU:HD23	2.52	0.44
5:1E:7:PHE:HB3	7:1G:175:THR:HG23	1.99	0.44
5:1E:144:CYS:HB2	48:1E:301:FES:S2	2.52	0.44
6:1F:83:ASN:ND2	6:1F:128:ALA:O	2.50	0.44
6:1F:188:GLU:OE2	6:1F:405:CYS:HB2	2.16	0.44
6:1F:406:ALA:O	6:1F:410:GLY:N	2.41	0.44
7:1G:202:ILE:HD13	7:1G:202:ILE:HA	1.90	0.44
7:1G:347:GLU:HB2	7:1G:499:GLN:NE2	2.32	0.44
8:1H:153:VAL:HG13	8:1H:174:MET:CE	2.47	0.44
9:1I:27:TRP:CZ2	46:1I:203:PC1:H332	2.52	0.44
12:1L:48:LEU:O	12:1L:52:LEU:HD12	2.16	0.44
12:1L:136:ASN:OD1	12:1L:139:GLN:N	2.40	0.44
12:1L:398:ALA:O	12:1L:402:SER:OG	2.34	0.44
13:1M:14:MET:SD	31:1f:12:VAL:HG12	2.58	0.44
14:1N:153:LEU:O	14:1N:157:MET:HG2	2.17	0.44
16:1P:240:ASP:O	16:1P:244:TYR:N	2.39	0.44
17:1Q:57:MET:HB3	17:1Q:84:LEU:HB2	1.99	0.44
20:1U:70:LEU:HD12	20:1U:75:GLU:HB3	1.98	0.44
22:1W:52:LEU:HD12	22:1W:52:LEU:HA	1.56	0.44
31:1f:24:CYS:O	31:1f:28:ARG:NE	2.42	0.44
31:1f:42:LEU:HD23	31:1f:42:LEU:H	1.82	0.44
32:1g:47:TYR:CD2	32:1g:58:MET:HG2	2.52	0.44
35:1j:45:ASP:HB2	35:1j:50:HIS:HB2	1.98	0.44
35:1j:63:GLU:H	35:1j:63:GLU:HG3	1.65	0.44
5:1E:159:ASN:OD1	5:1E:161:TYR:CZ	2.70	0.44
6:1F:203:PRO:HD2	6:1F:359:CYS:SG	2.57	0.44
6:1F:256:PHE:CD1	6:1F:270:GLU:HB3	2.53	0.44
7:1G:100:ASN:ND2	7:1G:179:ASN:HD21	2.14	0.44
7:1G:521:VAL:HG12	7:1G:542:PHE:HB3	1.99	0.44
8:1H:89:LEU:HD13	8:1H:90:PRO:HD2	1.99	0.44
51:1M:501:PGT:H131	51:1M:501:PGT:H361	1.98	0.44
14:1N:333:SER:O	14:1N:333:SER:OG	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:60:ASP:OD2	15:1O:68:PRO:HA	2.17	0.44
17:1Q:27:GLU:OE2	17:1Q:27:GLU:N	2.47	0.44
20:1T:64:ASP:HB3	22:1W:30:ARG:CZ	2.48	0.44
21:1V:91:ARG:O	21:1V:95:ARG:NH2	2.50	0.44
28:1c:16:LYS:HE2	28:1c:16:LYS:HB2	1.70	0.44
2:1B:99:ALA:O	2:1B:102:LYS:HG2	2.18	0.44
4:1D:424:VAL:O	4:1D:428:VAL:HG12	2.16	0.44
5:1E:110:LEU:HB3	6:1F:261:HIS:CE1	2.52	0.44
5:1E:159:ASN:ND2	5:1E:184:PRO:HG3	2.31	0.44
6:1F:92:TYR:CE1	6:1F:133:ALA:HB3	2.53	0.44
7:1G:74:MET:H	7:1G:77:TRP:HE3	1.65	0.44
7:1G:571:ALA:HB3	7:1G:583:THR:HB	1.99	0.44
7:1G:591:GLY:HA2	16:1P:6:ILE:HD13	2.00	0.44
13:1M:39:LEU:HA	13:1M:42:LEU:HD23	1.98	0.44
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.52	0.44
13:1M:207:MET:HE1	13:1M:240:GLY:HA2	1.98	0.44
13:1M:425:ASN:HD21	38:1m:58:VAL:HG13	1.82	0.44
14:1N:241:THR:HB	14:1N:301:SER:HB3	1.99	0.44
16:1P:91:VAL:C	16:1P:92:ILE:HD12	2.41	0.44
16:1P:93:ASN:HD22	16:1P:117:ILE:HG12	1.83	0.44
20:1U:43:ASP:OD2	20:1U:43:ASP:C	2.59	0.44
21:1V:37:ILE:O	21:1V:44:ARG:NH2	2.47	0.44
23:1X:138:GLU:OE1	23:1X:138:GLU:N	2.42	0.44
26:1a:43:TYR:HA	26:1a:46:ASN:HD21	1.82	0.44
35:1j:70:ASP:OD2	35:1j:70:ASP:C	2.61	0.44
38:1m:32:GLN:HA	38:1m:35:ARG:HG2	2.00	0.44
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.42	0.44
2:1B:158:TYR:CG	9:1I:138:GLU:HB3	2.52	0.44
3:1C:100:ARG:HD3	43:1r:100:ILE:HG22	2.00	0.44
4:1D:391:ILE:N	4:1D:430:ARG:HH22	2.13	0.44
5:1E:101:GLN:CD	5:1E:142:VAL:HG21	2.42	0.44
5:1E:175:GLU:HB2	5:1E:180:LYS:HG3	1.98	0.44
6:1F:250:ASN:ND2	6:1F:319:PHE:H	2.14	0.44
7:1G:195:LEU:HD12	7:1G:198:ASN:HD21	1.81	0.44
12:1L:407:TRP:CE2	12:1L:411:MET:HE1	2.52	0.44
14:1N:329:MET:HE2	14:1N:329:MET:HA	2.00	0.44
15:1O:147:GLN:CD	15:1O:147:GLN:H	2.24	0.44
15:1O:181:SER:O	15:1O:184:GLN:NE2	2.51	0.44
16:1P:57:MET:SD	16:1P:60:ARG:NH1	2.91	0.44
20:1U:42:LEU:HD12	20:1U:46:ASP:HB3	2.00	0.44
21:1V:34:LEU:O	21:1V:44:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:71:LEU:O	24:1Y:75:ILE:HG12	2.17	0.44
24:1Y:93:GLY:HA3	24:1Y:118:GLY:HA2	1.98	0.44
25:1Z:101:VAL:HG21	25:1Z:104:TRP:HB3	2.00	0.44
32:1g:47:TYR:CE2	32:1g:58:MET:HG2	2.52	0.44
39:1n:93:TYR:CD2	39:1n:93:TYR:N	2.84	0.44
2:1B:39:TRP:HA	2:1B:42:ARG:HG2	1.99	0.44
2:1B:47:PRO:HD2	2:1B:75:VAL:O	2.18	0.44
2:1B:57:VAL:HG11	4:1D:108:TYR:O	2.17	0.44
3:1C:58:ILE:HD11	3:1C:118:GLU:HB2	1.99	0.44
4:1D:34:ASN:ND2	15:1O:158:VAL:HA	2.31	0.44
6:1F:137:TYR:CG	6:1F:192:LEU:HD21	2.51	0.44
6:1F:318:ASP:O	6:1F:321:ALA:N	2.48	0.44
7:1G:104:ASP:O	7:1G:108:CYS:N	2.50	0.44
7:1G:248:MET:HE2	7:1G:248:MET:N	2.32	0.44
7:1G:376:VAL:HB	7:1G:439:PHE:HZ	1.82	0.44
7:1G:391:PHE:CE1	7:1G:395:ILE:HD11	2.52	0.44
7:1G:589:PRO:O	22:1W:126:HIS:HE1	2.00	0.44
7:1G:675:ASP:OD1	7:1G:676:SER:N	2.49	0.44
8:1H:141:SER:O	8:1H:144:VAL:HG22	2.17	0.44
12:1L:132:VAL:O	12:1L:262:ARG:NH2	2.38	0.44
13:1M:277:LEU:HD23	13:1M:277:LEU:HA	1.79	0.44
15:1O:140:ARG:HH22	15:1O:208:LYS:NZ	2.15	0.44
15:1O:151:HIS:HD2	15:1O:277:VAL:HB	1.83	0.44
15:1O:214:MET:O	15:1O:218:CYS:N	2.48	0.44
16:1P:310:LEU:HD23	16:1P:310:LEU:C	2.43	0.44
17:1Q:49:VAL:O	17:1Q:51:ASN:N	2.46	0.44
19:1S:40:TYR:O	19:1S:43:LEU:HG	2.17	0.44
23:1X:112:ASP:OD1	23:1X:113:LYS:HG2	2.18	0.44
25:1Z:98:MET:C	25:1Z:99:LYS:HZ2	2.25	0.44
26:1a:42:SER:O	26:1a:46:ASN:ND2	2.51	0.44
26:1a:48:MET:HE3	26:1a:48:MET:HB3	1.80	0.44
34:1i:64:TYR:CD1	34:1i:64:TYR:C	2.96	0.44
34:1i:85:LEU:HA	34:1i:89:VAL:HG12	1.99	0.44
35:1j:27:PHE:C	35:1j:27:PHE:HD1	2.26	0.44
35:1j:67:LEU:HG	40:1o:29:GLY:HA2	1.99	0.44
37:1l:3:HIS:CG	37:1l:4:VAL:N	2.85	0.44
37:1l:3:HIS:CE1	37:1l:4:VAL:HG12	2.53	0.44
1:1A:73:LEU:HD23	1:1A:73:LEU:HA	1.78	0.44
4:1D:204:PRO:HA	9:1I:175:TYR:CZ	2.53	0.44
6:1F:64:GLY:HA3	6:1F:249:ARG:HH22	1.82	0.44
8:1H:92:PRO:HA	8:1H:255:TYR:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	1.99	0.44
11:1K:40:LEU:HD23	11:1K:40:LEU:HA	1.76	0.44
12:1L:107:TYR:HD2	12:1L:108:MET:HG2	1.83	0.44
12:1L:293:ILE:HD11	45:1L:703:3PE:H242	1.99	0.44
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.53	0.44
13:1M:342:MET:HG3	13:1M:413:THR:HG21	2.00	0.44
14:1N:294:MET:O	14:1N:298:TYR:N	2.47	0.44
15:1O:315:LYS:HD2	15:1O:316:TRP:H	1.82	0.44
16:1P:206:TYR:CD2	16:1P:209:ASP:OD1	2.71	0.44
17:1Q:19:ILE:O	17:1Q:23:THR:HG23	2.18	0.44
20:1U:70:LEU:HD11	20:1U:76:ILE:HA	2.00	0.44
33:1h:7:ARG:HH11	34:1i:27:LEU:HD12	1.83	0.44
37:1l:8:MET:H	37:1l:8:MET:HG2	1.65	0.44
38:1m:69:TYR:CZ	38:1m:74:ASN:HB2	2.53	0.44
2:1B:104:TYR:CE1	2:1B:111:ARG:HD2	2.53	0.44
3:1C:150:ARG:HD2	3:1C:155:TYR:HA	1.99	0.44
5:1E:162:GLU:N	5:1E:162:GLU:OE1	2.51	0.44
6:1F:141:GLU:OE1	6:1F:141:GLU:N	2.51	0.44
7:1G:238:ILE:O	7:1G:253:ARG:NH1	2.50	0.44
7:1G:287:GLU:H	7:1G:287:GLU:CD	2.26	0.44
9:1I:64:GLU:HB2	9:1I:139:PHE:CE1	2.53	0.44
10:1J:107:ALA:HA	10:1J:119:PHE:HZ	1.82	0.44
12:1L:10:THR:HG21	34:1i:78:VAL:HA	2.00	0.44
12:1L:298:ILE:HD11	12:1L:359:MET:HE1	1.99	0.44
13:1M:76:MET:HE2	13:1M:99:LEU:HD22	1.99	0.44
14:1N:119:THR:O	14:1N:176:ARG:HD2	2.18	0.44
15:1O:25:ILE:HD12	15:1O:168:VAL:HB	2.00	0.44
16:1P:206:TYR:CE1	16:1P:208:VAL:HG23	2.53	0.44
18:1R:38:ASN:OD1	18:1R:38:ASN:N	2.50	0.44
20:1U:55:GLU:CD	39:1n:81:PHE:CE1	2.95	0.44
21:1V:50:ILE:C	21:1V:54:LYS:HZ2	2.25	0.44
25:1Z:9:ASP:O	25:1Z:10:MET:HE2	2.18	0.44
31:1f:45:LYS:HE2	31:1f:45:LYS:HB3	1.78	0.44
32:1g:50:ASP:C	32:1g:50:ASP:OD1	2.60	0.44
38:1m:26:PRO:HA	38:1m:29:ARG:HB2	1.98	0.44
40:1o:112:LYS:CG	40:1o:116:GLN:NE2	2.69	0.44
42:1q:9:ARG:CZ	52:1q:201:CDL:HA61	2.47	0.44
1:1A:5:LEU:O	1:1A:9:THR:HG22	2.18	0.44
3:1C:169:SER:OG	3:1C:190:LEU:HD11	2.18	0.44
4:1D:19:MET:HE1	14:1N:295:ARG:NE	2.32	0.44
4:1D:83:LEU:HD22	4:1D:425:PHE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:393:ALA:HB3	4:1D:396:PHE:HB2	2.00	0.44
6:1F:49:LEU:HA	6:1F:127:ARG:HG2	2.00	0.44
6:1F:185:ILE:HD13	6:1F:407:LEU:HB2	2.00	0.44
8:1H:150:LEU:HD23	8:1H:150:LEU:HA	1.76	0.44
10:1J:57:PHE:HA	10:1J:61:LEU:HD23	1.99	0.44
12:1L:4:PHE:HE1	12:1L:50:PRO:HB3	1.83	0.44
13:1M:207:MET:HG2	13:1M:298:ILE:HG13	1.99	0.44
13:1M:301:ILE:HD13	13:1M:301:ILE:HA	1.87	0.44
14:1N:236:LYS:HB2	14:1N:311:MET:SD	2.57	0.44
16:1P:172:PHE:HB2	16:1P:179:LEU:HD11	1.99	0.44
20:1T:12:LYS:O	20:1T:16:LEU:HG	2.18	0.44
22:1W:21:PHE:CB	22:1W:31:ARG:HH22	2.30	0.44
22:1W:88:MET:HE3	22:1W:91:GLU:OE2	2.17	0.44
29:1d:30:ARG:HE	29:1d:30:ARG:HB2	1.55	0.44
29:1d:49:ARG:HD2	29:1d:51:ARG:NH2	2.33	0.44
34:1i:4:THR:OG1	34:1i:6:ASP:OD1	2.23	0.44
38:1m:62:PRO:HB2	38:1m:66:ARG:NH1	2.33	0.44
39:1n:123:GLN:O	39:1n:127:LEU:HG	2.18	0.44
43:1r:32:LYS:HE2	43:1r:34:THR:O	2.18	0.44
2:1B:165:ARG:NH1	42:1q:77:VAL:O	2.51	0.43
4:1D:147:LEU:O	4:1D:304:MET:HE1	2.18	0.43
7:1G:91:GLU:OE2	7:1G:125:SER:HB2	2.18	0.43
7:1G:258:ILE:HD11	7:1G:579:ARG:NH2	2.33	0.43
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	2.00	0.43
7:1G:522:LEU:HB3	7:1G:543:ILE:HD13	2.00	0.43
9:1I:57:LEU:HD23	42:1q:91:HIS:HB3	1.99	0.43
12:1L:197:ASP:O	12:1L:201:ILE:HG13	2.18	0.43
12:1L:303:ALA:O	12:1L:306:THR:OG1	2.20	0.43
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.18	0.43
14:1N:147:GLN:NE2	33:1h:125:TYR:HD1	2.16	0.43
14:1N:335:LEU:O	29:1d:33:TYR:OH	2.28	0.43
16:1P:281:ARG:HA	16:1P:284:VAL:HG13	2.00	0.43
17:1Q:81:ASN:C	17:1Q:82:LEU:HD23	2.43	0.43
19:1S:33:ARG:O	19:1S:36:ILE:HG22	2.17	0.43
19:1S:35:PHE:CZ	19:1S:90:LEU:HD21	2.53	0.43
21:1V:65:LYS:HD3	21:1V:65:LYS:N	2.33	0.43
40:1o:112:LYS:CA	40:1o:116:GLN:HE21	2.31	0.43
42:1q:132:LYS:NZ	42:1q:135:GLN:HA	2.33	0.43
2:1B:81:ARG:NH2	8:1H:220:PHE:CD2	2.86	0.43
3:1C:87:GLN:H	3:1C:87:GLN:NE2	2.15	0.43
4:1D:399:LEU:HD12	4:1D:402:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:101:GLN:NE2	5:1E:142:VAL:HG11	2.33	0.43
9:1I:17:VAL:HG11	27:1b:9:LYS:HE2	2.00	0.43
12:1L:271:LYS:HE2	12:1L:271:LYS:HB2	1.72	0.43
14:1N:40:MET:SD	14:1N:134:GLN:NE2	2.91	0.43
17:1Q:40:PRO:HG3	17:1Q:56:LYS:HE2	2.00	0.43
23:1X:40:LYS:HB3	23:1X:130:VAL:HG11	2.00	0.43
26:1a:68:ASN:C	26:1a:68:ASN:HD22	2.25	0.43
34:1i:127:HIS:HB3	40:1o:84:HIS:CE1	2.53	0.43
38:1m:69:TYR:CE2	38:1m:74:ASN:HB2	2.53	0.43
40:1o:14:LYS:HE3	40:1o:14:LYS:HA	2.00	0.43
40:1o:53:GLN:HB2	40:1o:54:GLN:NE2	2.33	0.43
44:1s:67:SER:O	44:1s:67:SER:OG	2.33	0.43
1:1A:102:LEU:HD21	8:1H:295:PRO:HG3	2.00	0.43
3:1C:82:ASP:HB2	3:1C:138:PHE:HE1	1.83	0.43
6:1F:36:ALA:HB1	6:1F:41:ASP:HB2	2.00	0.43
6:1F:202:LYS:NZ	6:1F:361:GLN:HB3	2.33	0.43
7:1G:213:TYR:O	7:1G:216:THR:OG1	2.24	0.43
7:1G:261:GLU:OE2	17:1Q:42:ARG:NH2	2.51	0.43
7:1G:396:ARG:HH22	44:1s:74:ARG:NH2	2.16	0.43
7:1G:599:ILE:HG22	22:1W:122:PHE:CZ	2.53	0.43
7:1G:613:TYR:HE2	7:1G:622:ARG:HE	1.66	0.43
8:1H:85:MET:CG	8:1H:233:MET:HG3	2.47	0.43
8:1H:181:LEU:O	8:1H:185:TRP:N	2.44	0.43
8:1H:252:PRO:O	8:1H:256:THR:HG23	2.18	0.43
8:1H:299:ALA:HB1	27:1b:24:ILE:HB	2.01	0.43
12:1L:96:VAL:O	12:1L:100:ILE:HG12	2.18	0.43
12:1L:141:PHE:HB2	12:1L:186:MET:HE3	1.99	0.43
12:1L:145:GLU:OE1	12:1L:176:ARG:NH1	2.52	0.43
12:1L:278:LEU:CD2	12:1L:318:GLY:HA3	2.48	0.43
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	2.01	0.43
13:1M:82:SER:HB3	13:1M:432:ARG:HH12	1.84	0.43
13:1M:200:ILE:O	13:1M:204:MET:HG2	2.18	0.43
15:1O:320:LYS:NZ	28:1c:10:GLY:O	2.37	0.43
16:1P:234:ASN:OD1	16:1P:236:TYR:CE1	2.72	0.43
17:1Q:20:THR:HB	17:1Q:30:ILE:HD11	2.00	0.43
19:1S:86:VAL:O	19:1S:90:LEU:HG	2.18	0.43
20:1T:14:ARG:CD	20:1T:57:GLU:OE2	2.66	0.43
20:1T:52:MET:HE2	22:1W:37:ARG:CB	2.48	0.43
25:1Z:105:LYS:HE2	25:1Z:105:LYS:HB2	1.82	0.43
34:1i:19:ARG:HA	34:1i:19:ARG:HD3	1.82	0.43
34:1i:105:PRO:O	40:1o:67:LYS:NZ	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:95:VAL:O	40:1o:99:LYS:HG3	2.19	0.43
41:1p:2:ASP:OD2	41:1p:3:SER:N	2.52	0.43
41:1p:140:ASP:O	41:1p:161:ARG:NH2	2.51	0.43
2:1B:91:THR:HA	2:1B:119:CYS:HB3	1.99	0.43
3:1C:28:TYR:O	3:1C:32:ILE:HG13	2.18	0.43
3:1C:53:HIS:CG	3:1C:54:PRO:HD2	2.53	0.43
3:1C:125:LYS:NZ	4:1D:253:TYR:HE2	2.16	0.43
4:1D:391:ILE:HB	4:1D:430:ARG:CZ	2.49	0.43
5:1E:95:VAL:HG22	5:1E:138:THR:HG21	1.99	0.43
7:1G:59:ILE:HG23	7:1G:62:ALA:HB3	1.99	0.43
7:1G:107:ILE:HG12	18:1R:86:TYR:CZ	2.53	0.43
7:1G:247:VAL:O	7:1G:248:MET:HE2	2.18	0.43
7:1G:339:ASP:OD1	19:1S:69:ALA:HB1	2.19	0.43
8:1H:39:VAL:HA	42:1q:31:ASN:CG	2.43	0.43
8:1H:43:TYR:CZ	52:1q:201:CDL:H141	2.53	0.43
9:1I:174:LEU:HD12	43:1r:38:PRO:HD2	1.99	0.43
10:1J:167:VAL:O	10:1J:171:ILE:HG13	2.18	0.43
12:1L:209:PRO:HB2	12:1L:213:LEU:HG	2.00	0.43
12:1L:331:MET:HE2	12:1L:465:GLY:CA	2.44	0.43
16:1P:55:ASP:OD1	16:1P:55:ASP:N	2.51	0.43
16:1P:126:VAL:HG22	16:1P:127:GLU:N	2.33	0.43
18:1R:2:VAL:HG13	18:1R:10:LYS:HZ1	1.82	0.43
24:1Y:80:ARG:HB2	24:1Y:82:LYS:HZ3	1.83	0.43
32:1g:87:GLU:O	32:1g:91:ARG:NE	2.47	0.43
35:1j:55:ASP:C	35:1j:55:ASP:OD1	2.61	0.43
41:1p:48:ARG:O	41:1p:51:ILE:HG13	2.18	0.43
3:1C:72:PHE:CE1	3:1C:98:SER:HB3	2.54	0.43
3:1C:206:PHE:O	3:1C:206:PHE:CD1	2.72	0.43
4:1D:265:ILE:HD12	21:1V:10:LEU:HD23	2.00	0.43
4:1D:283:PHE:O	9:1I:1:THR:OG1	2.35	0.43
4:1D:357:GLN:OE1	43:1r:59:ARG:NH1	2.52	0.43
5:1E:173:ILE:HA	5:1E:176:LEU:HB2	2.00	0.43
6:1F:108:ARG:HG2	6:1F:112:ARG:HD3	2.01	0.43
7:1G:285:ARG:NH1	7:1G:289:GLY:O	2.45	0.43
8:1H:2:PHE:CE1	8:1H:6:ILE:HD11	2.53	0.43
8:1H:287:HIS:HA	8:1H:291:LYS:HZ2	1.84	0.43
9:1I:18:THR:HA	27:1b:12:TRP:CH2	2.53	0.43
12:1L:71:LEU:HD13	13:1M:307:TRP:CH2	2.54	0.43
12:1L:209:PRO:C	12:1L:212:PRO:HD2	2.43	0.43
12:1L:425:ARG:NH2	45:1L:703:3PE:O13	2.51	0.43
13:1M:134:THR:HG21	14:1N:298:TYR:CE1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:262:LEU:HD11	13:1M:302:MET:HB3	2.00	0.43
13:1M:423:ILE:HA	38:1m:58:VAL:HG12	1.99	0.43
14:1N:142:LEU:HB3	14:1N:194:LEU:CD2	2.48	0.43
14:1N:339:MET:HE2	14:1N:339:MET:HA	2.00	0.43
15:1O:14:THR:HA	15:1O:17:LYS:NZ	2.32	0.43
19:1S:55:ARG:NE	19:1S:55:ARG:N	2.66	0.43
23:1X:157:LEU:HD23	23:1X:157:LEU:HA	1.87	0.43
33:1h:64:TRP:CD1	33:1h:77:ARG:HG3	2.53	0.43
35:1j:19:ARG:HH11	35:1j:23:ILE:HG21	1.82	0.43
42:1q:49:TYR:HD1	42:1q:61:TRP:CE2	2.36	0.43
46:1A:202:PC1:H32	10:1J:151:THR:OG1	2.18	0.43
2:1B:81:ARG:HH12	2:1B:82:GLN:HA	1.77	0.43
2:1B:82:GLN:HG3	8:1H:220:PHE:CE2	2.53	0.43
3:1C:153:THR:OG1	3:1C:154:GLY:N	2.50	0.43
3:1C:194:PHE:HD2	17:1Q:81:ASN:HD22	1.65	0.43
4:1D:128:ILE:HD13	4:1D:128:ILE:HA	1.85	0.43
4:1D:352:TYR:HD2	9:1I:86:VAL:HG21	1.82	0.43
5:1E:102:VAL:HG12	5:1E:140:ILE:O	2.18	0.43
7:1G:58:GLU:HG2	7:1G:59:ILE:N	2.33	0.43
7:1G:74:MET:HE1	7:1G:77:TRP:CZ3	2.53	0.43
7:1G:255:HIS:ND1	7:1G:258:ILE:HB	2.33	0.43
7:1G:364:LEU:HD13	7:1G:491:ASN:ND2	2.34	0.43
7:1G:657:LEU:H	7:1G:657:LEU:HD12	1.83	0.43
10:1J:121:GLY:H	30:1e:73:LYS:NZ	2.17	0.43
11:1K:80:MET:O	11:1K:84:THR:HG23	2.18	0.43
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.54	0.43
13:1M:121:LEU:H	13:1M:121:LEU:HG	1.65	0.43
13:1M:168:GLN:NE2	33:1h:104:ARG:HD3	2.34	0.43
13:1M:442:LEU:HD13	13:1M:442:LEU:HA	1.88	0.43
14:1N:228:LEU:HD13	15:1O:278:TYR:HE2	1.84	0.43
15:1O:171:TYR:HD2	15:1O:211:LEU:HD11	1.83	0.43
15:1O:260:ARG:HA	15:1O:263:VAL:HG22	2.01	0.43
16:1P:256:TYR:HE2	16:1P:258:LEU:HD12	1.83	0.43
22:1W:126:HIS:CD2	22:1W:126:HIS:H	2.37	0.43
36:1k:30:THR:O	36:1k:34:LYS:HG2	2.18	0.43
38:1m:59:ILE:HD13	38:1m:59:ILE:HA	1.87	0.43
2:1B:43:SER:HB2	8:1H:40:VAL:HG21	2.00	0.43
3:1C:200:ASN:OD1	3:1C:200:ASN:N	2.51	0.43
4:1D:10:TRP:CZ2	13:1M:143:LEU:HD12	2.54	0.43
7:1G:533:THR:OG1	7:1G:534:ARG:N	2.52	0.43
8:1H:19:PHE:HB3	26:1a:12:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:128:MET:HE3	12:1L:251:THR:O	2.19	0.43
12:1L:240:PRO:HD2	12:1L:243:VAL:HG21	2.01	0.43
12:1L:597:ILE:HG13	12:1L:602:PHE:CE2	2.54	0.43
13:1M:11:LEU:HD22	13:1M:100:ILE:HD12	2.01	0.43
13:1M:35:SER:O	13:1M:38:SER:OG	2.26	0.43
13:1M:306:PRO:O	13:1M:310:MET:HG3	2.18	0.43
14:1N:167:TRP:CD1	14:1N:288:LEU:HD21	2.53	0.43
52:1N:402:CDL:H752	52:1N:402:CDL:H792	2.01	0.43
19:1S:88:ARG:NH2	19:1S:92:ASN:HB3	2.34	0.43
45:1Y:202:3PE:H251	45:1Y:202:3PE:H332	2.01	0.43
33:1h:63:HIS:CE1	33:1h:64:TRP:HD1	2.35	0.43
37:1l:100:THR:O	37:1l:104:HIS:ND1	2.45	0.43
7:1G:378:LEU:HD12	7:1G:439:PHE:CE2	2.54	0.43
7:1G:478:ARG:HG2	7:1G:643:GLN:HE22	1.84	0.43
7:1G:524:LEU:N	7:1G:544:ILE:O	2.48	0.43
8:1H:110:SER:O	8:1H:113:VAL:HG12	2.19	0.43
9:1I:92:ILE:HD11	47:1I:201:SF4:S4	2.59	0.43
46:1I:204:PC1:C14	25:1Z:35:MET:HE1	2.40	0.43
10:1J:7:PHE:O	10:1J:11:THR:HG22	2.19	0.43
10:1J:139:GLU:O	10:1J:143:ILE:HD12	2.18	0.43
13:1M:408:LEU:O	13:1M:412:ILE:HG12	2.19	0.43
15:1O:97:GLN:HG2	15:1O:135:LEU:HB2	2.01	0.43
15:1O:179:ILE:O	15:1O:183:ILE:HG13	2.17	0.43
16:1P:194:ILE:HB	16:1P:288:HIS:NE2	2.34	0.43
19:1S:24:GLN:OE1	19:1S:25:ARG:HD3	2.18	0.43
21:1V:46:TYR:O	21:1V:50:ILE:HG23	2.18	0.43
21:1V:92:LYS:HB3	21:1V:96:TRP:HE1	1.84	0.43
25:1Z:32:GLY:HA2	25:1Z:35:MET:HE3	2.00	0.43
27:1b:40:TYR:O	27:1b:44:ILE:HG23	2.19	0.43
37:1l:156:TYR:HB3	40:1o:33:ARG:NE	2.34	0.43
39:1n:135:GLU:HB2	39:1n:164:PRO:HA	2.01	0.43
1:1A:54:LYS:HD3	1:1A:54:LYS:H	1.84	0.43
1:1A:65:PHE:O	1:1A:69:ILE:HG12	2.19	0.43
4:1D:100:LEU:HD11	4:1D:115:GLU:HG2	1.99	0.43
4:1D:113:CYS:SG	4:1D:370:PRO:HD3	2.59	0.43
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.49	0.43
4:1D:245:VAL:CG1	4:1D:250:ALA:HB2	2.49	0.43
5:1E:86:PHE:HD2	7:1G:177:ARG:HB2	1.84	0.43
5:1E:134:ASP:OD2	5:1E:177:LYS:NZ	2.40	0.43
7:1G:84:GLU:O	7:1G:88:LYS:HG2	2.19	0.43
7:1G:402:ASN:OD1	7:1G:402:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:415:LEU:HB3	7:1G:417:TYR:CE1	2.54	0.43
8:1H:20:LEU:HD12	26:1a:12:MET:CE	2.42	0.43
12:1L:49:VAL:CG1	12:1L:50:PRO:HD3	2.48	0.43
12:1L:465:GLY:O	12:1L:469:SER:OG	2.26	0.43
13:1M:71:TRP:O	13:1M:74:PRO:HD2	2.19	0.43
13:1M:114:GLU:OE2	13:1M:174:LEU:HB3	2.18	0.43
14:1N:1:FME:HE3	14:1N:1:FME:HB2	1.88	0.43
14:1N:162:ILE:HD13	14:1N:282:MET:HB3	2.01	0.43
15:1O:26:THR:HG22	15:1O:124:LEU:HD21	2.01	0.43
15:1O:80:GLU:HB3	15:1O:190:HIS:NE2	2.34	0.43
15:1O:198:TYR:O	15:1O:202:ILE:HG12	2.18	0.43
16:1P:64:ASP:OD1	16:1P:65:LEU:N	2.51	0.43
21:1V:82:GLN:HA	21:1V:85:ASN:HD21	1.83	0.43
22:1W:70:ASN:HD22	22:1W:82:LEU:HD11	1.84	0.43
23:1X:127:VAL:O	27:1b:66:PRO:HD2	2.19	0.43
28:1c:42:TYR:CZ	29:1d:22:PRO:HG3	2.54	0.43
31:1f:3:VAL:O	31:1f:7:VAL:HG22	2.19	0.43
31:1f:11:TRP:O	31:1f:14:ILE:HG22	2.18	0.43
31:1f:31:ASP:OD1	33:1h:89:LYS:HD3	2.18	0.43
35:1j:67:LEU:HD13	35:1j:71:GLU:HG3	2.01	0.43
37:1l:14:PRO:HB2	37:1l:20:ARG:HG2	2.00	0.43
37:1l:139:TYR:OH	37:1l:145:ASP:O	2.34	0.43
40:1o:61:TYR:CD2	40:1o:89:CYS:HB2	2.54	0.43
42:1q:144:TYR:CE2	42:1q:145:LYS:HE3	2.54	0.43
1:1A:92:LEU:O	1:1A:96:ILE:HG12	2.19	0.43
2:1B:54:CYS:CA	4:1D:108:TYR:HB2	2.49	0.43
4:1D:178:PHE:CE2	4:1D:189:MET:HG3	2.54	0.43
6:1F:20:ARG:CZ	6:1F:269:GLU:HB2	2.48	0.43
6:1F:378:ARG:O	6:1F:383:ASP:N	2.52	0.43
7:1G:74:MET:SD	7:1G:77:TRP:CE3	3.12	0.43
7:1G:250:ILE:HG12	7:1G:271:TYR:HD2	1.83	0.43
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	2.00	0.43
9:1I:81:LYS:HA	9:1I:94:ILE:HD11	2.00	0.43
12:1L:292:ALA:HB2	12:1L:304:PHE:HB3	2.01	0.43
12:1L:363:TYR:HA	12:1L:370:THR:HG21	2.00	0.43
14:1N:106:LEU:HD21	14:1N:138:PRO:HB2	2.01	0.43
14:1N:211:MET:CE	14:1N:251:MET:HA	2.49	0.43
15:1O:167:HIS:O	15:1O:218:CYS:HB2	2.19	0.43
15:1O:191:GLU:O	15:1O:194:ILE:HG12	2.19	0.43
16:1P:81:ILE:O	16:1P:84:VAL:HG22	2.19	0.43
17:1Q:28:GLU:OE2	17:1Q:32:THR:OG1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:11:ILE:O	20:1T:15:VAL:HG23	2.18	0.43
20:1U:12:LYS:HB3	20:1U:12:LYS:HE3	1.74	0.43
21:1V:43:TYR:CE2	21:1V:93:MET:SD	3.12	0.43
21:1V:115:ILE:H	21:1V:115:ILE:HG12	1.63	0.43
22:1W:63:VAL:O	22:1W:67:PHE:HD2	2.02	0.43
22:1W:90:LEU:O	22:1W:93:THR:OG1	2.32	0.43
23:1X:44:LEU:HD23	23:1X:134:ARG:NH1	2.34	0.43
25:1Z:89:GLU:OE1	25:1Z:90:ASN:ND2	2.52	0.43
30:1e:73:LYS:HD3	30:1e:73:LYS:HA	1.39	0.43
32:1g:59:ARG:O	32:1g:63:PHE:HB2	2.19	0.43
33:1h:62:GLU:HB2	33:1h:65:GLU:HB2	2.01	0.43
34:1i:81:ILE:HD13	34:1i:81:ILE:HA	1.85	0.43
35:1j:32:MET:C	35:1j:32:MET:SD	3.02	0.43
42:1q:38:LEU:HD13	42:1q:39:VAL:N	2.34	0.43
43:1r:35:GLN:HE21	43:1r:36:PRO:HD2	1.84	0.43
1:1A:102:LEU:HD12	1:1A:102:LEU:O	2.19	0.42
2:1B:71:ARG:HH21	8:1H:38:ASN:ND2	2.16	0.42
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.54	0.42
4:1D:284:ASP:HB2	4:1D:306:GLN:CD	2.44	0.42
4:1D:329:LYS:HE2	43:1r:53:TYR:CE2	2.54	0.42
4:1D:428:VAL:HG13	4:1D:429:ASP:OD1	2.19	0.42
6:1F:15:LEU:HB2	6:1F:271:GLU:N	2.33	0.42
7:1G:21:GLU:OE2	7:1G:22:PRO:HD2	2.19	0.42
7:1G:40:PHE:CZ	7:1G:116:LEU:HA	2.53	0.42
7:1G:57:VAL:HA	7:1G:86:SER:HB2	2.01	0.42
7:1G:261:GLU:O	17:1Q:44:ASN:ND2	2.52	0.42
7:1G:345:THR:HG22	7:1G:508:LYS:O	2.18	0.42
8:1H:37:PRO:HB3	8:1H:47:GLN:HG2	2.01	0.42
11:1K:12:PHE:CZ	11:1K:36:MET:HE3	2.53	0.42
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.52	0.42
12:1L:309:GLN:O	12:1L:313:MET:HG2	2.19	0.42
12:1L:324:LEU:HD11	12:1L:476:THR:HG21	2.00	0.42
13:1M:52:PHE:HA	33:1h:89:LYS:NZ	2.34	0.42
13:1M:126:LEU:HD21	13:1M:153:THR:HG21	2.01	0.42
13:1M:196:TRP:CE3	13:1M:257:MET:HG3	2.53	0.42
13:1M:263:MET:HE1	38:1m:104:PHE:CD2	2.54	0.42
14:1N:9:LEU:HD21	14:1N:42:PRO:CG	2.49	0.42
16:1P:48:PRO:HA	16:1P:71:MET:O	2.19	0.42
16:1P:128:LYS:HE2	16:1P:128:LYS:HB3	1.88	0.42
17:1Q:19:ILE:N	17:1Q:98:LYS:O	2.52	0.42
20:1T:60:PHE:CE2	20:1T:62:ILE:HG12	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:92:GLU:HB3	22:1W:98:LYS:HG3	2.01	0.42
24:1Y:12:PRO:HG2	24:1Y:15:THR:OG1	2.18	0.42
25:1Z:125:TYR:O	25:1Z:127:LEU:N	2.51	0.42
31:1f:25:TYR:O	31:1f:28:ARG:HG2	2.19	0.42
33:1h:79:PHE:CD1	33:1h:79:PHE:N	2.85	0.42
37:1l:73:TRP:O	38:1m:42:LEU:HD23	2.19	0.42
40:1o:14:LYS:HZ2	40:1o:112:LYS:HB3	1.84	0.42
40:1o:18:PRO:HA	40:1o:21:MET:SD	2.59	0.42
41:1p:27:ASN:HD21	41:1p:29:VAL:HB	1.84	0.42
41:1p:126:LYS:HB3	41:1p:126:LYS:HE3	1.74	0.42
43:1r:100:ILE:HG23	43:1r:102:ARG:NH1	2.34	0.42
3:1C:136:ASP:OD1	3:1C:150:ARG:HA	2.18	0.42
4:1D:278:TYR:O	4:1D:281:VAL:HG12	2.20	0.42
5:1E:132:THR:OG1	5:1E:136:LEU:N	2.50	0.42
6:1F:31:TRP:NE1	44:1s:42:GLN:OE1	2.52	0.42
8:1H:53:LEU:HA	8:1H:56:VAL:HG12	2.01	0.42
9:1I:53:GLU:HG3	42:1q:58:ARG:HA	2.01	0.42
9:1I:128:VAL:HG12	18:1R:68:HIS:HB2	2.01	0.42
11:1K:73:LEU:HD21	14:1N:41:ILE:HG21	2.01	0.42
13:1M:43:ASN:HB2	32:1g:80:LEU:HD13	2.00	0.42
13:1M:75:LEU:HD13	13:1M:440:HIS:NE2	2.34	0.42
13:1M:450:ASN:HD22	13:1M:453:MET:HG2	1.82	0.42
14:1N:326:LEU:O	14:1N:330:ILE:HG12	2.19	0.42
15:1O:82:PHE:CZ	15:1O:138:MET:CE	3.02	0.42
16:1P:172:PHE:CZ	16:1P:310:LEU:HA	2.54	0.42
18:1R:74:ASN:OD1	18:1R:75:LEU:N	2.52	0.42
19:1S:65:TRP:CD2	19:1S:75:ASN:ND2	2.87	0.42
22:1W:70:ASN:ND2	22:1W:82:LEU:HD11	2.33	0.42
25:1Z:32:GLY:HA2	25:1Z:35:MET:CE	2.50	0.42
28:1c:27:LEU:HD12	29:1d:70:PHE:CG	2.53	0.42
44:1s:63:MET:HB2	44:1s:64:PRO:HD3	2.01	0.42
1:1A:73:LEU:N	1:1A:74:PRO:HD2	2.34	0.42
6:1F:77:LEU:H	6:1F:77:LEU:HD12	1.83	0.42
7:1G:375:ASP:OD1	7:1G:376:VAL:N	2.52	0.42
7:1G:703:ILE:HD13	7:1G:703:ILE:HA	1.85	0.42
10:1J:113:VAL:HG23	10:1J:119:PHE:HE1	1.84	0.42
11:1K:23:ARG:HD2	11:1K:23:ARG:HA	1.74	0.42
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.55	0.42
12:1L:489:THR:HG22	58:1l:201:MYR:H121	1.99	0.42
45:1L:701:3PE:H252	45:1L:701:3PE:O32	2.18	0.42
13:1M:6:ILE:HD11	31:1f:26:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:22:MET:HE3	13:1M:25:ILE:HD13	2.01	0.42
13:1M:50:LEU:N	13:1M:58:SER:O	2.50	0.42
13:1M:252:PRO:HG3	29:1d:117:HIS:CD2	2.54	0.42
20:1U:22:TYR:CZ	20:1U:24:LYS:HE3	2.54	0.42
21:1V:22:ARG:HD2	21:1V:26:LEU:HD21	2.00	0.42
23:1X:58:GLU:H	23:1X:58:GLU:CD	2.24	0.42
31:1f:7:VAL:HG23	31:1f:8:ARG:H	1.84	0.42
33:1h:9:PHE:CE2	33:1h:11:ILE:HG12	2.53	0.42
39:1n:93:TYR:HD2	39:1n:93:TYR:N	2.17	0.42
41:1p:50:PHE:O	41:1p:53:GLN:HG3	2.19	0.42
42:1q:32:ASP:OD2	42:1q:32:ASP:C	2.62	0.42
1:1A:15:SER:HA	8:1H:76:ILE:HD11	2.01	0.42
1:1A:57:LEU:HD23	10:1J:172:THR:HG21	2.01	0.42
3:1C:209:TYR:N	3:1C:209:TYR:CD1	2.87	0.42
4:1D:168:PHE:HB2	8:1H:32:GLN:HB3	2.02	0.42
4:1D:236:ARG:HA	4:1D:239:THR:HG22	2.01	0.42
5:1E:129:GLY:N	5:1E:139:LEU:O	2.38	0.42
6:1F:8:LYS:NZ	6:1F:247:ARG:HE	2.17	0.42
6:1F:33:LEU:HD22	6:1F:155:GLU:HB3	2.00	0.42
6:1F:249:ARG:NH1	6:1F:249:ARG:HA	2.34	0.42
6:1F:431:GLN:OE1	6:1F:431:GLN:N	2.46	0.42
7:1G:61:LYS:HD2	7:1G:61:LYS:O	2.20	0.42
7:1G:231:MET:HE1	7:1G:677:ILE:HG21	2.01	0.42
7:1G:300:LEU:HD23	7:1G:300:LEU:H	1.84	0.42
7:1G:399:TRP:HA	7:1G:404:LEU:HB3	2.02	0.42
7:1G:552:VAL:O	7:1G:555:PRO:HD2	2.20	0.42
8:1H:76:ILE:HD13	8:1H:76:ILE:HA	1.91	0.42
9:1I:44:GLU:CA	26:1a:1:MET:HE1	2.44	0.42
9:1I:141:THR:OG1	9:1I:142:GLU:N	2.52	0.42
12:1L:100:ILE:O	12:1L:104:SER:OG	2.28	0.42
12:1L:528:TYR:CG	37:1l:101:MET:HE1	2.55	0.42
12:1L:564:LYS:HD2	12:1L:564:LYS:HA	1.79	0.42
13:1M:16:TRP:HA	13:1M:93:LYS:HD2	2.00	0.42
15:1O:94:TYR:CG	15:1O:148:CYS:HB3	2.53	0.42
18:1R:28:PHE:CD1	18:1R:33:LYS:HB2	2.55	0.42
22:1W:84:ILE:O	22:1W:88:MET:N	2.49	0.42
23:1X:73:ILE:HD13	23:1X:81:PHE:CD2	2.55	0.42
26:1a:54:ILE:O	26:1a:54:ILE:HG13	2.19	0.42
36:1k:13:MET:HE3	36:1k:13:MET:HB3	1.97	0.42
38:1m:27:GLU:H	38:1m:27:GLU:CD	2.20	0.42
5:1E:136:LEU:HD23	5:1E:136:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:23:THR:OG1	6:1F:39:ARG:HB2	2.19	0.42
6:1F:403:THR:C	7:1G:53:ARG:HH12	2.27	0.42
7:1G:379:LEU:HB2	7:1G:408:LEU:HB2	2.01	0.42
7:1G:399:TRP:HD1	7:1G:404:LEU:O	2.02	0.42
7:1G:449:PRO:HG2	7:1G:477:ILE:HG12	2.01	0.42
7:1G:514:ILE:HD11	7:1G:522:LEU:CD1	2.50	0.42
8:1H:91:MET:O	8:1H:93:TYR:N	2.52	0.42
9:1I:150:ASN:C	9:1I:150:ASN:OD1	2.62	0.42
12:1L:194:ASN:ND2	41:1p:106:GLN:OE1	2.53	0.42
51:1M:501:PGT:H442	51:1M:501:PGT:H412	1.83	0.42
14:1N:282:MET:H	14:1N:282:MET:HG3	1.68	0.42
15:1O:86:PRO:HA	15:1O:143:PHE:CZ	2.54	0.42
17:1Q:28:GLU:O	17:1Q:32:THR:OG1	2.36	0.42
19:1S:44:LYS:NZ	19:1S:50:LEU:O	2.52	0.42
20:1T:62:ILE:HD13	20:1T:62:ILE:HA	1.89	0.42
28:1c:48:LEU:H	28:1c:48:LEU:HD12	1.84	0.42
30:1e:20:GLN:HG2	30:1e:36:GLU:OE1	2.18	0.42
35:1j:71:GLU:O	40:1o:114:ARG:NH2	2.52	0.42
37:1l:112:MET:HA	37:1l:112:MET:HE3	2.01	0.42
38:1m:82:THR:HG23	38:1m:84:LYS:N	2.35	0.42
39:1n:38:TYR:CD1	39:1n:38:TYR:C	2.98	0.42
43:1r:109:GLN:OE1	43:1r:111:TYR:N	2.53	0.42
6:1F:237:ARG:HH21	6:1F:241:TRP:HD1	1.68	0.42
7:1G:216:THR:O	7:1G:243:ARG:NH1	2.30	0.42
7:1G:231:MET:HE1	7:1G:566:TYR:HE1	1.84	0.42
8:1H:30:TYR:OH	26:1a:4:GLU:OE1	2.35	0.42
9:1I:43:ARG:HG3	43:1r:11:ARG:CZ	2.50	0.42
13:1M:166:TYR:O	13:1M:170:THR:OG1	2.31	0.42
13:1M:278:ARG:HH22	37:1l:83:MET:HE1	1.85	0.42
19:1S:25:ARG:HH21	19:1S:58:SER:HA	1.85	0.42
19:1S:44:LYS:HZ3	19:1S:52:ILE:HG23	1.84	0.42
20:1U:71:MET:HE2	20:1U:71:MET:HB2	1.82	0.42
21:1V:85:ASN:O	21:1V:89:LEU:N	2.44	0.42
23:1X:37:LYS:HB2	23:1X:37:LYS:HE3	1.78	0.42
25:1Z:104:TRP:CZ2	30:1e:74:ARG:HD2	2.55	0.42
34:1i:93:PRO:HG3	41:1p:9:TYR:CE2	2.55	0.42
36:1k:32:GLN:O	36:1k:35:LEU:HD23	2.19	0.42
39:1n:155:PRO:HD2	39:1n:157:ARG:HH21	1.84	0.42
42:1q:68:MET:HE2	42:1q:68:MET:HA	2.01	0.42
1:1A:104:TYR:HE2	10:1J:166:VAL:HG23	1.84	0.42
3:1C:90:PHE:CD2	3:1C:140:VAL:HB	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:407:LYS:HA	4:1D:407:LYS:HD2	1.76	0.42
5:1E:161:TYR:C	5:1E:164:LEU:HD21	2.45	0.42
6:1F:19:ASP:OD1	6:1F:19:ASP:N	2.52	0.42
11:1K:11:ALA:HA	11:1K:14:ILE:HD12	2.02	0.42
12:1L:119:LYS:HB3	12:1L:119:LYS:HE2	1.93	0.42
12:1L:249:SER:OG	12:1L:250:SER:N	2.51	0.42
12:1L:368:PHE:HE1	35:1j:28:PHE:HD2	1.67	0.42
13:1M:216:LEU:HB2	13:1M:217:PRO:HD3	2.02	0.42
14:1N:26:TRP:CE2	14:1N:86:ILE:HG12	2.54	0.42
14:1N:206:LEU:HD12	14:1N:206:LEU:H	1.85	0.42
15:1O:242:LYS:HD2	15:1O:242:LYS:O	2.20	0.42
22:1W:80:ASP:HA	22:1W:83:VAL:HG12	2.02	0.42
27:1b:6:SER:O	27:1b:10:ASN:N	2.42	0.42
30:1e:7:LYS:HB3	30:1e:7:LYS:HE3	1.76	0.42
33:1h:50:ALA:HB2	41:1p:60:TYR:CE2	2.55	0.42
42:1q:60:ARG:NH2	42:1q:95:ASP:OD1	2.51	0.42
4:1D:307:SER:HA	4:1D:310:ILE:HD12	2.01	0.42
5:1E:27:ASN:HD21	5:1E:53:LEU:HD11	1.85	0.42
5:1E:86:PHE:HE2	7:1G:177:ARG:HG3	1.85	0.42
7:1G:391:PHE:CZ	7:1G:395:ILE:HD11	2.54	0.42
12:1L:89:PHE:CE1	12:1L:93:ALA:HB2	2.55	0.42
13:1M:129:THR:HG21	13:1M:235:LEU:HD11	2.00	0.42
17:1Q:59:PHE:CZ	17:1Q:79:LEU:HD12	2.55	0.42
17:1Q:106:GLU:HA	17:1Q:106:GLU:OE1	2.20	0.42
19:1S:23:CYS:C	19:1S:33:ARG:HH21	2.28	0.42
25:1Z:12:PRO:HD2	25:1Z:16:TYR:CE2	2.55	0.42
25:1Z:104:TRP:HE1	30:1e:74:ARG:CZ	2.32	0.42
32:1g:90:ARG:HA	41:1p:100:GLU:HG2	2.00	0.42
40:1o:75:ASN:O	40:1o:75:ASN:OD1	2.37	0.42
44:1s:50:THR:O	44:1s:54:LEU:HD23	2.20	0.42
1:1A:90:MET:HA	1:1A:90:MET:HE2	2.00	0.42
3:1C:210:ARG:NH1	7:1G:35:MET:HG3	2.35	0.42
5:1E:177:LYS:HA	5:1E:177:LYS:HD3	1.78	0.42
6:1F:97:ALA:HA	6:1F:107:ASP:CG	2.44	0.42
6:1F:312:CYS:O	6:1F:313:GLU:C	2.63	0.42
10:1J:163:ILE:O	10:1J:166:VAL:HG12	2.20	0.42
12:1L:83:ASP:OD1	12:1L:83:ASP:C	2.63	0.42
12:1L:288:THR:HG21	12:1L:307:SER:OG	2.19	0.42
13:1M:44:GLN:HG3	13:1M:60:SER:HA	2.02	0.42
14:1N:89:MET:SD	14:1N:98:MET:CE	3.07	0.42
23:1X:84:TYR:HE1	23:1X:99:CYS:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:23:ARG:CG	25:1Z:25:LEU:HD23	2.49	0.42
29:1d:108:THR:HA	41:1p:77:GLU:HA	2.01	0.42
37:1l:131:LYS:HG3	37:1l:133:TYR:CD1	2.51	0.42
39:1n:38:TYR:HE1	39:1n:42:LEU:HD21	1.85	0.42
41:1p:22:GLN:OE1	41:1p:22:GLN:N	2.52	0.42
42:1q:47:LYS:HE3	42:1q:47:LYS:HB3	1.93	0.42
42:1q:134:ILE:O	42:1q:134:ILE:HG22	2.20	0.42
2:1B:62:MET:CE	2:1B:156:LEU:HD11	2.50	0.42
3:1C:92:ILE:HD11	3:1C:140:VAL:HG11	2.02	0.42
3:1C:113:GLU:HG3	17:1Q:19:ILE:HG21	2.02	0.42
3:1C:151:ILE:HD12	3:1C:151:ILE:HA	1.89	0.42
3:1C:159:GLY:O	3:1C:160:HIS:ND1	2.53	0.42
3:1C:204:GLU:HG3	3:1C:205:ALA:O	2.20	0.42
4:1D:305:ARG:HB3	25:1Z:21:TYR:O	2.20	0.42
5:1E:89:MET:HG2	6:1F:181:ALA:O	2.20	0.42
5:1E:176:LEU:HD23	5:1E:176:LEU:HA	1.88	0.42
6:1F:89:ARG:HG2	6:1F:217:GLY:O	2.20	0.42
6:1F:132:ARG:NH2	44:1s:66:PRO:HD3	2.33	0.42
7:1G:48:VAL:HG21	17:1Q:118:TYR:HA	2.00	0.42
8:1H:230:ASN:O	8:1H:234:MET:HB2	2.19	0.42
9:1I:14:MET:O	9:1I:18:THR:OG1	2.35	0.42
10:1J:52:LEU:N	10:1J:139:GLU:OE2	2.48	0.42
12:1L:297:ASP:HB3	12:1L:300:LYS:HB2	2.02	0.42
12:1L:415:ALA:HA	12:1L:418:LEU:HB2	2.02	0.42
13:1M:25:ILE:O	13:1M:29:VAL:HG13	2.19	0.42
13:1M:255:ASN:OD1	13:1M:255:ASN:N	2.53	0.42
14:1N:58:LYS:O	14:1N:62:THR:HG22	2.19	0.42
15:1O:13:ARG:HB2	15:1O:16:ARG:CD	2.50	0.42
15:1O:94:TYR:CD1	15:1O:148:CYS:HB3	2.55	0.42
18:1R:46:GLU:OE2	18:1R:46:GLU:N	2.37	0.42
23:1X:143:SER:OG	23:1X:146:ARG:NH1	2.52	0.42
25:1Z:104:TRP:HE1	30:1e:74:ARG:NH1	2.18	0.42
29:1d:58:LEU:HD12	29:1d:58:LEU:HA	1.87	0.42
34:1i:76:ILE:HB	34:1i:77:PRO:HD3	2.01	0.42
40:1o:90:GLU:O	40:1o:93:ASP:OD2	2.37	0.42
43:1r:18:ASP:C	43:1r:18:ASP:OD2	2.62	0.42
3:1C:66:ASP:OD1	3:1C:66:ASP:N	2.53	0.41
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	2.02	0.41
3:1C:93:VAL:HG22	3:1C:108:LYS:HG2	2.00	0.41
4:1D:115:GLU:OE1	4:1D:194:ILE:N	2.49	0.41
5:1E:194:GLU:CD	6:1F:28:ARG:HH22	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:15:LEU:HG	6:1F:19:ASP:HB2	2.01	0.41
7:1G:121:MET:HE3	7:1G:121:MET:HB3	1.78	0.41
7:1G:299:ALA:O	7:1G:303:VAL:HG23	2.19	0.41
7:1G:562:PRO:HB2	7:1G:593:ALA:HB2	2.01	0.41
7:1G:599:ILE:HG22	22:1W:122:PHE:HZ	1.84	0.41
7:1G:647:GLU:H	7:1G:647:GLU:HG2	1.64	0.41
9:1I:65:HIS:CD2	9:1I:133:GLU:HG3	2.55	0.41
10:1J:119:PHE:HA	11:1K:6:MET:SD	2.59	0.41
10:1J:124:ASP:O	10:1J:127:ILE:HG12	2.20	0.41
12:1L:158:TRP:CZ2	39:1n:92:ARG:HD3	2.55	0.41
14:1N:25:HIS:HD2	30:1e:18:THR:HA	1.84	0.41
14:1N:124:LEU:HD23	14:1N:220:ILE:HD13	2.02	0.41
17:1Q:91:ASP:OD1	17:1Q:91:ASP:N	2.53	0.41
39:1n:103:LEU:HD23	39:1n:121:ARG:HD3	2.00	0.41
39:1n:144:PRO:HG2	39:1n:148:PRO:HA	2.02	0.41
40:1o:14:LYS:HZ3	40:1o:109:GLN:HA	1.83	0.41
42:1q:86:TRP:CZ3	42:1q:98:PRO:HD2	2.55	0.41
4:1D:332:PRO:HB3	4:1D:352:TYR:HE1	1.84	0.41
4:1D:373:GLU:C	4:1D:394:PRO:HG3	2.46	0.41
6:1F:20:ARG:HH22	6:1F:269:GLU:H	1.67	0.41
6:1F:140:GLY:HA2	6:1F:179:ARG:NE	2.25	0.41
7:1G:569:LYS:HE2	7:1G:596:ASP:HB2	2.02	0.41
10:1J:82:VAL:HG13	10:1J:84:VAL:N	2.26	0.41
12:1L:101:MET:HG3	12:1L:118:PHE:CE2	2.55	0.41
14:1N:25:HIS:CD2	30:1e:18:THR:HA	2.55	0.41
16:1P:95:VAL:HG11	16:1P:113:ILE:HG21	2.02	0.41
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.85	0.41
19:1S:88:ARG:HH21	19:1S:92:ASN:H	1.68	0.41
20:1T:17:TYR:HD1	20:1T:20:LYS:NZ	2.18	0.41
30:1e:74:ARG:O	30:1e:78:ILE:HG12	2.20	0.41
37:1l:74:GLY:N	38:1m:61:ASP:OD1	2.52	0.41
38:1m:17:LEU:HD23	38:1m:17:LEU:HA	1.92	0.41
40:1o:62:LEU:HD13	40:1o:86:TRP:CE2	2.54	0.41
52:1q:201:CDL:H531	52:1q:201:CDL:H711	2.01	0.41
43:1r:102:ARG:N	43:1r:102:ARG:HD2	2.35	0.41
3:1C:135:TRP:HZ2	22:1W:88:MET:HG3	1.85	0.41
4:1D:184:VAL:HG23	4:1D:185:SER:H	1.84	0.41
6:1F:91:LYS:HG2	6:1F:129:MET:O	2.19	0.41
10:1J:129:ASP:OD1	11:1K:52:HIS:NE2	2.53	0.41
11:1K:54:THR:HG21	30:1e:28:ILE:HB	2.01	0.41
12:1L:71:LEU:HD11	13:1M:380:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:194:ASN:OD1	38:1m:127:SER:HB2	2.20	0.41
12:1L:562:LEU:HD23	12:1L:562:LEU:HA	1.82	0.41
15:1O:61:SER:HA	15:1O:66:GLY:HA2	2.03	0.41
15:1O:191:GLU:HA	15:1O:194:ILE:HD11	2.03	0.41
16:1P:175:GLU:N	16:1P:175:GLU:OE2	2.53	0.41
21:1V:68:GLU:OE2	21:1V:76:ILE:HG12	2.21	0.41
22:1W:36:TYR:CE1	22:1W:40:TYR:CE1	3.09	0.41
31:1f:41:SER:O	31:1f:45:LYS:N	2.48	0.41
37:1l:10:PRO:O	38:1m:74:ASN:ND2	2.53	0.41
40:1o:38:MET:HG3	40:1o:40:ALA:O	2.20	0.41
42:1q:78:ASP:H	42:1q:81:MET:HE1	1.84	0.41
4:1D:347:HIS:NE2	7:1G:125:SER:O	2.43	0.41
5:1E:98:TYR:HE2	5:1E:136:LEU:HD13	1.85	0.41
6:1F:144:ASN:OD1	6:1F:144:ASN:N	2.51	0.41
6:1F:154:ARG:NH2	44:1s:54:LEU:O	2.54	0.41
6:1F:166:ALA:O	6:1F:167:CYS:HB2	2.21	0.41
7:1G:73:VAL:HA	7:1G:77:TRP:CE3	2.55	0.41
7:1G:138:GLU:OE1	7:1G:138:GLU:N	2.42	0.41
7:1G:230:VAL:HG21	7:1G:566:TYR:CD1	2.55	0.41
7:1G:385:ARG:HD2	7:1G:414:ASP:O	2.19	0.41
7:1G:451:VAL:HG11	7:1G:470:VAL:HG23	2.02	0.41
8:1H:124:ASN:C	8:1H:124:ASN:ND2	2.78	0.41
8:1H:136:VAL:HG12	8:1H:140:ILE:HD13	2.03	0.41
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.55	0.41
9:1I:146:GLU:HG2	42:1q:124:TYR:HB3	2.02	0.41
10:1J:74:MET:O	10:1J:76:THR:HG22	2.20	0.41
13:1M:77:LEU:HD23	13:1M:77:LEU:HA	1.92	0.41
13:1M:360:LEU:O	13:1M:364:LEU:HG	2.20	0.41
14:1N:71:MET:HE3	14:1N:74:ILE:HB	2.02	0.41
15:1O:195:THR:HG22	15:1O:198:TYR:H	1.86	0.41
19:1S:70:PHE:CD1	19:1S:70:PHE:O	2.74	0.41
29:1d:113:LEU:HD23	29:1d:113:LEU:C	2.46	0.41
31:1f:4:LEU:O	31:1f:4:LEU:HD23	2.20	0.41
34:1i:69:PHE:O	34:1i:73:HIS:HB2	2.20	0.41
40:1o:74:PRO:O	40:1o:75:ASN:C	2.63	0.41
1:1A:67:LEU:HB3	11:1K:65:VAL:HG23	2.03	0.41
2:1B:71:ARG:HH21	8:1H:38:ASN:HD21	1.69	0.41
6:1F:258:ILE:HD13	6:1F:284:ALA:HB2	2.02	0.41
6:1F:426:LEU:HD12	6:1F:426:LEU:HA	1.88	0.41
7:1G:8:LEU:HA	7:1G:22:PRO:HD3	2.02	0.41
7:1G:104:ASP:HB2	7:1G:152:ARG:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:300:LEU:HD12	7:1G:606:ILE:HG21	2.03	0.41
9:1I:169:ILE:O	9:1I:173:TYR:HD2	2.04	0.41
10:1J:12:ILE:O	10:1J:15:ILE:HG13	2.20	0.41
12:1L:108:MET:HE2	12:1L:108:MET:HB3	1.85	0.41
12:1L:138:PHE:HA	12:1L:186:MET:HE1	2.02	0.41
16:1P:224:LYS:H	16:1P:224:LYS:HG3	1.54	0.41
18:1R:28:PHE:CE1	18:1R:33:LYS:HB2	2.55	0.41
20:1U:55:GLU:HG2	20:1U:60:PHE:O	2.20	0.41
21:1V:103:VAL:HG23	21:1V:104:GLU:H	1.84	0.41
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.55	0.41
37:1l:98:TRP:NE1	37:1l:102:CYS:SG	2.94	0.41
38:1m:43:LYS:HD3	38:1m:43:LYS:HA	1.82	0.41
2:1B:51:GLY:HA2	2:1B:56:ALA:HB1	2.01	0.41
2:1B:87:ILE:CG2	2:1B:116:MET:HE2	2.50	0.41
3:1C:73:LYS:HA	3:1C:124:TYR:OH	2.20	0.41
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.46	0.41
3:1C:161:PRO:HA	3:1C:166:PHE:CD2	2.55	0.41
3:1C:179:GLU:HG3	16:1P:33:TYR:HD2	1.84	0.41
6:1F:101:GLU:CD	6:1F:302:SER:H	2.27	0.41
7:1G:92:GLY:O	7:1G:95:GLU:HG3	2.20	0.41
7:1G:404:LEU:HD13	7:1G:405:LYS:N	2.36	0.41
8:1H:108:MET:SD	8:1H:108:MET:C	3.04	0.41
11:1K:2:PRO:HD2	11:1K:5:TYR:HD2	1.86	0.41
12:1L:401:MET:HA	37:1l:126:GLN:HG2	2.01	0.41
12:1L:552:LEU:HD21	38:1m:88:LEU:C	2.46	0.41
12:1L:599:MET:HE2	12:1L:599:MET:HB3	1.96	0.41
13:1M:361:MET:HA	13:1M:364:LEU:CG	2.51	0.41
14:1N:160:LEU:O	14:1N:164:ILE:HG22	2.21	0.41
15:1O:204:ASN:O	15:1O:208:LYS:HG2	2.21	0.41
16:1P:48:PRO:O	16:1P:73:TRP:NE1	2.54	0.41
16:1P:249:ALA:HB2	16:1P:318:LEU:HD21	2.01	0.41
18:1R:37:GLU:H	18:1R:37:GLU:CD	2.23	0.41
19:1S:31:GLY:HA3	19:1S:81:PHE:O	2.21	0.41
19:1S:65:TRP:HA	19:1S:75:ASN:HB3	2.03	0.41
20:1T:16:LEU:O	20:1T:20:LYS:HG3	2.21	0.41
20:1U:35:HIS:CE1	20:1U:71:MET:HG2	2.55	0.41
22:1W:65:GLU:OE2	22:1W:65:GLU:C	2.64	0.41
24:1Y:74:CYS:SG	24:1Y:75:ILE:N	2.93	0.41
29:1d:34:MET:HB3	29:1d:37:LEU:HD12	2.03	0.41
33:1h:87:TYR:O	33:1h:91:MET:HE2	2.19	0.41
35:1j:12:ARG:HD3	36:1k:50:TRP:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:45:ASP:HB2	35:1j:50:HIS:CB	2.50	0.41
38:1m:44:ARG:NH2	39:1n:148:PRO:HB3	2.35	0.41
38:1m:110:LYS:O	38:1m:114:LEU:HG	2.21	0.41
39:1n:24:ARG:HD3	39:1n:24:ARG:HA	1.82	0.41
41:1p:145:LEU:HD23	41:1p:145:LEU:HA	1.87	0.41
42:1q:6:VAL:O	42:1q:9:ARG:HG3	2.20	0.41
3:1C:129:TRP:HZ2	4:1D:78:PRO:HD2	1.84	0.41
3:1C:203:TRP:CZ3	7:1G:36:GLN:HB3	2.55	0.41
4:1D:349:PHE:HD2	7:1G:105:CYS:HB3	1.84	0.41
4:1D:410:MET:SD	4:1D:411:LEU:N	2.93	0.41
5:1E:10:ARG:HH21	18:1R:77:LYS:HA	1.85	0.41
5:1E:27:ASN:OD1	5:1E:53:LEU:HD11	2.21	0.41
5:1E:116:ILE:HD11	5:1E:152:PRO:HB2	2.03	0.41
6:1F:84:LYS:HB2	6:1F:85:PRO:HD3	2.02	0.41
6:1F:275:PRO:HG2	6:1F:278:GLU:HG2	2.01	0.41
7:1G:305:GLY:HA3	7:1G:306:MET:HE2	2.01	0.41
7:1G:397:LYS:HG3	7:1G:401:HIS:ND1	2.36	0.41
7:1G:558:ASP:HB3	42:1q:144:TYR:OH	2.21	0.41
8:1H:92:PRO:HB2	8:1H:93:TYR:H	1.74	0.41
8:1H:157:ASN:HD22	8:1H:165:LEU:HD13	1.84	0.41
12:1L:7:LEU:HB3	12:1L:46:LEU:HD21	2.02	0.41
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.17	0.41
13:1M:88:THR:HG23	13:1M:91:ARG:H	1.86	0.41
13:1M:165:VAL:HG23	14:1N:271:THR:HG21	2.03	0.41
15:1O:135:LEU:HA	15:1O:138:MET:HB3	2.03	0.41
15:1O:320:LYS:HG3	28:1c:12:PRO:HG3	2.03	0.41
16:1P:90:VAL:HG11	16:1P:218:ILE:HD12	2.03	0.41
19:1S:18:ILE:HD12	19:1S:66:ALA:HA	2.01	0.41
20:1U:47:GLN:HA	20:1U:50:ILE:HG12	2.03	0.41
21:1V:8:THR:HG21	21:1V:13:LEU:HD12	2.02	0.41
23:1X:39:ASN:HB3	25:1Z:73:PRO:HG2	2.03	0.41
29:1d:107:LYS:HA	29:1d:107:LYS:HD2	1.64	0.41
30:1e:68:ARG:HH11	30:1e:71:THR:HG21	1.85	0.41
33:1h:79:PHE:N	33:1h:79:PHE:HD1	2.19	0.41
34:1i:32:PRO:HB3	39:1n:114:TYR:CE2	2.51	0.41
2:1B:72:PHE:HA	8:1H:39:VAL:HG12	2.02	0.41
2:1B:95:LYS:HD3	3:1C:154:GLY:HA2	2.01	0.41
3:1C:160:HIS:O	3:1C:163:ARG:HB2	2.20	0.41
5:1E:156:ILE:HG12	5:1E:161:TYR:CE2	2.55	0.41
6:1F:395:ILE:HD12	6:1F:396:SER:N	2.35	0.41
10:1J:33:LEU:CD2	10:1J:65:LEU:HG	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:7:LEU:O	12:1L:10:THR:OG1	2.30	0.41
12:1L:71:LEU:N	12:1L:74:VAL:O	2.54	0.41
12:1L:152:PHE:CD1	12:1L:168:ALA:HB1	2.55	0.41
12:1L:295:GLN:NE2	12:1L:524:ASN:O	2.54	0.41
12:1L:502:LEU:HD13	36:1k:62:PHE:CD2	2.56	0.41
13:1M:23:ILE:HD11	13:1M:92:LYS:HE3	2.03	0.41
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.21	0.41
13:1M:190:TRP:CG	24:1Y:126:MET:HE1	2.55	0.41
13:1M:275:ILE:HG21	13:1M:288:TYR:CG	2.55	0.41
14:1N:200:MET:HE2	14:1N:269:GLU:HB2	2.02	0.41
14:1N:344:SER:O	29:1d:82:MET:HG3	2.20	0.41
15:1O:279:LEU:HD12	15:1O:279:LEU:HA	1.82	0.41
24:1Y:43:LYS:HZ3	45:1Y:201:3PE:P	2.44	0.41
24:1Y:44:PRO:HA	24:1Y:45:PRO:HD3	1.93	0.41
24:1Y:89:TYR:O	24:1Y:93:GLY:N	2.39	0.41
25:1Z:23:ARG:HG2	25:1Z:25:LEU:H	1.86	0.41
32:1g:58:MET:HE3	32:1g:58:MET:HB3	1.72	0.41
32:1g:93:ALA:O	32:1g:97:VAL:HG23	2.20	0.41
34:1i:109:ILE:CD1	34:1i:112:THR:H	2.34	0.41
37:1l:133:TYR:HD2	37:1l:138:LEU:HD13	1.86	0.41
39:1n:92:ARG:HG2	39:1n:93:TYR:CE2	2.56	0.41
43:1r:104:GLU:C	43:1r:104:GLU:OE1	2.64	0.41
3:1C:73:LYS:NZ	4:1D:251:LEU:HG	2.33	0.41
3:1C:116:PRO:O	3:1C:117:ILE:HD13	2.21	0.41
4:1D:110:SER:C	4:1D:111:MET:HE2	2.45	0.41
5:1E:93:LYS:HE3	5:1E:93:LYS:HB2	1.79	0.41
5:1E:98:TYR:CE2	5:1E:136:LEU:HB3	2.56	0.41
5:1E:99:HIS:HA	5:1E:138:THR:OG1	2.20	0.41
5:1E:196:ALA:HB3	6:1F:264:HIS:ND1	2.36	0.41
5:1E:199:LEU:HD22	5:1E:201:SER:O	2.21	0.41
6:1F:362:CYS:SG	6:1F:364:PRO:HD2	2.61	0.41
7:1G:36:GLN:OE1	17:1Q:49:VAL:HG12	2.21	0.41
7:1G:53:ARG:N	48:1G:803:FES:S1	2.92	0.41
7:1G:94:MET:SD	7:1G:120:SER:OG	2.77	0.41
7:1G:266:LYS:HD2	7:1G:672:TYR:HA	2.03	0.41
7:1G:378:LEU:HD12	7:1G:439:PHE:CD2	2.56	0.41
7:1G:524:LEU:HD23	7:1G:524:LEU:HA	1.97	0.41
7:1G:594:ARG:NH2	22:1W:125:GLY:HA2	2.36	0.41
8:1H:12:PRO:O	8:1H:16:ALA:N	2.39	0.41
8:1H:317:GLN:H	8:1H:317:GLN:HG3	1.67	0.41
11:1K:34:GLU:O	11:1K:37:MET:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:205:ASN:ND2	12:1L:207:GLU:OE2	2.54	0.41
12:1L:295:GLN:O	12:1L:425:ARG:NH1	2.54	0.41
12:1L:604:TYR:CE2	14:1N:153:LEU:HD23	2.56	0.41
13:1M:160:LEU:HG	13:1M:164:LEU:CD1	2.51	0.41
13:1M:214:LEU:HA	13:1M:214:LEU:HD23	1.83	0.41
14:1N:83:GLN:NE2	30:1e:36:GLU:OE2	2.46	0.41
15:1O:189:PRO:HD2	15:1O:190:HIS:CD2	2.56	0.41
16:1P:13:ARG:NH2	16:1P:63:GLY:O	2.53	0.41
18:1R:3:ARG:O	18:1R:11:VAL:HG12	2.20	0.41
20:1T:55:GLU:OE1	20:1T:60:PHE:CE2	2.74	0.41
20:1U:9:GLU:HA	20:1U:12:LYS:HE3	2.03	0.41
20:1U:55:GLU:OE1	39:1n:81:PHE:CE1	2.74	0.41
23:1X:40:LYS:HB3	23:1X:130:VAL:CG1	2.50	0.41
25:1Z:58:ARG:HE	25:1Z:58:ARG:HB3	1.67	0.41
25:1Z:120:MET:HG3	30:1e:68:ARG:NE	2.35	0.41
26:1a:1:MET:O	26:1a:4:GLU:HG3	2.21	0.41
30:1e:83:ASP:OD1	30:1e:83:ASP:C	2.64	0.41
32:1g:67:SER:HA	32:1g:71:VAL:HG23	2.01	0.41
33:1h:56:PRO:HD3	41:1p:63:TYR:CE2	2.56	0.41
34:1i:21:TRP:CD2	39:1n:171:THR:HG22	2.56	0.41
35:1j:61:ASP:OD1	35:1j:61:ASP:N	2.53	0.41
37:1l:55:GLN:HG2	37:1l:84:TYR:O	2.21	0.41
37:1l:115:MET:HA	37:1l:118:VAL:HG22	2.02	0.41
38:1m:126:ILE:HA	41:1p:139:GLN:OE1	2.21	0.41
39:1n:133:GLU:O	39:1n:137:LYS:HB2	2.20	0.41
40:1o:80:LYS:HE3	40:1o:80:LYS:HB3	1.92	0.41
4:1D:159:LEU:HA	4:1D:159:LEU:HD23	1.82	0.41
4:1D:371:LYS:HB2	4:1D:422:ASP:OD2	2.21	0.41
5:1E:51:LEU:HD12	5:1E:51:LEU:HA	1.89	0.41
6:1F:280:ILE:H	6:1F:280:ILE:HG13	1.66	0.41
6:1F:282:LYS:HB3	6:1F:282:LYS:HE2	1.60	0.41
6:1F:427:GLU:O	6:1F:431:GLN:NE2	2.53	0.41
7:1G:49:ALA:HB2	7:1G:161:ARG:CZ	2.51	0.41
7:1G:278:ARG:HD2	7:1G:278:ARG:HA	1.92	0.41
7:1G:283:MET:HE2	7:1G:283:MET:HA	2.02	0.41
7:1G:355:GLY:HA2	7:1G:361:ASN:HD22	1.86	0.41
7:1G:383:ASN:HD22	7:1G:383:ASN:HA	1.68	0.41
7:1G:598:LYS:HG3	22:1W:118:PHE:CZ	2.55	0.41
8:1H:17:VAL:HG21	8:1H:229:ALA:HB2	2.03	0.41
8:1H:144:VAL:O	8:1H:148:ILE:HG12	2.21	0.41
10:1J:84:VAL:HG22	10:1J:90:PHE:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:112:GLU:OE1	10:1J:120:ASN:ND2	2.54	0.41
12:1L:211:MET:HE3	12:1L:211:MET:HB2	1.74	0.41
12:1L:556:ILE:HD13	12:1L:556:ILE:HA	1.82	0.41
13:1M:191:SER:HB2	51:1M:501:PGT:H31	2.03	0.41
13:1M:243:MET:HE2	13:1M:301:ILE:HG21	2.03	0.41
13:1M:457:PRO:HA	32:1g:84:ARG:NH2	2.33	0.41
14:1N:7:THR:HG21	52:1N:402:CDL:H322	2.03	0.41
14:1N:198:THR:O	14:1N:202:ILE:HG12	2.21	0.41
15:1O:224:SER:H	15:1O:227:GLU:HB2	1.85	0.41
15:1O:295:LYS:O	15:1O:298:GLU:HG3	2.21	0.41
19:1S:15:LEU:HD13	19:1S:15:LEU:HA	1.95	0.41
20:1T:72:CYS:HB2	20:1T:74:GLN:OE1	2.21	0.41
20:1U:49:GLU:CD	36:1k:44:TRP:HE1	2.28	0.41
21:1V:92:LYS:HB3	21:1V:96:TRP:CE2	2.56	0.41
22:1W:114:ARG:HB3	22:1W:115:PRO:HD3	2.02	0.41
31:1f:5:GLN:O	31:1f:9:ASP:HB3	2.21	0.41
46:1f:101:PC1:H362	33:1h:79:PHE:CE2	2.55	0.41
33:1h:87:TYR:OH	41:1p:86:GLU:OE1	2.33	0.41
36:1k:20:GLN:OE1	36:1k:20:GLN:N	2.49	0.41
38:1m:28:THR:HA	38:1m:31:ALA:HB3	2.03	0.41
2:1B:98:PRO:HG3	22:1W:101:THR:HG21	2.03	0.40
4:1D:306:GLN:O	4:1D:309:ARG:HG2	2.22	0.40
6:1F:45:THR:HG23	6:1F:236:ARG:HH21	1.86	0.40
6:1F:74:PRO:HG2	6:1F:77:LEU:HD13	2.03	0.40
8:1H:183:MET:HB2	9:1I:27:TRP:CH2	2.56	0.40
8:1H:286:MET:HE2	8:1H:286:MET:HA	2.02	0.40
10:1J:174:GLY:HA2	14:1N:48:PHE:CE2	2.56	0.40
12:1L:247:LEU:HB3	12:1L:252:MET:HB2	2.03	0.40
12:1L:310:LEU:HA	12:1L:313:MET:HG2	2.03	0.40
12:1L:379:ALA:O	12:1L:388:GLY:HA3	2.21	0.40
13:1M:359:TRP:CB	13:1M:415:GLN:HE21	2.34	0.40
14:1N:2:ASN:OD1	14:1N:4:ILE:HG22	2.21	0.40
14:1N:175:LEU:HD11	14:1N:225:THR:HA	2.03	0.40
15:1O:30:ASN:O	15:1O:35:LYS:NZ	2.52	0.40
15:1O:138:MET:SD	15:1O:144:ILE:CG2	3.08	0.40
17:1Q:20:THR:HG22	17:1Q:99:ASN:C	2.46	0.40
20:1U:15:VAL:HA	20:1U:54:MET:HE1	2.03	0.40
20:1U:32:VAL:O	20:1U:74:GLN:N	2.49	0.40
21:1V:8:THR:HG23	21:1V:10:LEU:H	1.85	0.40
24:1Y:130:GLU:HG2	24:1Y:132:TRP:HE1	1.85	0.40
27:1b:62:MET:SD	27:1b:62:MET:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1c:34:GLN:HG2	29:1d:74:TYR:OH	2.21	0.40
29:1d:96:SER:OG	29:1d:97:HIS:ND1	2.46	0.40
30:1e:9:LEU:HB2	30:1e:11:LEU:CD2	2.51	0.40
31:1f:14:ILE:C	31:1f:17:PRO:HD2	2.46	0.40
32:1g:96:LEU:HD11	32:1g:100:ARG:HE	1.85	0.40
33:1h:74:TRP:O	33:1h:78:THR:HG22	2.21	0.40
33:1h:88:GLU:HA	33:1h:91:MET:HE2	2.00	0.40
34:1i:1:SAC:H2A1	34:1i:1:SAC:OG	2.21	0.40
37:1l:28:ASN:ND2	38:1m:42:LEU:HD11	2.36	0.40
37:1l:33:ASP:OD1	37:1l:33:ASP:N	2.42	0.40
38:1m:55:ARG:NH1	38:1m:57:GLY:O	2.54	0.40
42:1q:133:LYS:HD3	42:1q:133:LYS:HA	1.80	0.40
42:1q:134:ILE:HD13	42:1q:134:ILE:HA	1.84	0.40
43:1r:110:PRO:CD	43:1r:111:TYR:N	2.81	0.40
2:1B:175:ILE:HD13	2:1B:175:ILE:HA	1.91	0.40
3:1C:167:PRO:HB3	17:1Q:82:LEU:HD11	2.02	0.40
4:1D:416:ALA:O	4:1D:420:THR:HG22	2.21	0.40
5:1E:148:CYS:HB3	6:1F:103:GLY:HA2	2.02	0.40
5:1E:217:LEU:C	6:1F:47:GLU:HG3	2.46	0.40
6:1F:154:ARG:HH12	44:1s:57:GLU:CB	2.32	0.40
6:1F:154:ARG:NH1	44:1s:57:GLU:HB3	2.32	0.40
6:1F:200:GLN:HE22	6:1F:202:LYS:HD2	1.78	0.40
6:1F:327:THR:OG1	6:1F:328:GLY:N	2.54	0.40
8:1H:233:MET:SD	8:1H:233:MET:C	3.04	0.40
9:1I:113:MET:HE1	9:1I:118:TYR:CE2	2.56	0.40
12:1L:81:LYS:HB2	12:1L:135:ASN:ND2	2.35	0.40
12:1L:293:ILE:HG22	12:1L:422:TYR:HB3	2.03	0.40
12:1L:331:MET:HB3	12:1L:387:THR:HG22	2.03	0.40
14:1N:190:MET:HE1	14:1N:205:LEU:HA	2.02	0.40
14:1N:268:GLN:HG3	23:1X:167:PHE:CZ	2.52	0.40
15:1O:24:VAL:HB	15:1O:166:PRO:HA	2.03	0.40
15:1O:171:TYR:HD1	15:1O:172:VAL:N	2.19	0.40
16:1P:109:VAL:HG12	55:1P:501:NDP:H61A	1.85	0.40
16:1P:149:LYS:HA	16:1P:149:LYS:HD3	1.84	0.40
19:1S:72:GLN:HA	19:1S:74:LYS:HZ1	1.85	0.40
23:1X:75:ARG:HB3	23:1X:76:HIS:HD2	1.87	0.40
29:1d:45:ASP:O	29:1d:49:ARG:HG3	2.20	0.40
30:1e:68:ARG:HA	30:1e:68:ARG:HD3	1.80	0.40
30:1e:88:GLU:HG2	30:1e:90:LYS:HG2	2.03	0.40
31:1f:55:THR:O	31:1f:56:TRP:C	2.65	0.40
35:1j:12:ARG:NH1	36:1k:47:ASN:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:56:PRO:HA	35:1j:59:TRP:CE2	2.56	0.40
37:1l:138:LEU:HB2	37:1l:142:ARG:HH21	1.87	0.40
42:1q:22:GLY:O	42:1q:26:VAL:HG23	2.20	0.40
2:1B:33:LEU:HD23	2:1B:33:LEU:HA	1.89	0.40
2:1B:166:LYS:HG2	2:1B:169:ARG:HH12	1.86	0.40
3:1C:52:ILE:HG12	3:1C:109:THR:HG22	2.03	0.40
3:1C:80:ALA:HA	3:1C:91:GLU:O	2.22	0.40
3:1C:181:LYS:HA	3:1C:181:LYS:HD3	1.79	0.40
4:1D:226:GLU:CD	4:1D:301:VAL:HG11	2.46	0.40
6:1F:207:PRO:HD3	7:1G:71:MET:CE	2.51	0.40
6:1F:374:LYS:HB2	7:1G:132:GLU:HG3	2.04	0.40
7:1G:408:LEU:HG	7:1G:410:GLY:H	1.86	0.40
7:1G:629:ASN:HA	7:1G:637:GLU:HG2	2.03	0.40
8:1H:186:PHE:CD2	46:1I:203:PC1:H2E1	2.56	0.40
10:1J:146:LEU:HA	11:1K:58:MET:HE1	2.03	0.40
12:1L:559:GLU:HB3	13:1M:214:LEU:CD1	2.51	0.40
13:1M:229:MET:HB3	13:1M:324:SER:HB2	2.02	0.40
13:1M:403:THR:O	13:1M:407:SER:OG	2.30	0.40
14:1N:127:GLY:O	14:1N:131:LEU:HD12	2.21	0.40
14:1N:243:LEU:HD12	14:1N:243:LEU:H	1.87	0.40
16:1P:52:GLU:OE2	16:1P:53:PRO:HD2	2.22	0.40
16:1P:92:ILE:HG13	16:1P:130:ILE:HB	2.02	0.40
18:1R:41:ILE:H	18:1R:41:ILE:HG13	1.74	0.40
21:1V:50:ILE:HG13	21:1V:54:LYS:HZ1	1.81	0.40
23:1X:167:PHE:H	33:1h:104:ARG:HH12	1.69	0.40
25:1Z:31:SER:O	25:1Z:35:MET:HE2	2.21	0.40
33:1h:41:THR:O	33:1h:45:VAL:HG22	2.21	0.40
36:1k:87:LEU:HA	36:1k:90:GLN:HG2	2.03	0.40
37:1l:125:TYR:HD1	40:1o:3:HIS:HE1	1.69	0.40
2:1B:49:THR:HG21	2:1B:59:MET:HE3	2.03	0.40
2:1B:166:LYS:HG2	2:1B:169:ARG:NH1	2.37	0.40
3:1C:94:TYR:HB2	3:1C:107:VAL:CG2	2.50	0.40
4:1D:323:ILE:H	4:1D:323:ILE:HG12	1.72	0.40
6:1F:129:MET:HE2	6:1F:221:THR:HB	2.03	0.40
6:1F:245:PHE:HB3	6:1F:271:GLU:CD	2.45	0.40
6:1F:259:SER:HA	6:1F:265:PRO:HB3	2.03	0.40
7:1G:59:ILE:HD12	7:1G:78:ASN:C	2.46	0.40
7:1G:296:TRP:O	7:1G:300:LEU:HD23	2.21	0.40
7:1G:341:ASP:N	7:1G:341:ASP:OD1	2.54	0.40
7:1G:374:ALA:HB2	7:1G:487:TRP:HH2	1.86	0.40
8:1H:85:MET:O	8:1H:88:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:310:LEU:HA	12:1L:310:LEU:HD13	1.94	0.40
13:1M:25:ILE:H	13:1M:25:ILE:HD12	1.85	0.40
13:1M:33:LEU:O	13:1M:37:ILE:HG12	2.21	0.40
13:1M:215:TRP:HZ3	13:1M:231:LEU:HD11	1.85	0.40
13:1M:368:ALA:HB1	13:1M:375:LEU:HA	2.02	0.40
14:1N:45:MET:HE3	14:1N:45:MET:HB3	1.72	0.40
14:1N:55:ALA:HB1	14:1N:118:VAL:HA	2.03	0.40
14:1N:107:GLY:HA2	14:1N:111:PHE:O	2.20	0.40
14:1N:165:GLY:HA3	14:1N:185:ALA:HB2	2.03	0.40
16:1P:315:ILE:H	16:1P:315:ILE:HG12	1.64	0.40
17:1Q:130:VAL:HG12	17:1Q:132:THR:H	1.86	0.40
19:1S:16:ARG:O	19:1S:51:PRO:HD2	2.20	0.40
20:1T:10:ALA:HA	20:1T:13:ASP:OD2	2.22	0.40
20:1U:61:GLU:C	20:1U:61:GLU:OE1	2.64	0.40
23:1X:25:LYS:NZ	23:1X:94:GLN:O	2.47	0.40
23:1X:47:TRP:CZ3	33:1h:141:PRO:HG3	2.57	0.40
24:1Y:91:ILE:H	24:1Y:91:ILE:HG12	1.73	0.40
24:1Y:139:LYS:HE2	33:1h:112:ARG:HH11	1.86	0.40
30:1e:31:ARG:NH2	30:1e:68:ARG:HH21	2.17	0.40
31:1f:31:ASP:OD2	33:1h:85:LYS:NZ	2.54	0.40
39:1n:106:TRP:CE3	39:1n:110:GLU:HB3	2.56	0.40
41:1p:77:GLU:OE1	41:1p:80:ASP:HB2	2.22	0.40
2:1B:72:PHE:HA	8:1H:39:VAL:CG1	2.51	0.40
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	2.03	0.40
4:1D:350:LYS:HD2	4:1D:350:LYS:HA	1.73	0.40
4:1D:424:VAL:HB	4:1D:427:GLU:OE1	2.22	0.40
5:1E:120:ILE:CD1	5:1E:123:LYS:HD3	2.50	0.40
6:1F:56:ILE:CG2	6:1F:128:ALA:HB2	2.51	0.40
6:1F:395:ILE:HG13	6:1F:395:ILE:H	1.71	0.40
8:1H:74:ALA:HB3	8:1H:75:PRO:HD3	2.03	0.40
12:1L:144:TRP:CH2	12:1L:256:GLY:HA2	2.53	0.40
12:1L:145:GLU:OE2	12:1L:176:ARG:NH2	2.54	0.40
12:1L:420:ALA:O	12:1L:424:THR:HG23	2.21	0.40
13:1M:278:ARG:NH2	37:1l:82:ASP:OD1	2.55	0.40
14:1N:54:GLU:O	14:1N:58:LYS:HG3	2.22	0.40
14:1N:122:ILE:HD12	14:1N:126:ALA:HB3	2.03	0.40
14:1N:254:LEU:O	14:1N:257:LEU:HB2	2.21	0.40
15:1O:30:ASN:ND2	15:1O:203:GLU:HB3	2.37	0.40
15:1O:156:LYS:O	15:1O:160:ALA:N	2.51	0.40
16:1P:29:PHE:CD1	16:1P:175:GLU:OE1	2.70	0.40
17:1Q:33:ARG:NH2	17:1Q:59:PHE:HB3	2.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:124:TRP:HB3	17:1Q:126:LYS:HZ1	1.86	0.40
19:1S:26:SER:O	19:1S:33:ARG:NH1	2.52	0.40
21:1V:89:LEU:O	21:1V:93:MET:HG3	2.22	0.40
29:1d:16:ASN:HA	29:1d:19:ARG:HH11	1.86	0.40
33:1h:20:ARG:O	33:1h:24:LEU:HG	2.22	0.40
34:1i:65:ARG:HE	34:1i:68:ILE:HD11	1.86	0.40
40:1o:36:ARG:HB3	40:1o:57:TYR:CE2	2.56	0.40
41:1p:55:HIS:HB3	41:1p:59:ARG:CZ	2.51	0.40
41:1p:155:LEU:HD23	41:1p:155:LEU:HA	1.85	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	84/115 (73%)	78 (93%)	6 (7%)	0	100	100
2	1B	153/255 (60%)	138 (90%)	14 (9%)	1 (1%)	18	51
3	1C	207/264 (78%)	191 (92%)	16 (8%)	0	100	100
4	1D	390/476 (82%)	364 (93%)	26 (7%)	0	100	100
5	1E	212/249 (85%)	195 (92%)	16 (8%)	1 (0%)	24	57
6	1F	430/464 (93%)	401 (93%)	28 (6%)	1 (0%)	43	72
7	1G	697/727 (96%)	648 (93%)	48 (7%)	1 (0%)	48	79
8	1H	289/318 (91%)	270 (93%)	17 (6%)	2 (1%)	18	51
9	1I	174/239 (73%)	166 (95%)	8 (5%)	0	100	100
10	1J	173/175 (99%)	158 (91%)	14 (8%)	1 (1%)	21	54
11	1K	96/98 (98%)	90 (94%)	5 (5%)	1 (1%)	12	45
12	1L	604/606 (100%)	541 (90%)	61 (10%)	2 (0%)	36	65
13	1M	457/459 (100%)	441 (96%)	16 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	1N	345/347 (99%)	323 (94%)	22 (6%)	0	100	100
15	1O	318/357 (89%)	302 (95%)	16 (5%)	0	100	100
16	1P	340/377 (90%)	314 (92%)	25 (7%)	1 (0%)	36	65
17	1Q	127/175 (73%)	113 (89%)	13 (10%)	1 (1%)	16	49
18	1R	94/123 (76%)	87 (93%)	7 (7%)	0	100	100
19	1S	85/99 (86%)	73 (86%)	12 (14%)	0	100	100
20	1T	83/156 (53%)	79 (95%)	3 (4%)	1 (1%)	10	41
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	106 (94%)	7 (6%)	0	100	100
22	1W	113/128 (88%)	108 (96%)	5 (4%)	0	100	100
23	1X	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
24	1Y	137/141 (97%)	131 (96%)	6 (4%)	0	100	100
25	1Z	139/144 (96%)	122 (88%)	17 (12%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	71 (88%)	10 (12%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	106 (91%)	11 (9%)	0	100	100
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	7 (7%)	1 (1%)	12	45
33	1h	136/189 (72%)	124 (91%)	12 (9%)	0	100	100
34	1i	124/128 (97%)	117 (94%)	7 (6%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	71 (90%)	8 (10%)	0	100	100
37	1l	154/186 (83%)	143 (93%)	11 (7%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	5 (3%)	2 (1%)	10	41
40	1o	120/137 (88%)	111 (92%)	8 (7%)	1 (1%)	16	49
41	1p	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
42	1q	143/145 (99%)	130 (91%)	11 (8%)	2 (1%)	9	38
43	1r	90/114 (79%)	77 (86%)	13 (14%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	8101/9741 (83%)	7516 (93%)	566 (7%)	19 (0%)	44	72

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	1F	313	GLU
8	1H	92	PRO
8	1H	170	GLU
20	1T	23	ASP
42	1q	142	THR
10	1J	116	ILE
12	1L	601	LEU
16	1P	333	ASP
39	1n	54	LYS
12	1L	549	ALA
17	1Q	70	MET
32	1g	65	GLY
39	1n	31	VAL
40	1o	32	GLU
7	1G	186	TYR
5	1E	157	ASN
42	1q	143	PRO
2	1B	79	SER
11	1K	2	PRO

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	76/99 (77%)	76 (100%)	0	100	100
2	1B	131/209 (63%)	130 (99%)	1 (1%)	73	77
3	1C	190/227 (84%)	188 (99%)	2 (1%)	65	74
4	1D	341/405 (84%)	339 (99%)	2 (1%)	78	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	1E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	346 (100%)	0	100	100
7	1G	588/610 (96%)	585 (100%)	3 (0%)	81	80
8	1H	255/274 (93%)	255 (100%)	0	100	100
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/140 (100%)	138 (99%)	2 (1%)	59	71
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	536 (99%)	3 (1%)	78	79
13	1M	408/408 (100%)	408 (100%)	0	100	100
14	1N	310/310 (100%)	309 (100%)	1 (0%)	86	83
15	1O	283/307 (92%)	281 (99%)	2 (1%)	76	78
16	1P	296/323 (92%)	295 (100%)	1 (0%)	86	83
17	1Q	117/152 (77%)	116 (99%)	1 (1%)	70	76
18	1R	79/97 (81%)	78 (99%)	1 (1%)	61	72
19	1S	77/82 (94%)	77 (100%)	0	100	100
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	78 (99%)	1 (1%)	61	72
21	1V	100/101 (99%)	100 (100%)	0	100	100
22	1W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	100 (99%)	1 (1%)	68	75
25	1Z	123/124 (99%)	123 (100%)	0	100	100
26	1a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	44 (98%)	1 (2%)	45	65
29	1d	107/109 (98%)	107 (100%)	0	100	100
30	1e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	74
33	1h	121/158 (77%)	120 (99%)	1 (1%)	73	77
34	1i	119/120 (99%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	1j	62/84 (74%)	62 (100%)	0	100	100
36	1k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	141 (100%)	0	100	100
38	1m	113/114 (99%)	112 (99%)	1 (1%)	70	76
39	1n	156/160 (98%)	156 (100%)	0	100	100
40	1o	110/120 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	153 (99%)	1 (1%)	78	79
42	1q	131/131 (100%)	129 (98%)	2 (2%)	57	70
43	1r	85/98 (87%)	84 (99%)	1 (1%)	63	73
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7147/8269 (86%)	7118 (100%)	29 (0%)	81	81

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1B	94	ASN
3	1C	52	ILE
3	1C	97	LEU
4	1D	189	MET
4	1D	318	MET
7	1G	77	TRP
7	1G	307	LEU
7	1G	624	GLU
10	1J	61	LEU
10	1J	70	TYR
12	1L	147	VAL
12	1L	163	ASP
12	1L	331	MET
14	1N	211	MET
15	1O	143	PHE
15	1O	192	MET
16	1P	171	ILE
17	1Q	6	GLN
18	1R	54	SER
20	1U	87	TYR
24	1Y	42	LEU
28	1c	48	LEU
32	1g	120	LEU

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Mol	Chain	Res	Type
33	1h	34	ILE
38	1m	13	LEU
41	1p	35	ILE
42	1q	78	ASP
42	1q	135	GLN
43	1r	19	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
3	1C	41	GLN
3	1C	144	ASN
4	1D	116	GLN
5	1E	55	GLN
5	1E	121	GLN
5	1E	159	ASN
6	1F	29	HIS
6	1F	37	GLN
6	1F	83	ASN
6	1F	148	ASN
6	1F	165	ASN
6	1F	200	GLN
6	1F	324	GLN
6	1F	398	GLN
7	1G	100	ASN
7	1G	117	GLN
7	1G	255	HIS
7	1G	476	ASN
7	1G	549	HIS
7	1G	581	GLN
7	1G	665	GLN
8	1H	138	GLN
8	1H	287	HIS
9	1I	144	HIS
9	1I	157	ASN
12	1L	115	ASN
12	1L	165	ASN
12	1L	194	ASN
12	1L	320	ASN
12	1L	351	ASN
12	1L	506	ASN
12	1L	541	ASN

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Mol	Chain	Res	Type
13	1M	48	ASN
13	1M	168	GLN
13	1M	304	GLN
13	1M	366	ASN
13	1M	399	ASN
13	1M	415	GLN
13	1M	425	ASN
14	1N	204	ASN
14	1N	235	ASN
14	1N	322	GLN
14	1N	347	ASN
15	1O	50	HIS
15	1O	180	GLN
15	1O	190	HIS
15	1O	288	GLN
16	1P	36	ASN
16	1P	44	GLN
16	1P	134	HIS
16	1P	260	HIS
17	1Q	6	GLN
17	1Q	51	ASN
18	1R	93	GLN
19	1S	80	ASN
20	1T	35	HIS
20	1U	74	GLN
21	1V	49	GLN
21	1V	85	ASN
22	1W	126	HIS
24	1Y	88	ASN
28	1c	34	GLN
30	1e	20	GLN
33	1h	95	GLN
34	1i	13	GLN
34	1i	25	GLN
34	1i	88	HIS
35	1j	42	HIS
37	1l	55	GLN
38	1m	74	ASN
38	1m	125	ASN
39	1n	140	GLN
40	1o	49	GLN
40	1o	54	GLN

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Mol	Chain	Res	Type
40	1o	116	GLN
41	1p	27	ASN
41	1p	130	GLN
41	1p	148	HIS
42	1q	69	ASN
42	1q	91	HIS
42	1q	112	ASN
43	1r	20	GLN
43	1r	24	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	1.72	2 (25%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.09	1 (12%)
34	SAC	1i	1	-	7,8,9	0.53	0	7,9,11	1.54	1 (14%)
10	FME	1J	1	10	8,9,10	0.56	0	8,9,11	0.96	1 (12%)
14	FME	1N	1	14	8,9,10	0.52	0	8,9,11	1.03	1 (12%)
12	FME	1L	1	12	8,9,10	0.56	0	8,9,11	1.05	1 (12%)
1	FME	1A	1	1	8,9,10	0.53	0	8,9,11	0.99	1 (12%)
13	FME	1M	1	13	8,9,10	0.56	0	8,9,11	0.99	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
11	FME	1K	1	11	-	0/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
34	SAC	1i	1	-	-	5/7/8/10	-
10	FME	1J	1	10	-	0/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
1	FME	1A	1	1	-	2/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1K	1	FME	CA-N-CN	3.72	128.54	122.82
34	1i	1	SAC	O-C-CA	-2.98	117.10	124.77
8	1H	1	FME	O-C-CA	-2.80	117.57	124.77
12	1L	1	FME	O-C-CA	-2.71	117.81	124.77
14	1N	1	FME	O-C-CA	-2.66	117.94	124.77
11	1K	1	FME	O-C-CA	-2.56	118.19	124.77
13	1M	1	FME	O-C-CA	-2.54	118.23	124.77
1	1A	1	FME	O-C-CA	-2.52	118.30	124.77
10	1J	1	FME	O-C-CA	-2.48	118.39	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	N-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
34	1i	1	SAC	C-CA-CB-OG
34	1i	1	SAC	C2A-C1A-N-CA
34	1i	1	SAC	OAC-C1A-N-CA
34	1i	1	SAC	N-CA-CB-OG
1	1A	1	FME	C-CA-CB-CG
34	1i	1	SAC	C-CA-N-C1A

There are no ring outliers.

5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1K	1	FME	1	0
34	1i	1	SAC	2	0
14	1N	1	FME	3	0
1	1A	1	FME	1	0
13	1M	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
57	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.26	1 (2%)
48	FES	1E	301	5	0,4,4	-	-	-		
51	PGT	1M	501	-	50,50,50	0.50	0	53,56,56	0.50	0
45	3PE	1L	701	-	45,45,50	0.29	0	48,50,55	0.31	0
46	PC1	1I	204	9	43,43,53	0.30	0	49,51,61	0.35	0
57	EHZ	1W	201	-	31,36,37	0.21	0	36,44,47	1.09	1 (2%)
45	3PE	1L	703	-	41,41,50	0.31	0	44,46,55	1.27	5 (11%)
46	PC1	1A	202	1	34,34,53	0.32	0	40,42,61	0.36	0
45	3PE	1Y	202	-	50,50,50	0.26	0	53,55,55	0.41	0
52	CDL	1q	201	42,43	60,60,99	0.34	0	66,72,111	0.43	0
45	3PE	1N	401	13,14	50,50,50	0.27	0	53,55,55	0.41	0
46	PC1	1f	101	31	45,45,53	0.27	0	51,53,61	0.35	0
47	SF4	1I	202	9	0,12,12	-	-	-		
47	SF4	1I	201	9	0,12,12	-	-	-		
47	SF4	1B	201	2	0,12,12	-	-	-		
55	NDP	1P	501	-	51,52,52	0.53	0	71,80,80	0.73	1 (1%)
46	PC1	1L	702	-	43,43,53	0.30	0	49,51,61	0.38	0
52	CDL	1N	402	14	76,76,99	0.85	2 (2%)	82,88,111	0.63	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	1G	802	7	0,12,12	-	-	-		
47	SF4	1F	502	6	0,12,12	-	-	-		
45	3PE	1Y	201	-	30,30,50	0.34	0	33,35,55	0.60	1 (3%)
58	MYR	1l	201	-	13,14,15	0.30	0	12,13,15	0.30	0
49	FMN	1F	501	-	33,33,33	0.61	0	48,50,50	0.66	1 (2%)
46	PC1	1I	203	9	53,53,53	0.27	0	59,61,61	0.30	0
53	GTP	1O	401	54	33,34,34	0.59	0	50,54,54	0.61	0
47	SF4	1G	801	7	0,12,12	-	-	-		
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.38	0
48	FES	1G	803	7	0,4,4	-	-	-		

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
57	EHZ	1n	201	-	-	3/42/44/45	-
48	FES	1E	301	5	-	-	0/1/1/1
51	PGT	1M	501	-	-	22/55/55/55	-
45	3PE	1L	701	-	-	3/49/49/54	-
46	PC1	1I	204	9	-	4/47/47/57	-
57	EHZ	1W	201	-	-	14/42/44/45	-
45	3PE	1L	703	-	-	6/45/45/54	-
46	PC1	1A	202	1	-	4/38/38/57	-
45	3PE	1Y	202	-	-	8/54/54/54	-
52	CDL	1q	201	42,43	-	16/71/71/110	-
45	3PE	1N	401	13,14	-	5/54/54/54	-
46	PC1	1f	101	31	-	5/49/49/57	-
47	SF4	1I	202	9	-	-	0/6/5/5
47	SF4	1I	201	9	-	-	0/6/5/5
47	SF4	1B	201	2	-	-	0/6/5/5
55	NDP	1P	501	-	-	6/34/77/77	0/5/5/5
46	PC1	1L	702	-	-	4/47/47/57	-
52	CDL	1N	402	14	-	10/87/87/110	-
47	SF4	1G	802	7	-	-	0/6/5/5
47	SF4	1F	502	6	-	-	0/6/5/5
45	3PE	1Y	201	-	-	7/34/34/54	-
58	MYR	1l	201	-	-	1/12/12/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
46	PC1	1I	203	9	-	3/57/57/57	-
53	GTP	1O	401	54	-	0/22/38/38	0/3/3/3
47	SF4	1G	801	7	-	-	0/6/5/5
45	3PE	1A	201	-	-	2/50/50/54	-
48	FES	1G	803	7	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	1N	402	CDL	C15-C14	5.64	1.79	1.51
52	1N	402	CDL	C16-C15	3.03	1.66	1.51

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1n	201	EHZ	C10-S1-C9	7.14	122.94	101.84
57	1W	201	EHZ	C10-S1-C9	6.18	120.11	101.84
45	1L	703	3PE	O21-C21-C22	6.09	124.66	111.48
55	1P	501	NDP	P2B-O2B-C2B	-3.91	112.99	123.43
52	1N	402	CDL	C17-C16-C15	2.82	139.96	115.25
45	1L	703	3PE	O21-C21-O22	-2.73	117.31	123.70
45	1L	703	3PE	C2-O21-C21	2.65	124.14	117.80
52	1N	402	CDL	C16-C15-C14	2.52	127.13	114.37
45	1L	703	3PE	O21-C2-C1	2.38	116.87	108.34
45	1Y	201	3PE	O21-C21-C22	2.30	116.45	111.48
49	1F	501	FMN	C4-N3-C2	-2.12	121.88	125.64
45	1L	703	3PE	O21-C2-C3	2.09	115.83	108.34

There are no chirality outliers.

All (124) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2
45	1Y	201	3PE	O32-C31-O31-C3
45	1Y	201	3PE	C32-C31-O31-C3
45	1Y	201	3PE	O22-C21-O21-C2
45	1Y	201	3PE	C22-C21-O21-C2
45	1Y	202	3PE	C1-O11-P-O14
46	1A	202	PC1	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
46	1A	202	PC1	C1-O11-P-O13
46	1I	204	PC1	C11-O13-P-O14
46	1L	702	PC1	C1-O11-P-O14
46	1f	101	PC1	O32-C31-O31-C3
46	1f	101	PC1	C32-C31-O31-C3
51	1M	501	PGT	C32-C31-O2-C2
51	1M	501	PGT	C1-O3P-P-O1P
51	1M	501	PGT	C4-O4P-P-O3P
51	1M	501	PGT	O11-C11-O3-C3
51	1M	501	PGT	C12-C11-O3-C3
52	1q	201	CDL	CA3-OA5-PA1-OA2
52	1q	201	CDL	CA3-OA5-PA1-OA4
52	1q	201	CDL	CA4-CA3-OA5-PA1
52	1q	201	CDL	CB4-CB3-OB5-PB2
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	C16-C17-C20-O6
57	1W	201	EHZ	C18-C17-C20-O6
57	1W	201	EHZ	C19-C17-C20-O6
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	S1-C10-C11-N1
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
57	1W	201	EHZ	C13-C12-N1-C11
51	1M	501	PGT	O31-C31-O2-C2
45	1Y	202	3PE	C2-C1-O11-P
51	1M	501	PGT	C5-C4-O4P-P
57	1W	201	EHZ	O3-C12-N1-C11
51	1M	501	PGT	C31-C32-C33-C34
51	1M	501	PGT	C15-C16-C17-C18
52	1N	402	CDL	C12-C13-C14-C15
51	1M	501	PGT	C14-C15-C16-C17
52	1q	201	CDL	O1-C1-CB2-OB2
51	1M	501	PGT	C40-C41-C42-C43
46	1I	204	PC1	C36-C37-C38-C39
52	1N	402	CDL	C15-C16-C17-C18
51	1M	501	PGT	C22-C23-C24-C25
46	1I	204	PC1	O21-C2-C3-O31
49	1F	501	FMN	C4'-C5'-O5'-P
45	1N	401	3PE	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
57	1W	201	EHZ	O4-C15-C16-O5
46	1I	203	PC1	C24-C25-C26-C27
45	1N	401	3PE	C37-C38-C39-C3A
51	1M	501	PGT	C34-C35-C36-C37
46	1I	204	PC1	C1-C2-C3-O31
52	1q	201	CDL	CA3-CA4-CA6-OA8
45	1Y	202	3PE	C3C-C3D-C3E-C3F
57	1W	201	EHZ	C3-C4-C5-C6
58	1l	201	MYR	C2-C3-C4-C5
45	1L	703	3PE	O11-C1-C2-O21
51	1M	501	PGT	O3P-C1-C2-O2
57	1W	201	EHZ	C2-C3-C4-C5
52	1N	402	CDL	OA6-CA4-CA6-OA8
45	1Y	202	3PE	C35-C36-C37-C38
45	1N	401	3PE	C2-C3-O31-C31
51	1M	501	PGT	C32-C33-C34-C35
45	1N	401	3PE	O11-C1-C2-O21
51	1M	501	PGT	C44-C45-C46-C47
45	1A	201	3PE	O21-C2-C3-O31
52	1q	201	CDL	OB6-CB4-CB6-OB8
55	1P	501	NDP	C3B-C2B-O2B-P2B
45	1Y	202	3PE	O11-C1-C2-O21
52	1N	402	CDL	CA3-CA4-CA6-OA8
45	1A	201	3PE	C12-C11-O13-P
45	1Y	202	3PE	C12-C11-O13-P
46	1A	202	PC1	O13-C11-C12-N
52	1q	201	CDL	CA2-C1-CB2-OB2
51	1M	501	PGT	C16-C17-C18-C19
45	1Y	202	3PE	O11-C1-C2-C3
52	1N	402	CDL	C32-C33-C34-C35
57	1W	201	EHZ	C11-C10-S1-C9
55	1P	501	NDP	C1B-C2B-O2B-P2B
46	1I	203	PC1	C3A-C3B-C3C-C3D
51	1M	501	PGT	C21-C22-C23-C24
45	1Y	201	3PE	O21-C2-C3-O31
45	1Y	201	3PE	C1-O11-P-O14
46	1f	101	PC1	C11-O13-P-O14
51	1M	501	PGT	C4-O4P-P-O1P
52	1q	201	CDL	CA2-OA2-PA1-OA3
52	1q	201	CDL	CB3-OB5-PB2-OB3
52	1q	201	CDL	C1-CA2-OA2-PA1
55	1P	501	NDP	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
52	1q	201	CDL	C12-C13-C14-C15
52	1q	201	CDL	OA6-CA4-CA6-OA8
46	1L	702	PC1	C31-C32-C33-C34
51	1M	501	PGT	C41-C42-C43-C44
52	1q	201	CDL	C52-C51-CB5-OB6
46	1I	203	PC1	C32-C33-C34-C35
55	1P	501	NDP	O4D-C1D-N1N-C6N
52	1N	402	CDL	C55-C56-C57-C58
52	1N	402	CDL	C76-C77-C78-C79
45	1L	703	3PE	C1-C2-O21-C21
51	1M	501	PGT	O3P-C1-C2-C3
45	1N	401	3PE	C22-C23-C24-C25
46	1f	101	PC1	C21-C22-C23-C24
52	1N	402	CDL	CA7-C31-C32-C33
46	1A	202	PC1	O21-C2-C3-O31
52	1N	402	CDL	C53-C54-C55-C56
52	1q	201	CDL	CB3-CB4-CB6-OB8
46	1L	702	PC1	O11-C1-C2-C3
46	1f	101	PC1	C36-C37-C38-C39
45	1L	701	3PE	C22-C23-C24-C25
55	1P	501	NDP	C2D-C1D-N1N-C2N
45	1L	703	3PE	C1-C2-C3-O31
45	1L	703	3PE	C32-C33-C34-C35
45	1Y	201	3PE	C1-C2-C3-O31
45	1L	701	3PE	C33-C34-C35-C36
51	1M	501	PGT	C39-C40-C41-C42
55	1P	501	NDP	O4D-C1D-N1N-C2N
46	1L	702	PC1	O31-C31-C32-C33
45	1L	701	3PE	C37-C38-C39-C3A
52	1N	402	CDL	C33-C34-C35-C36
45	1Y	202	3PE	C24-C25-C26-C27
52	1q	201	CDL	O1-C1-CA2-OA2

There are no ring outliers.

23 monomers are involved in 85 short contacts:

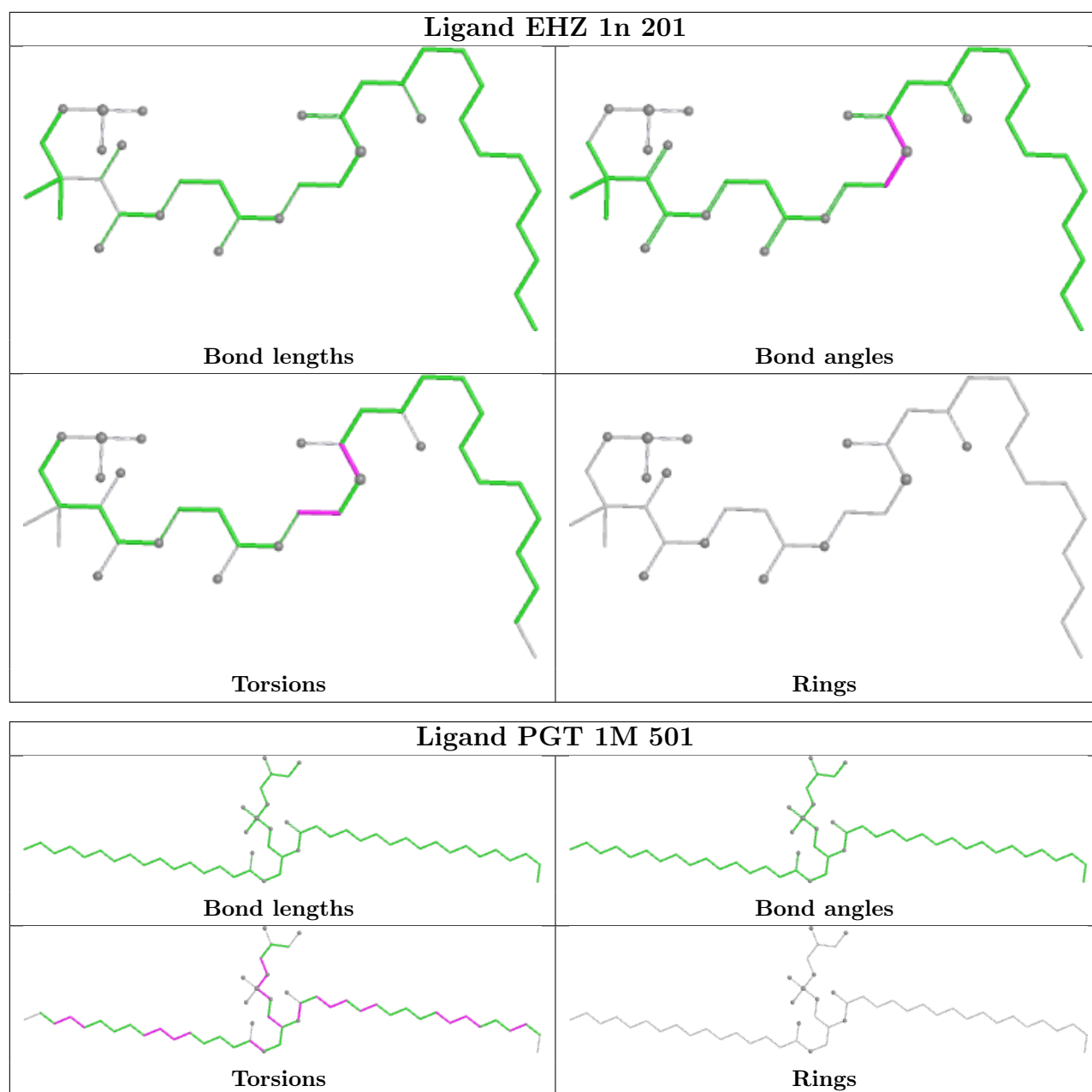
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	1E	301	FES	2	0
51	1M	501	PGT	8	0
45	1L	701	3PE	4	0
46	1I	204	PC1	5	0
57	1W	201	EHZ	1	0

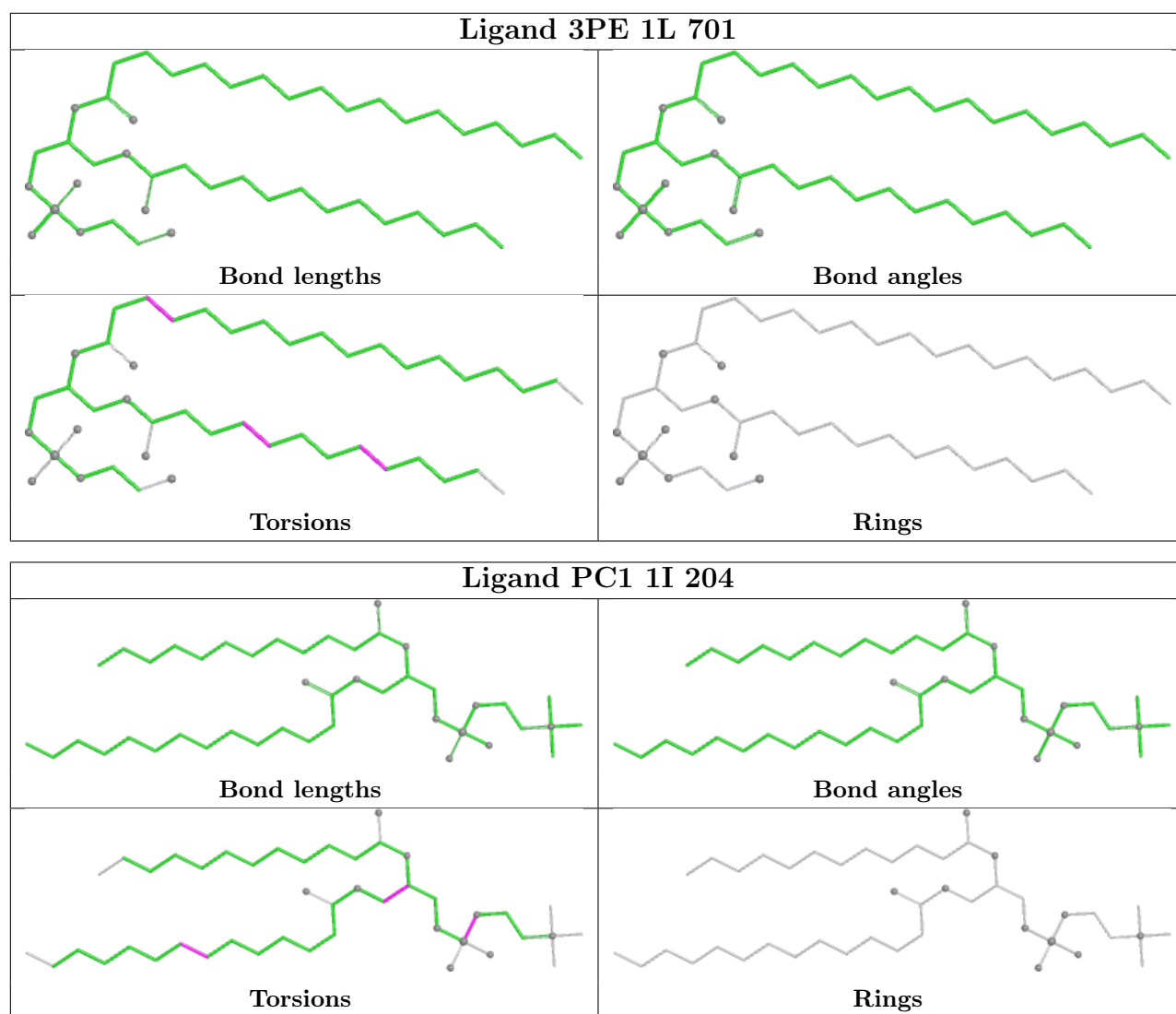
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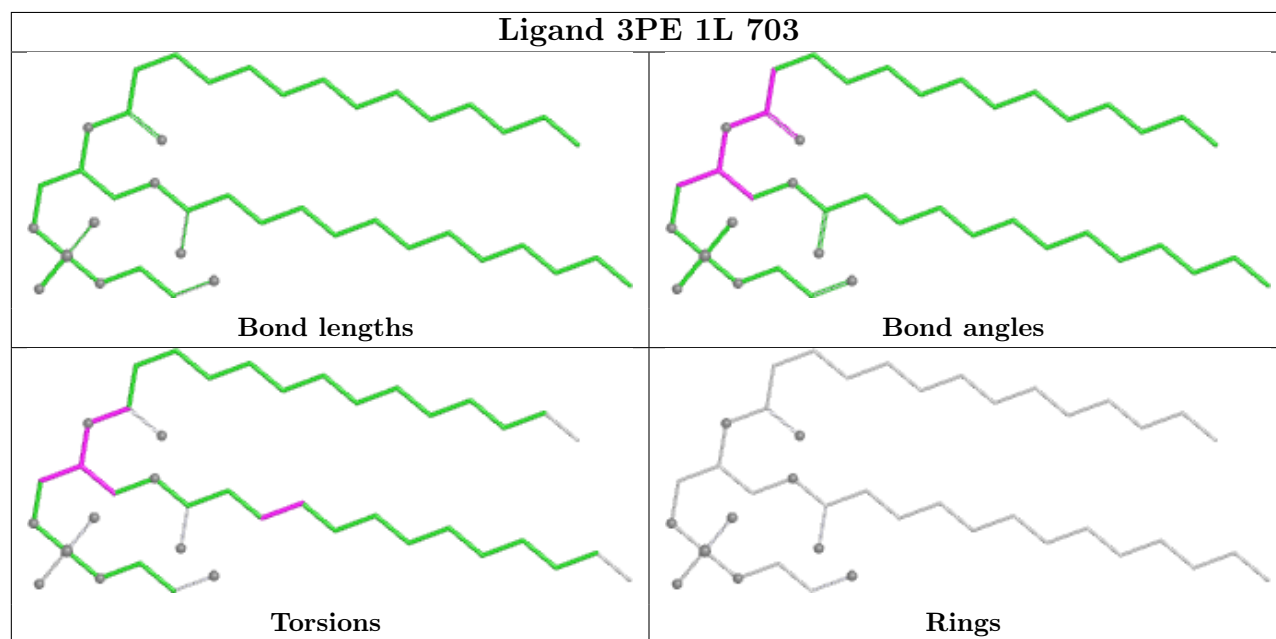
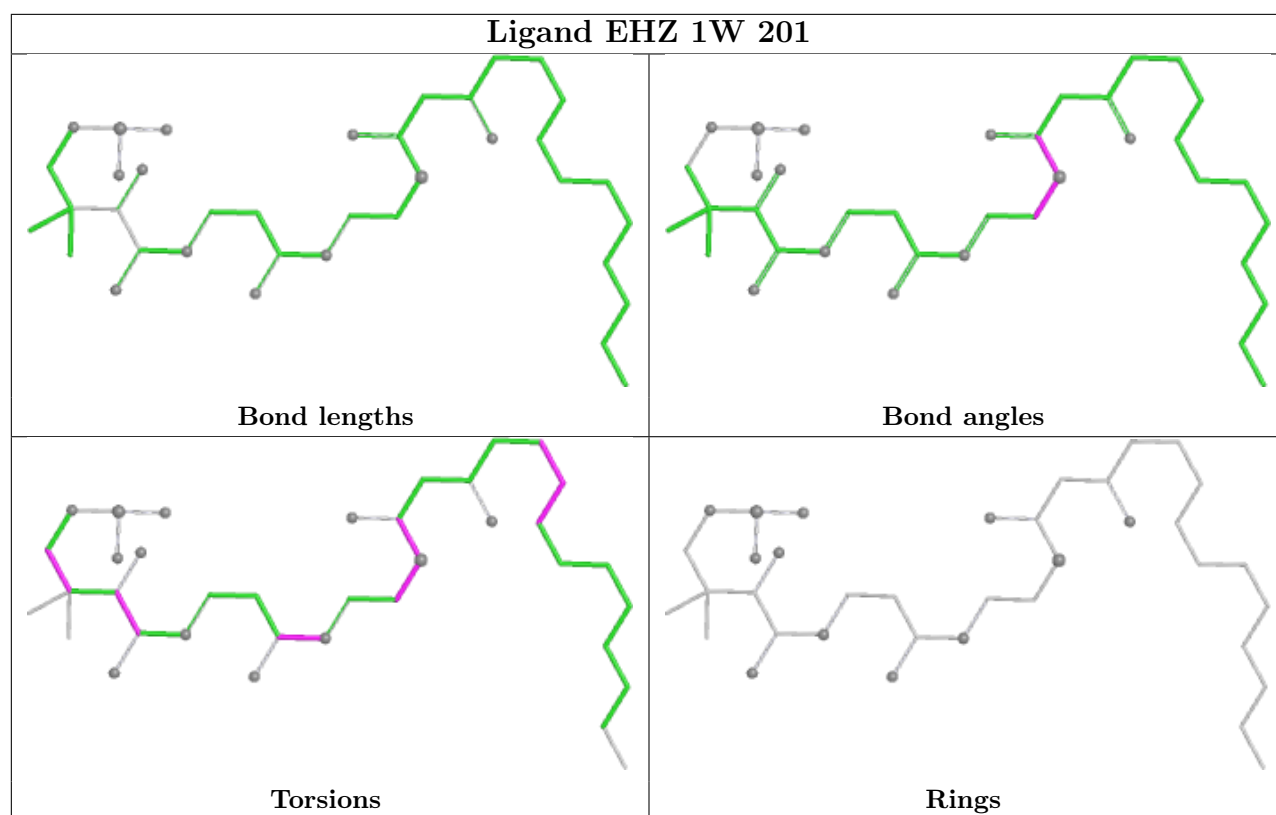
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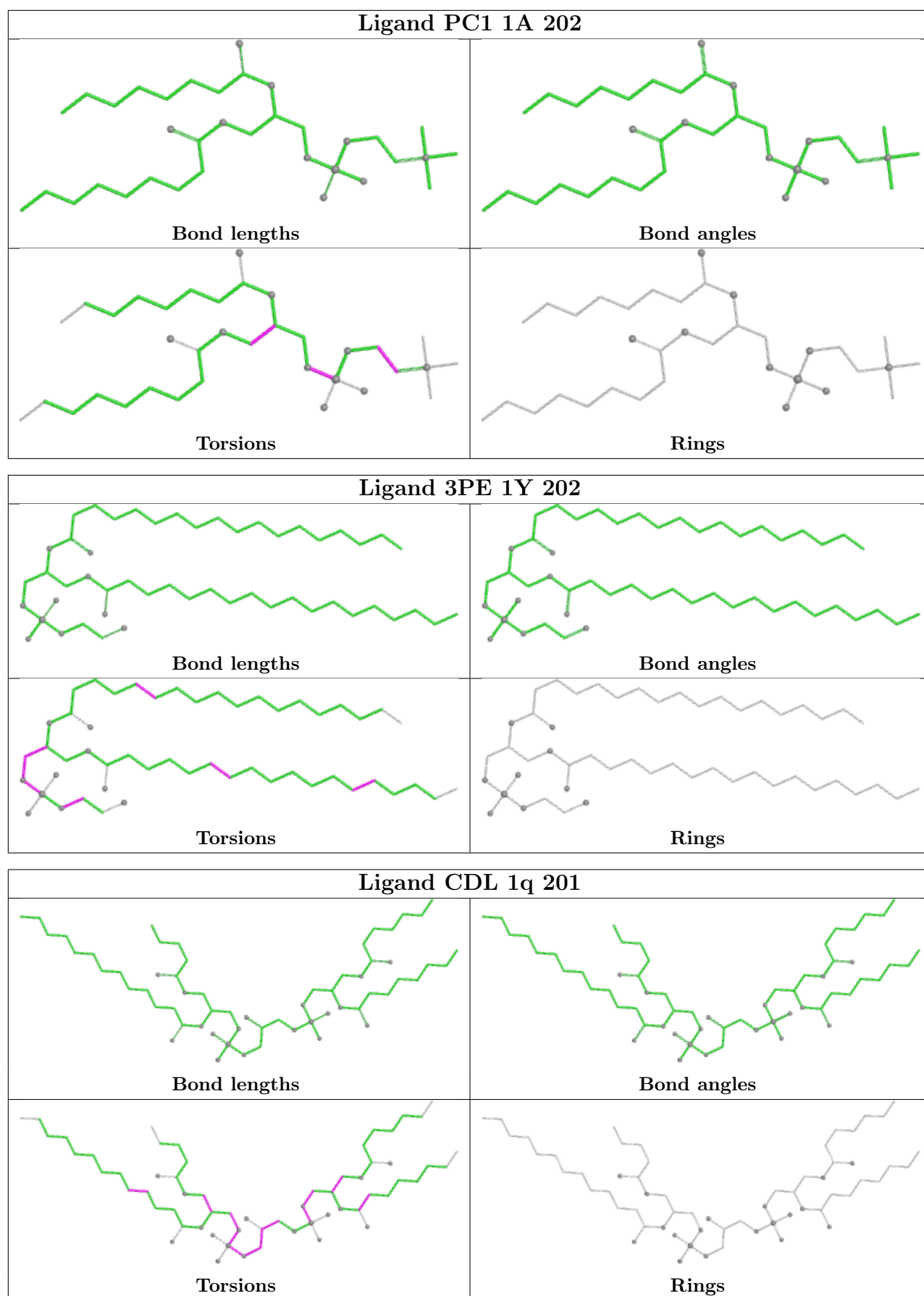
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1L	703	3PE	4	0
46	1A	202	PC1	1	0
45	1Y	202	3PE	4	0
52	1q	201	CDL	11	0
45	1N	401	3PE	2	0
46	1f	101	PC1	6	0
47	1I	201	SF4	1	0
47	1B	201	SF4	2	0
55	1P	501	NDP	6	0
46	1L	702	PC1	4	0
52	1N	402	CDL	6	0
47	1F	502	SF4	1	0
45	1Y	201	3PE	7	0
58	1l	201	MYR	1	0
46	1I	203	PC1	4	0
47	1G	801	SF4	2	0
45	1A	201	3PE	2	0
48	1G	803	FES	1	0

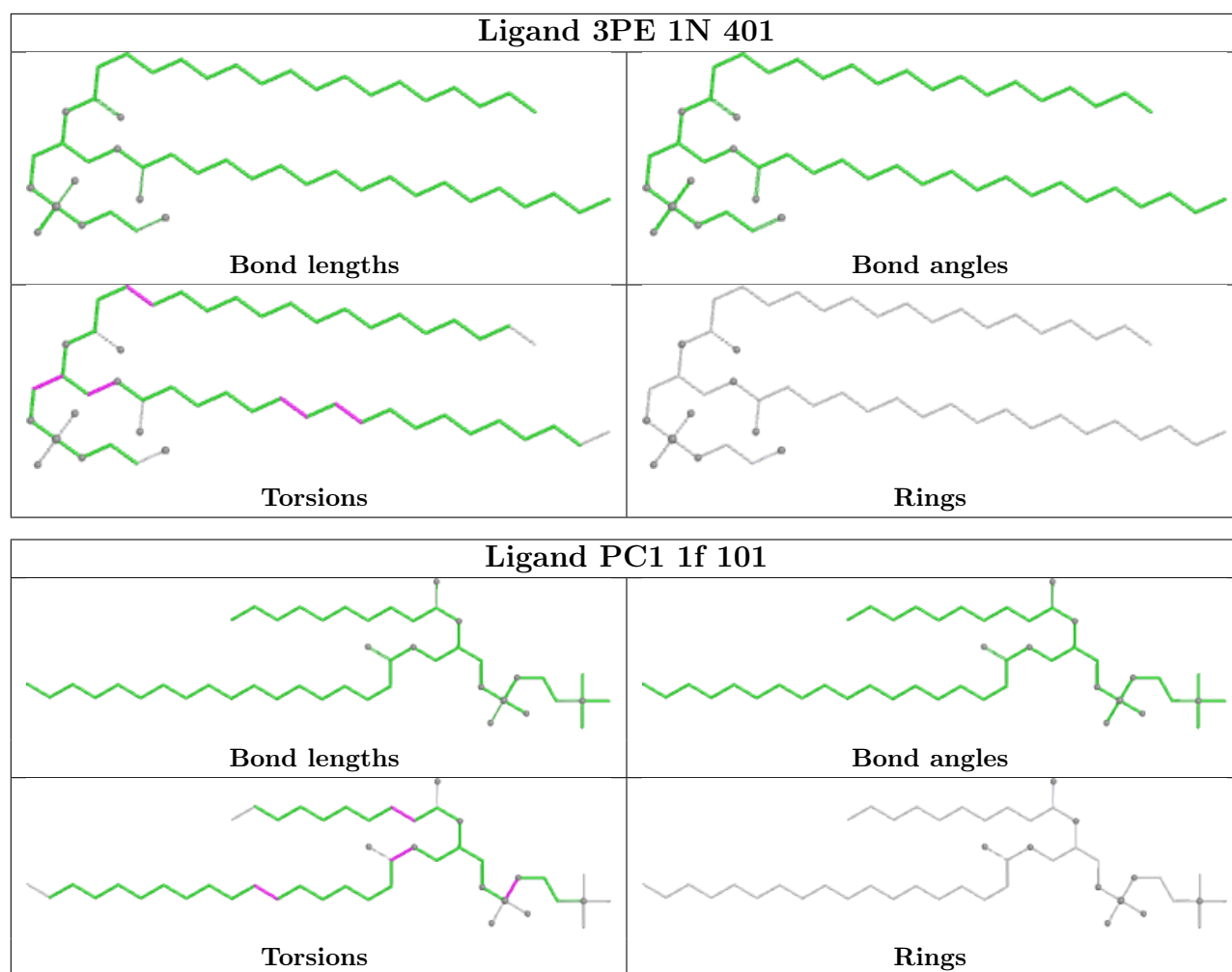
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

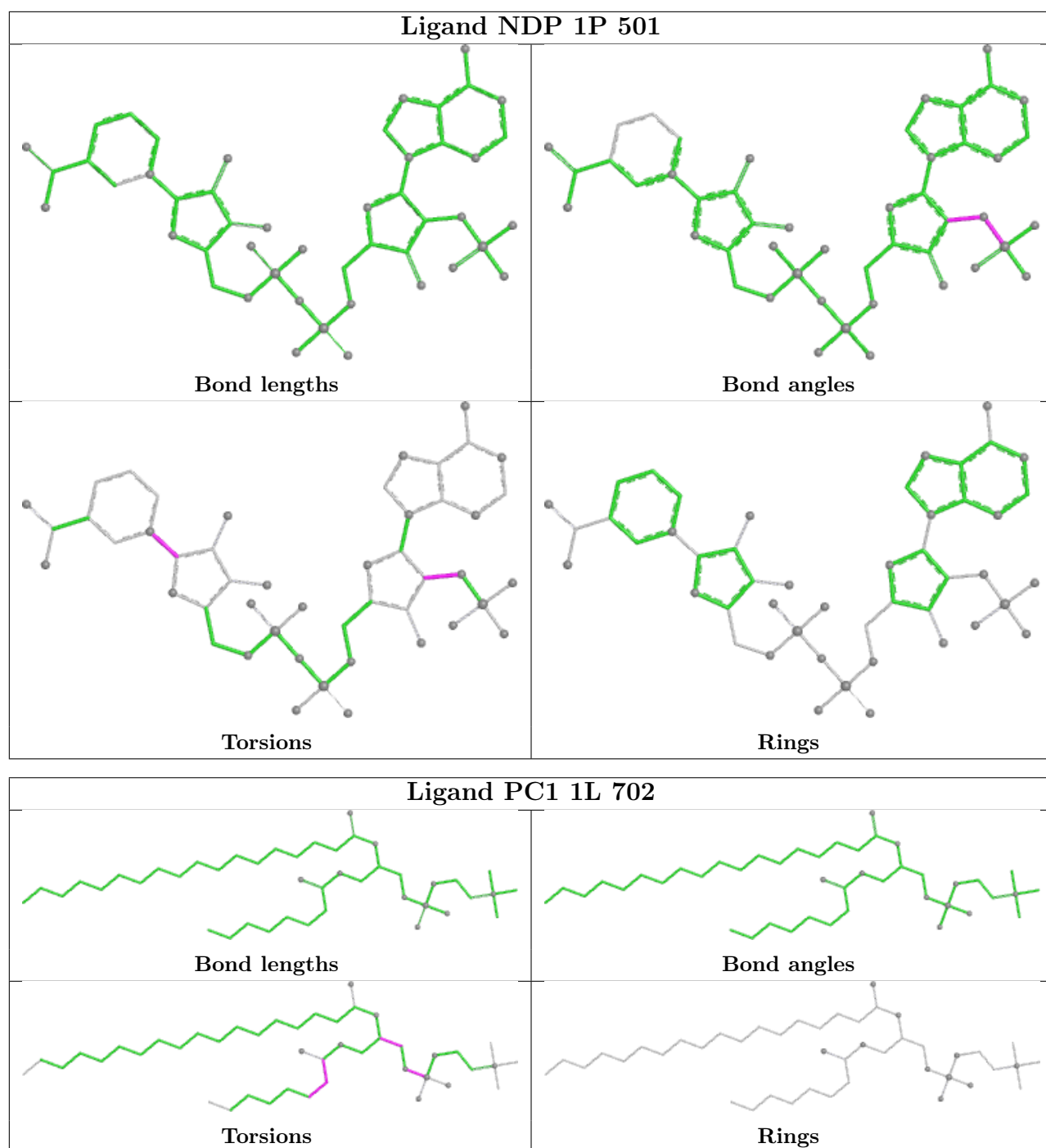


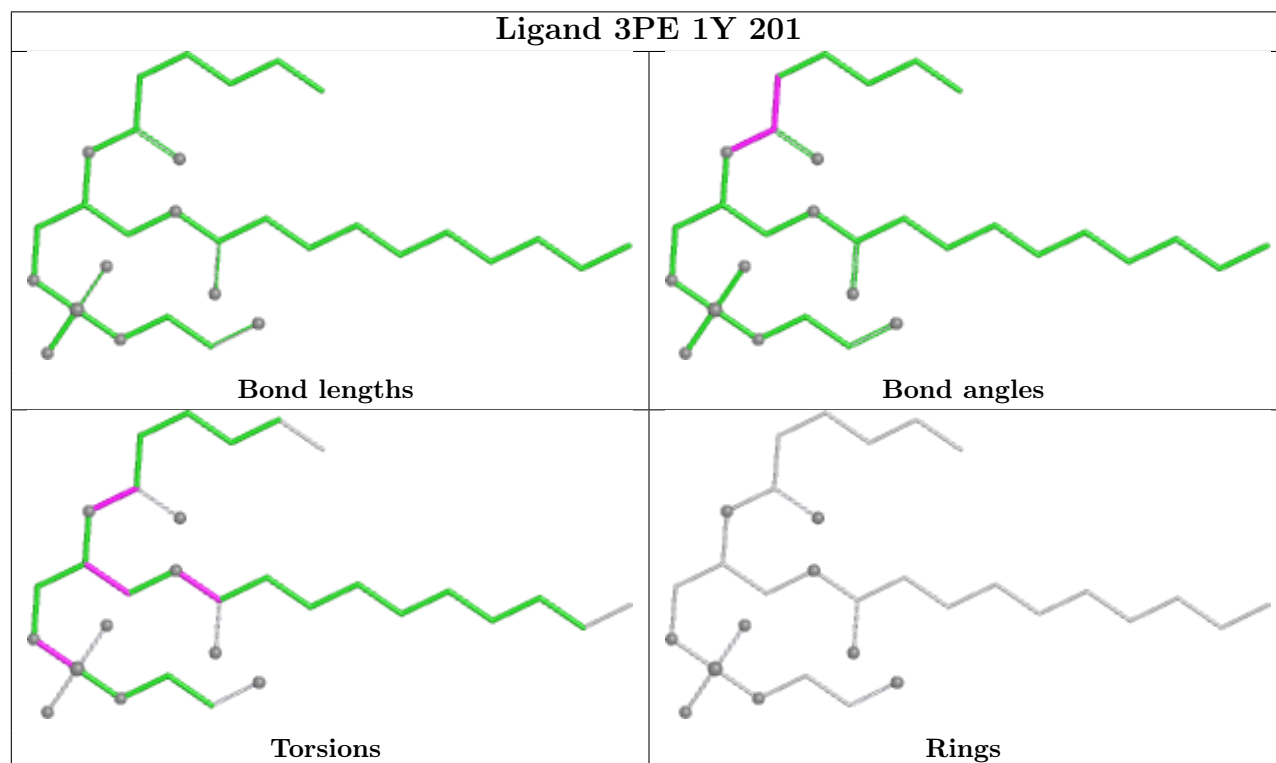
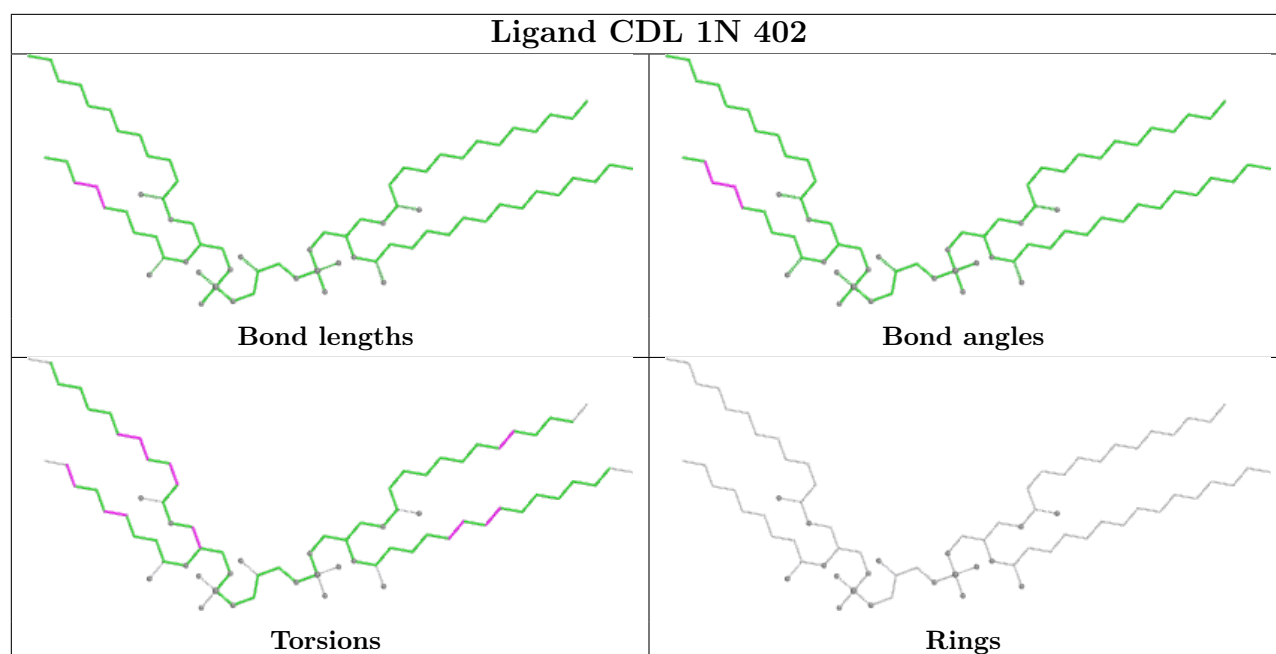


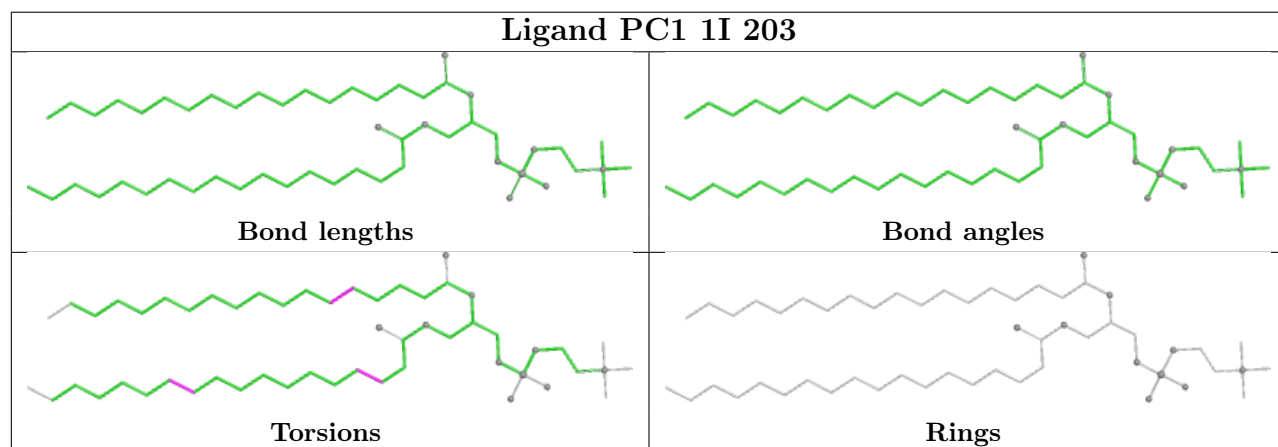
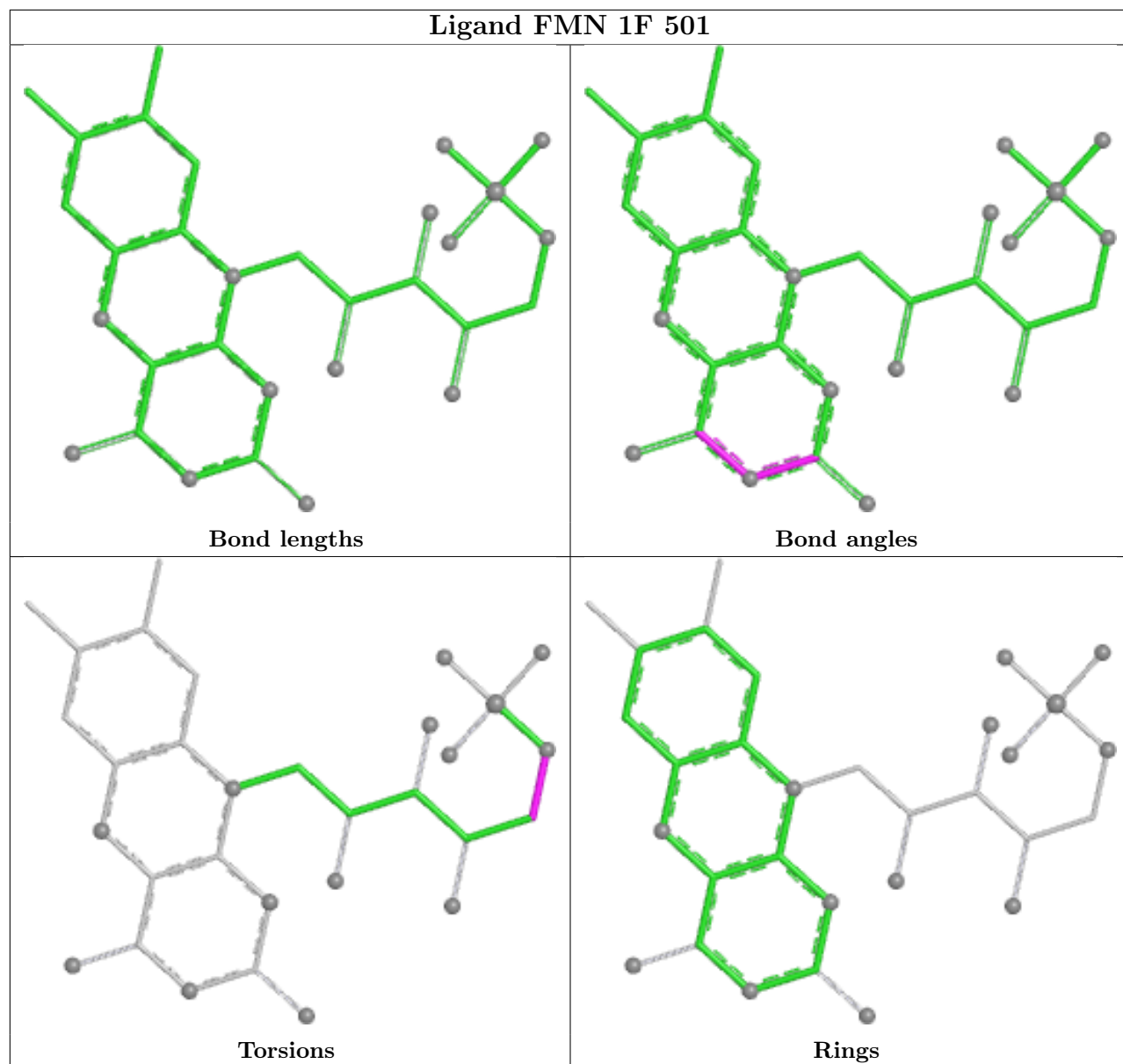


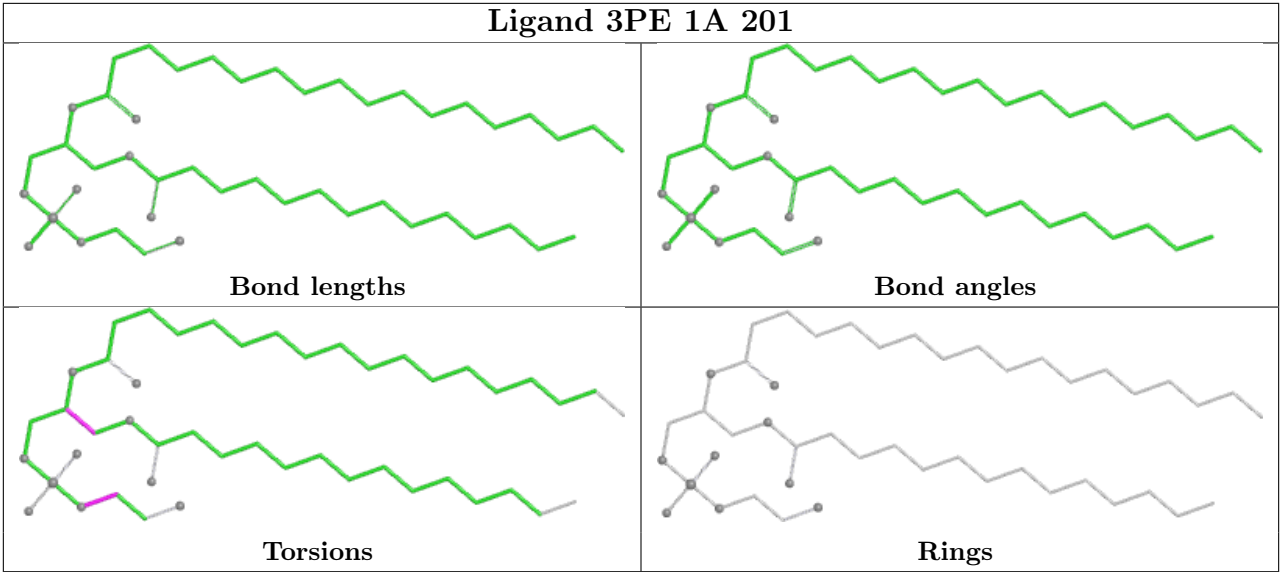












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	3.75
1	1r	1:ALA	C	2:SER	N	3.09

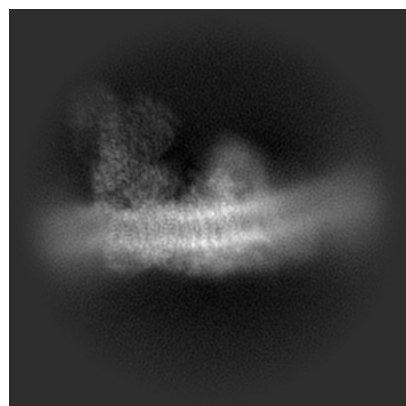
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42175. These allow visual inspection of the internal detail of the map and identification of artifacts.

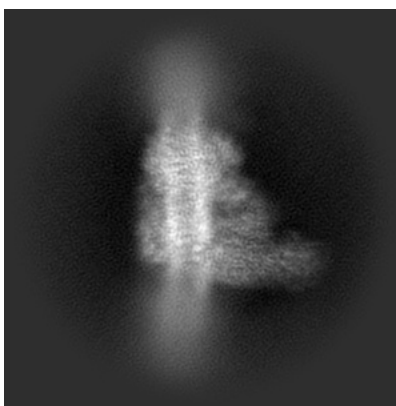
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

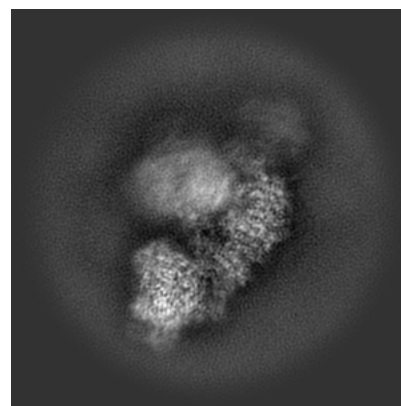
6.1.1 Primary map



X

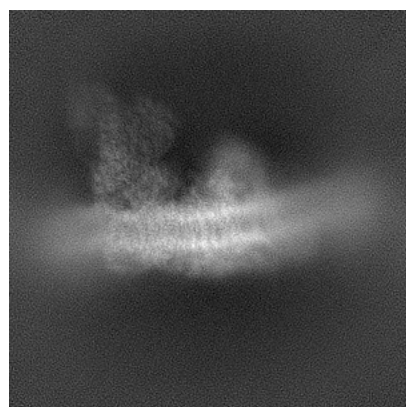


Y

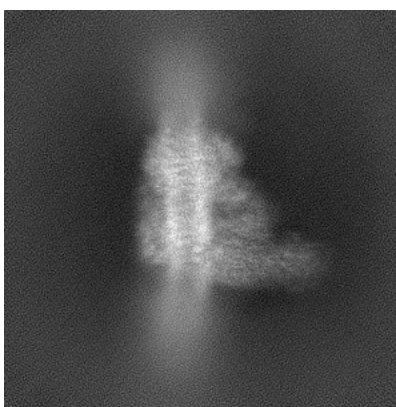


Z

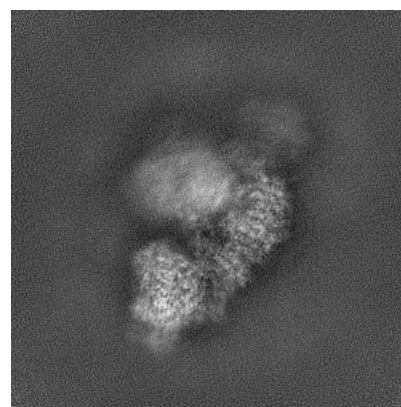
6.1.2 Raw map



X



Y

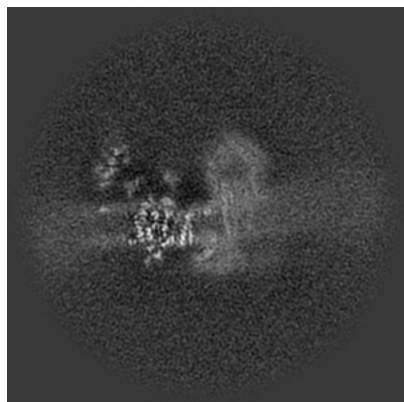


Z

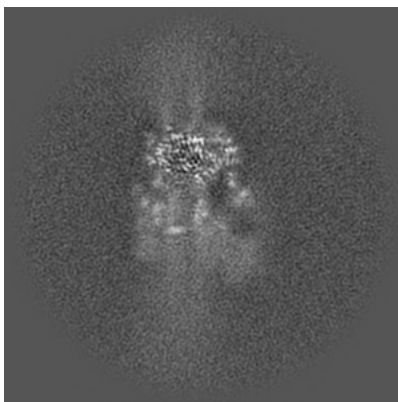
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

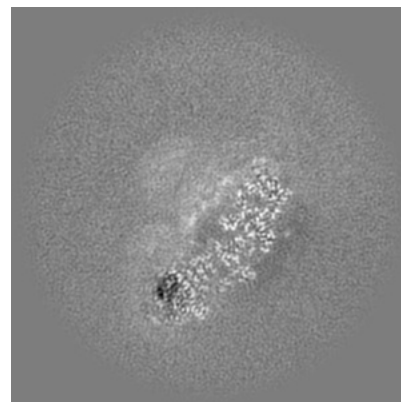
6.2.1 Primary map



X Index: 160



Y Index: 160

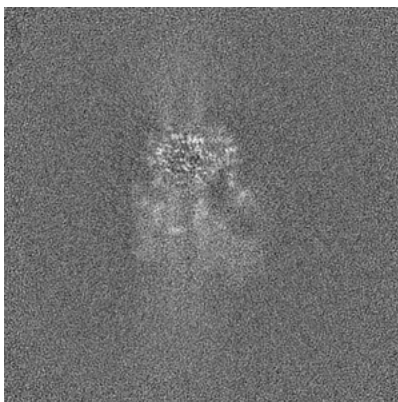


Z Index: 160

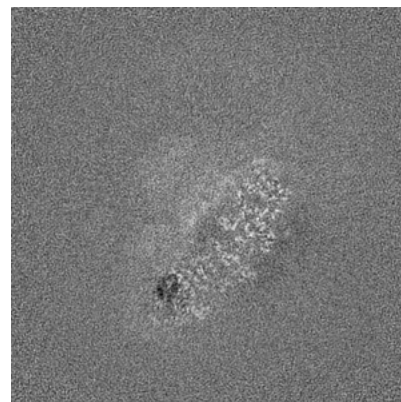
6.2.2 Raw map



X Index: 160



Y Index: 160

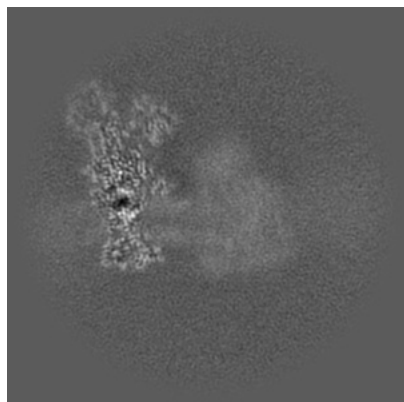


Z Index: 160

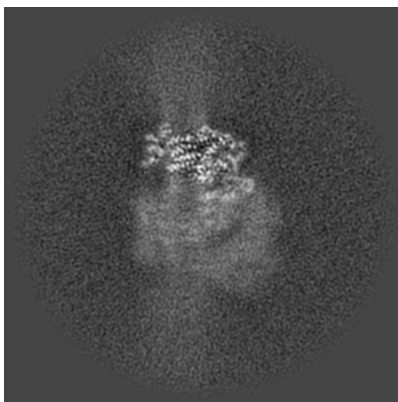
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

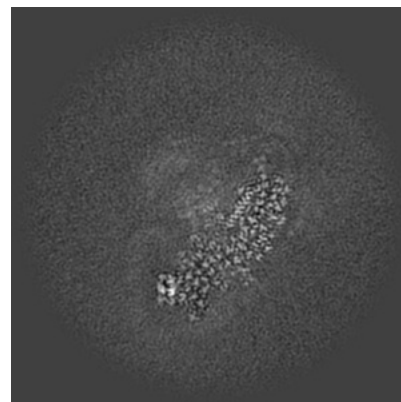
6.3.1 Primary map



X Index: 127

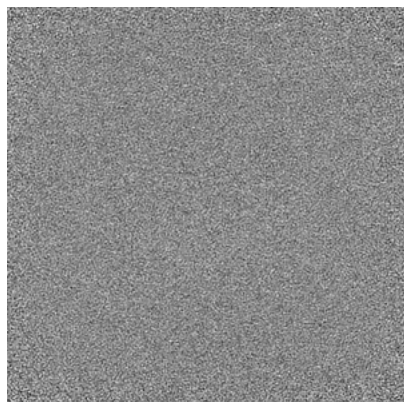


Y Index: 171

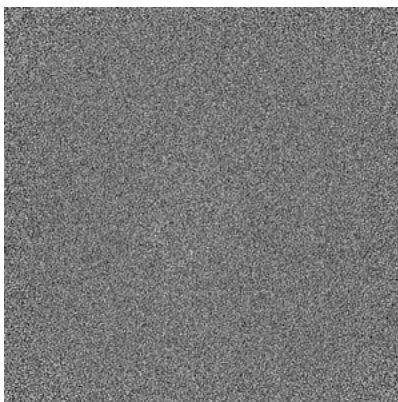


Z Index: 155

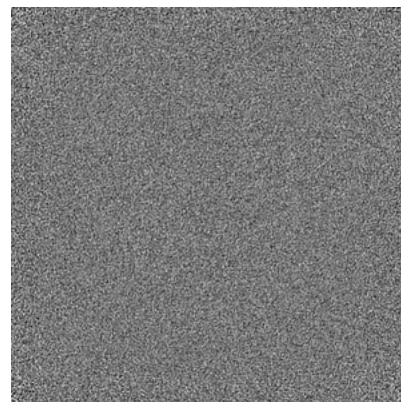
6.3.2 Raw map



X Index: 0



Y Index: 0

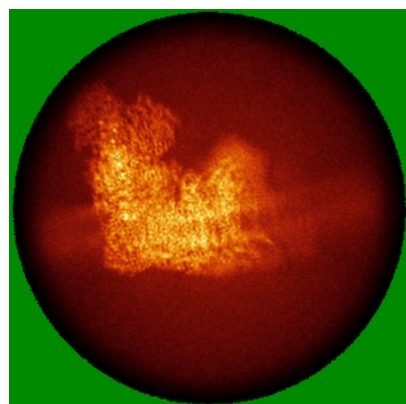


Z Index: 0

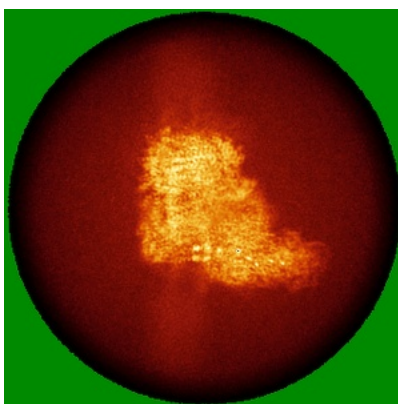
The images above show the largest variance slices of the map in three orthogonal directions.

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

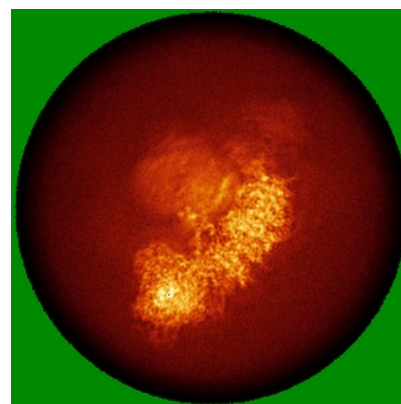
6.4.1 Primary map



X

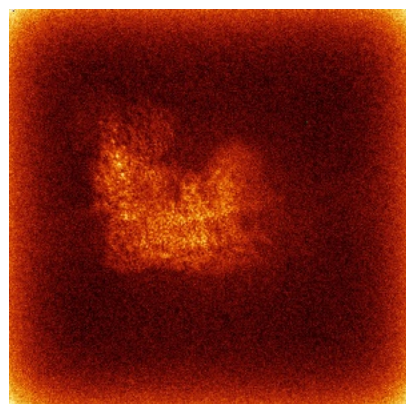


Y

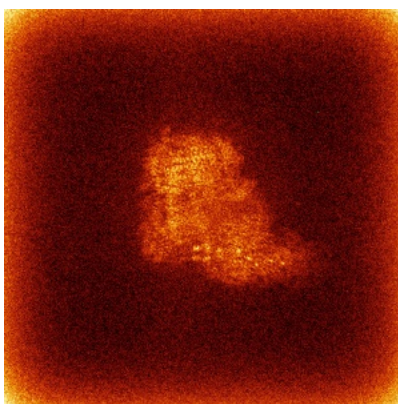


Z

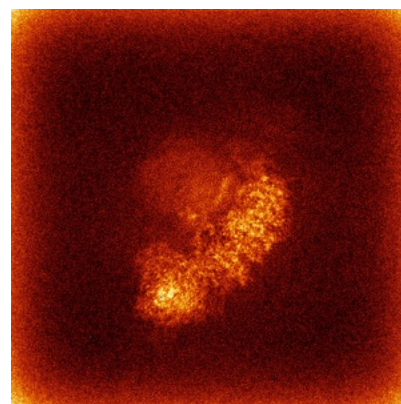
6.4.2 Raw map



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.

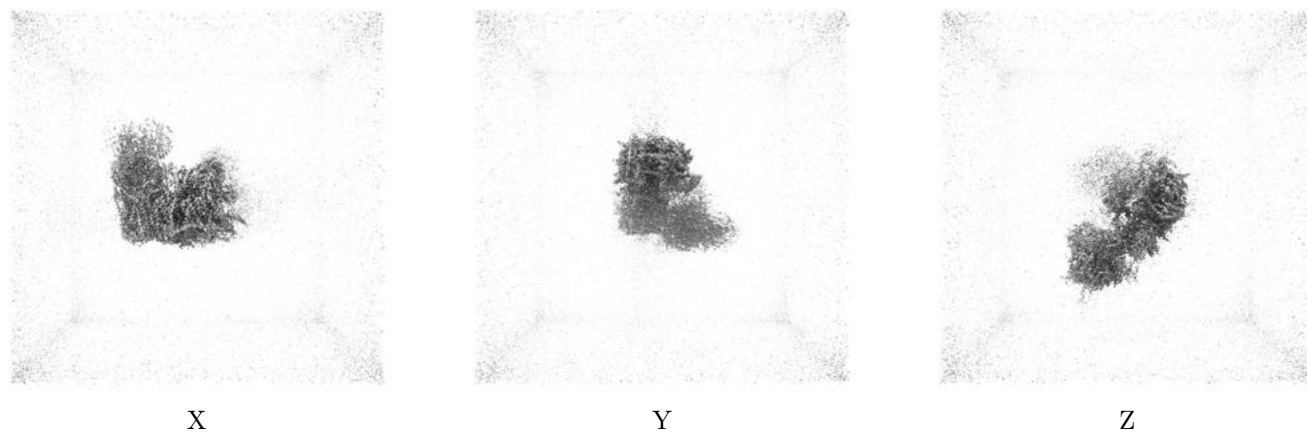
6.5 Orthogonal surface views [i](#)

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.

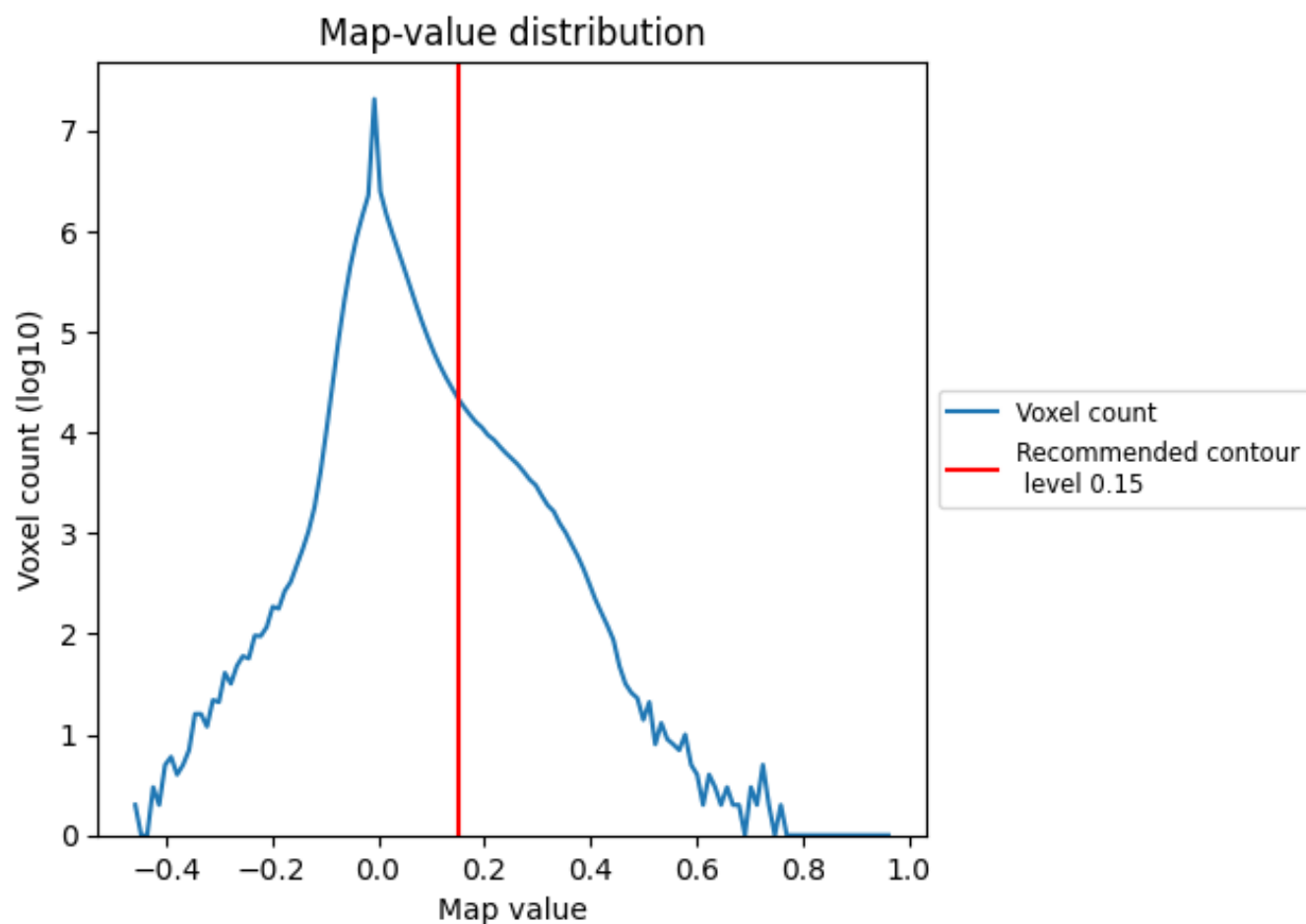
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

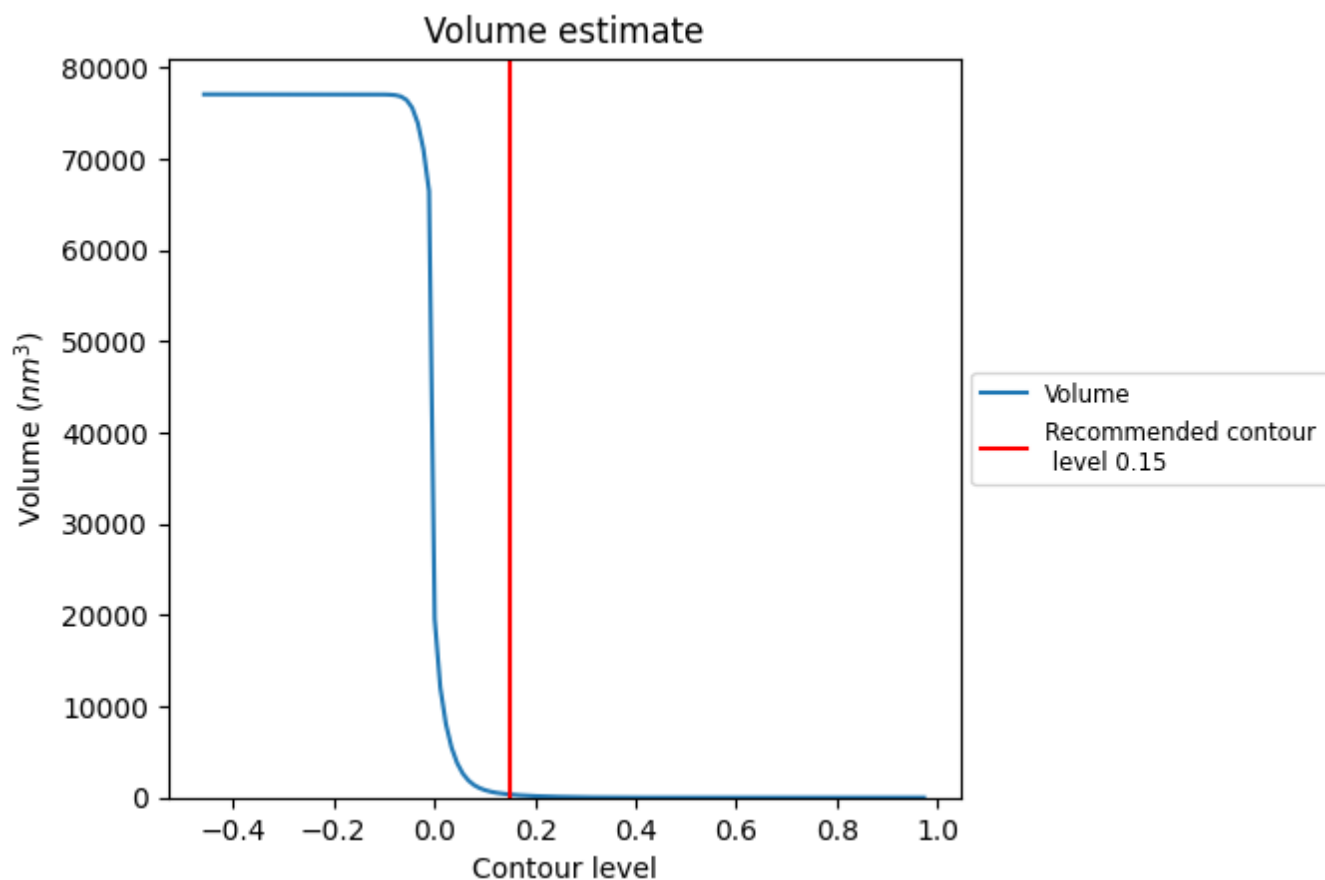
This section contains the results of statistical analysis of the map.

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.

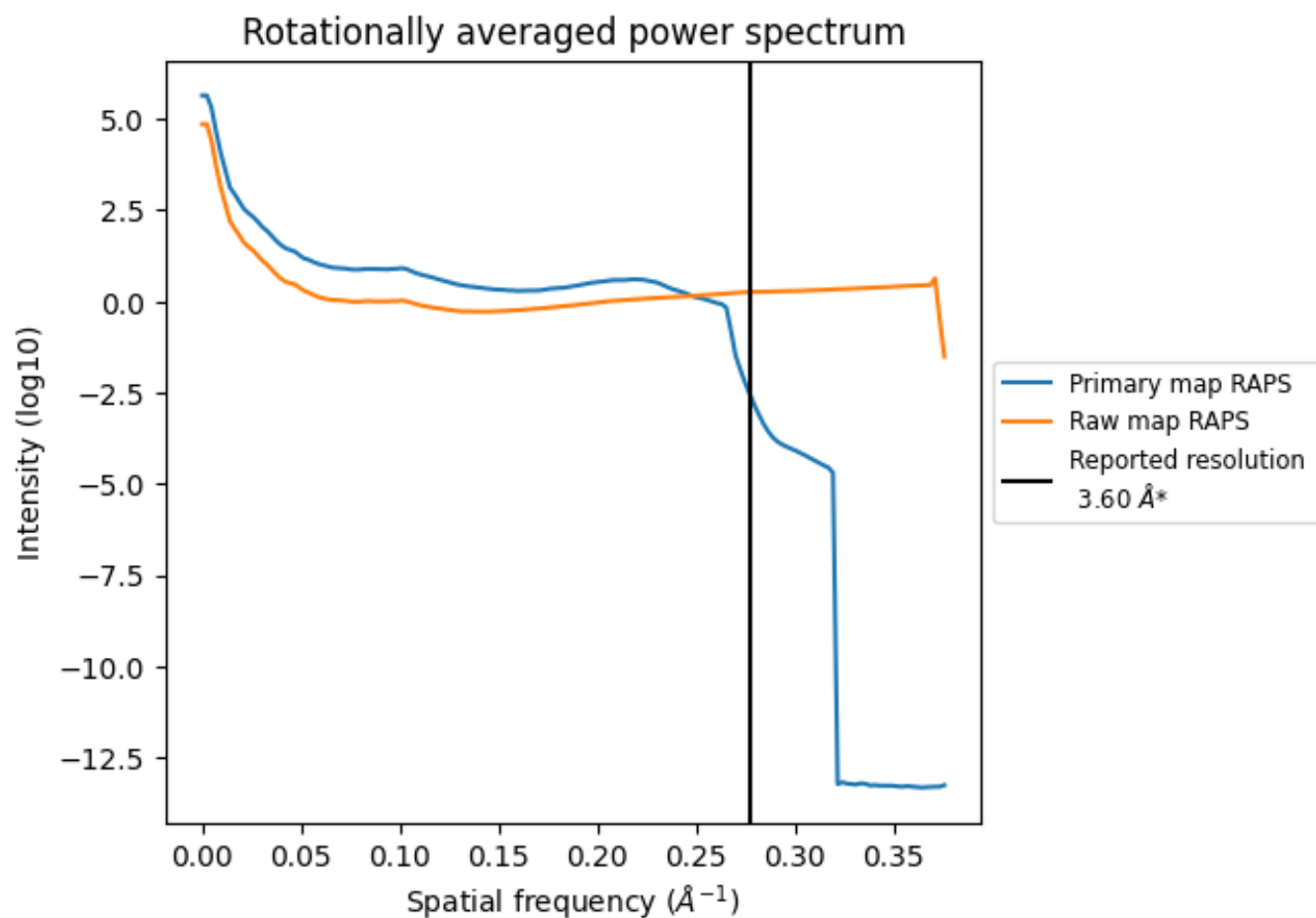
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 338 nm³; this corresponds to an approximate mass of 306 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 ⓘ

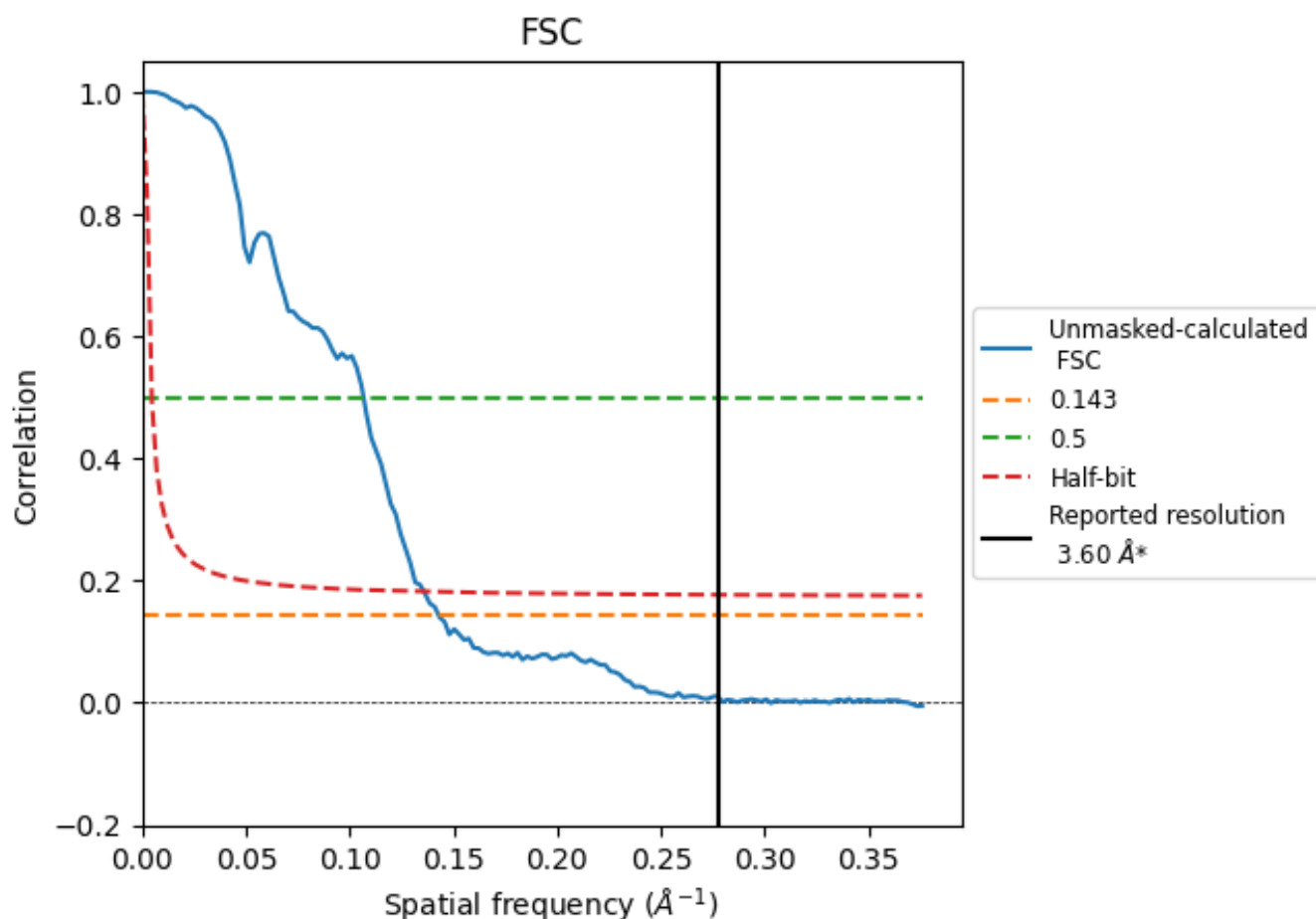


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

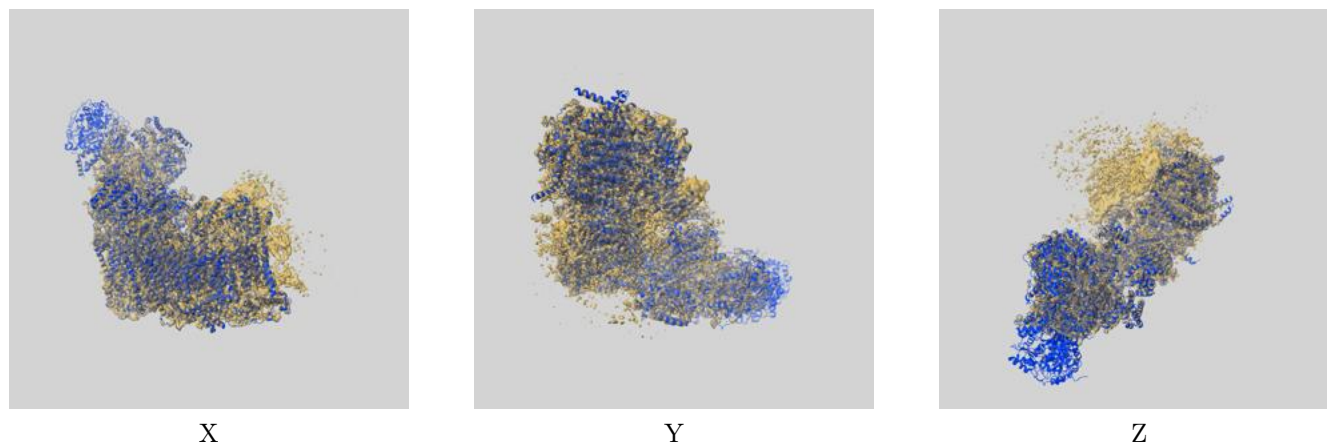
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.00	9.37	7.36

*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 7.00 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

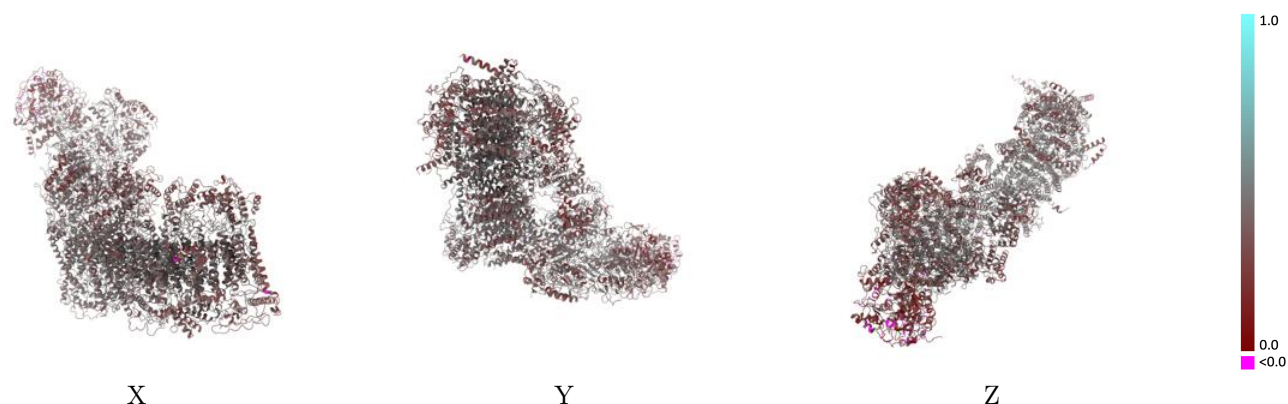
This section contains information regarding the fit between EMDB map EMD-42175 and PDB model 8UEY. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



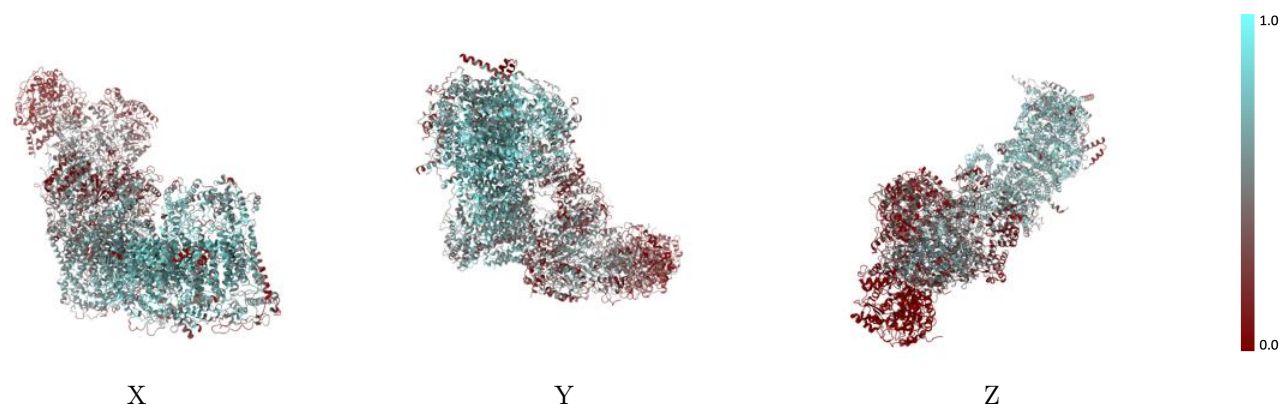
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



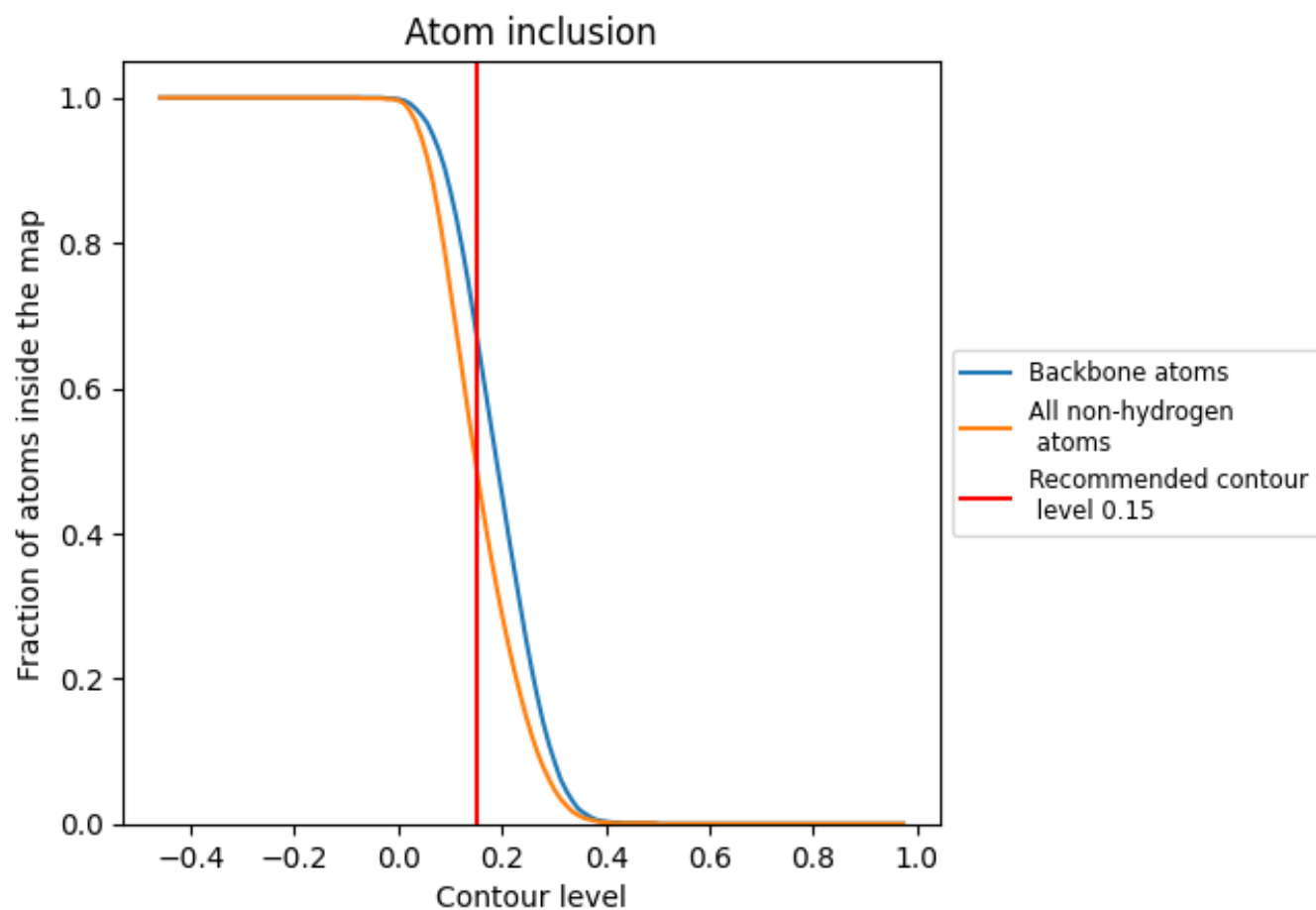
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 68% of all backbone atoms, 50% 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	0.4950	0.3830
1A	0.5300	0.4180
1B	0.5860	0.4290
1C	0.4340	0.4060
1D	0.5590	0.4080
1E	0.0450	0.2950
1F	0.0480	0.2570
1G	0.3120	0.3680
1H	0.5930	0.4130
1I	0.5670	0.4210
1J	0.5290	0.3800
1K	0.6290	0.4090
1L	0.7110	0.4100
1M	0.7630	0.4420
1N	0.6850	0.4310
1O	0.4050	0.3700
1P	0.3270	0.3470
1Q	0.3250	0.3840
1R	0.3320	0.4040
1S	0.1620	0.3070
1T	0.2640	0.2940
1U	0.6120	0.3580
1V	0.2440	0.3400
1W	0.3370	0.3580
1X	0.5630	0.4110
1Y	0.6790	0.3880
1Z	0.5820	0.4200
1a	0.6840	0.4140
1b	0.5690	0.4180
1c	0.4460	0.3740
1d	0.6800	0.4180
1e	0.6120	0.4290
1f	0.4740	0.3860
1g	0.5960	0.4040
1h	0.6890	0.4230



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Chain	Atom inclusion	Q-score
1i	 0.4070	 0.3590
1j	 0.5220	 0.3630
1k	 0.5200	 0.3610
1l	 0.6540	 0.3940
1m	 0.6900	 0.3870
1n	 0.6560	 0.3760
1o	 0.5350	 0.3320
1p	 0.6210	 0.3920
1q	 0.4310	 0.4050
1r	 0.4140	 0.3990
1s	 0.0000	 0.2350