



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 06:53 AM EDT

PDB ID : 8UEQ / pdb_00008ueq
EMDB ID : EMD-42167
Title : In-situ complex I with Q10 (State-beta)
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.40 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:

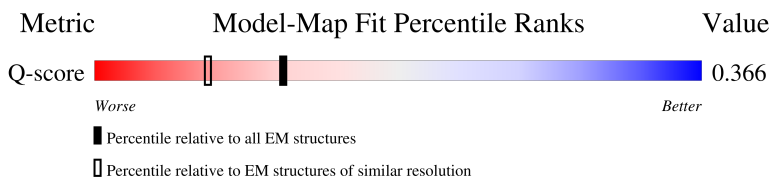
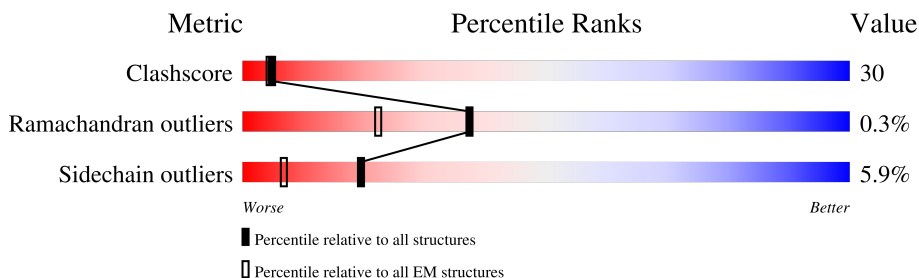
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.40 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	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1A	115	
2	1B	258	
3	1C	264	
4	1D	476	

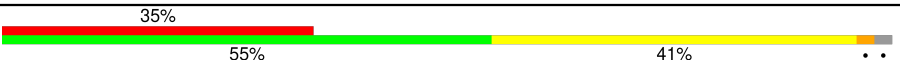
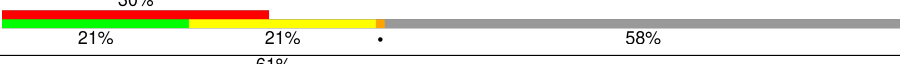
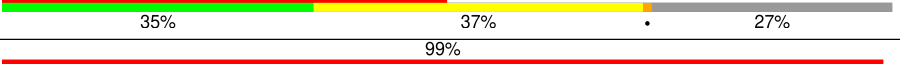
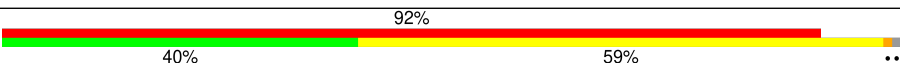
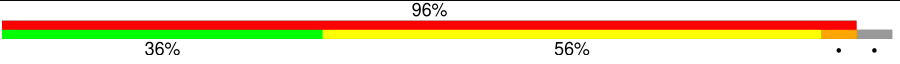
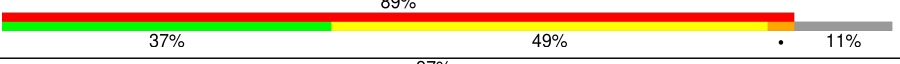
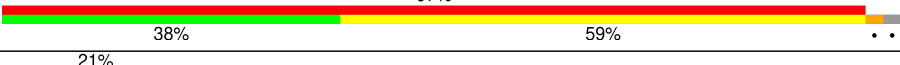
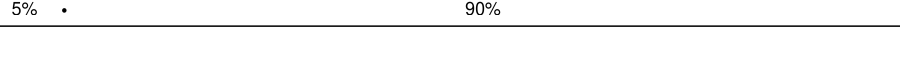
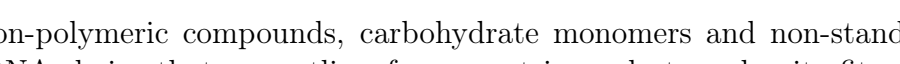
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24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

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Mol	Chain	Length	Quality of chain
29	1d	123	
30	1e	106	
31	1f	135	
32	1g	154	
33	1h	189	
34	1i	128	
35	1j	105	
36	1k	98	
37	1l	186	
38	1m	129	
39	1n	179	
40	1o	137	
41	1p	176	
42	1q	145	
43	1r	114	
44	1s	471	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1G	801	-	-	X	-
48	FES	1G	803	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67142 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	115	Total	C	N	O	S	0	0
			916	616	134	159	7		

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

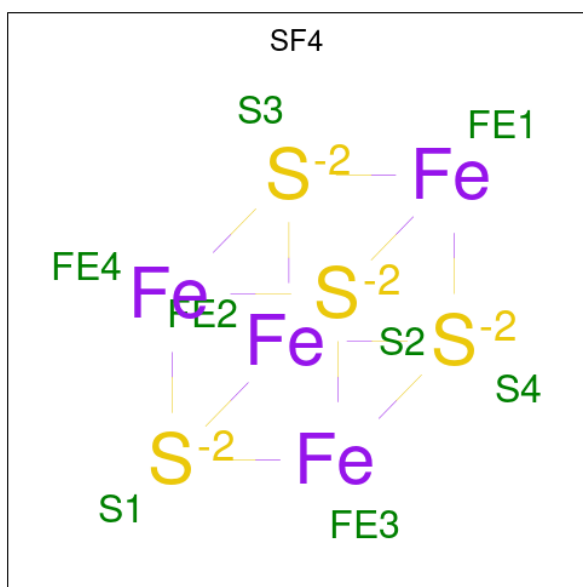
There is a discrepancy between the modelled and reference sequences:

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

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

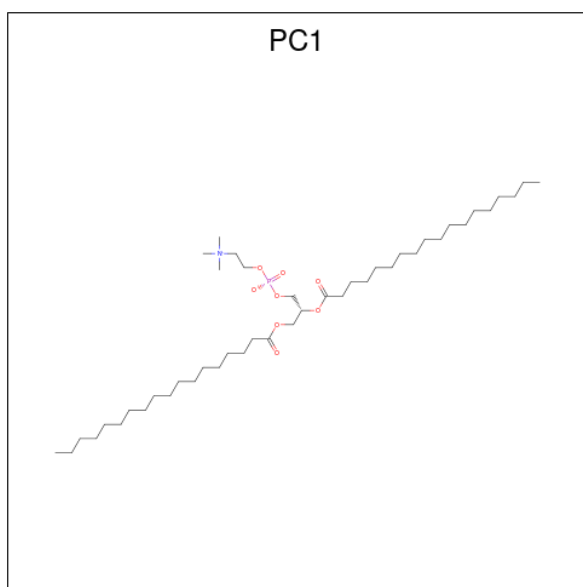
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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



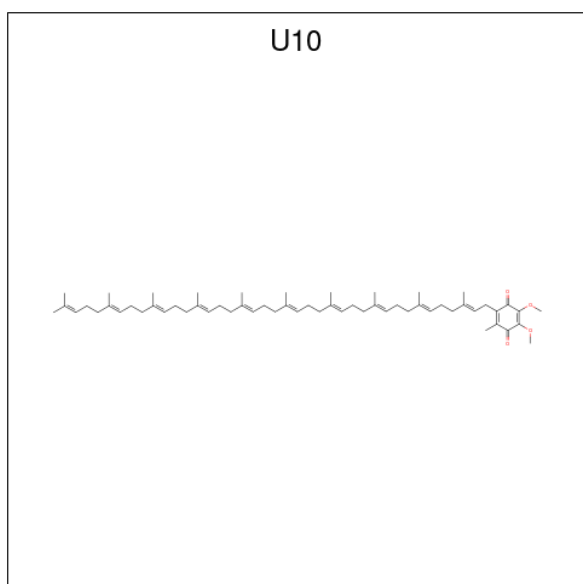
Mol	Chain	Residues	Atoms			AltConf
45	1B	1	Total	Fe	S	0
			8	4	4	
45	1F	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	

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



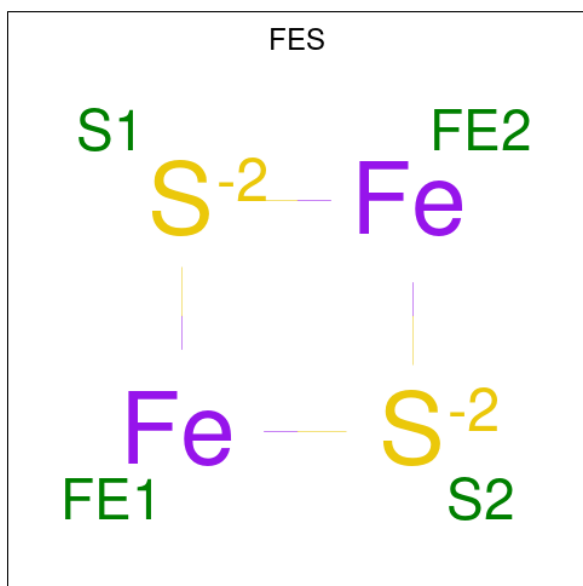
Mol	Chain	Residues	Atoms					AltConf
46	1B	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1q	1	Total	C	N	O	P	0
			48	38	1	8	1	

- Molecule 47 is UBIQUINONE-10 (CCD ID: U10) (formula: C₅₉H₉₀O₄) (labeled as "Ligand of Interest" by depositor).



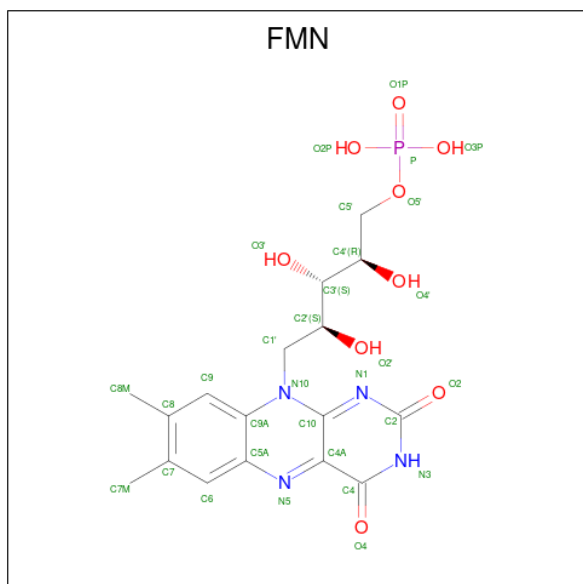
Mol	Chain	Residues	Atoms			AltConf
47	1D	1	Total	C	O	0
			63	59	4	

- 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: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).

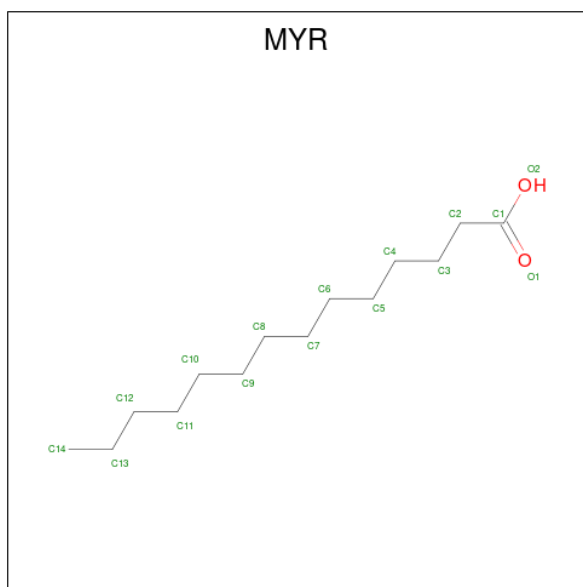


Mol	Chain	Residues	Atoms					AltConf
49	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

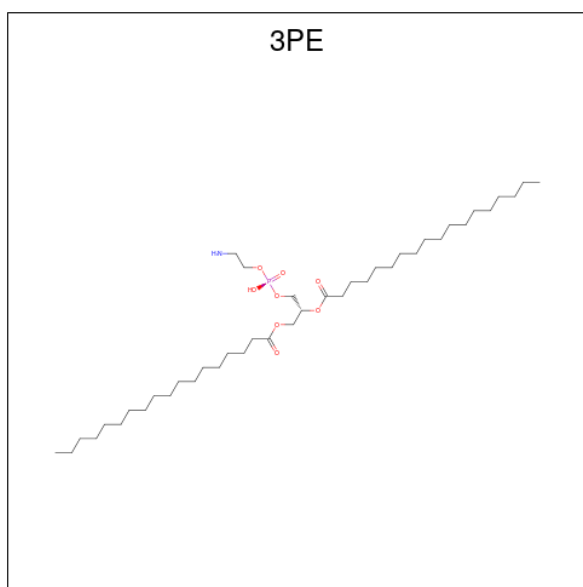
Mol	Chain	Residues	Atoms		AltConf
50	1G	1	Total	K	0
			1	1	

- Molecule 51 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



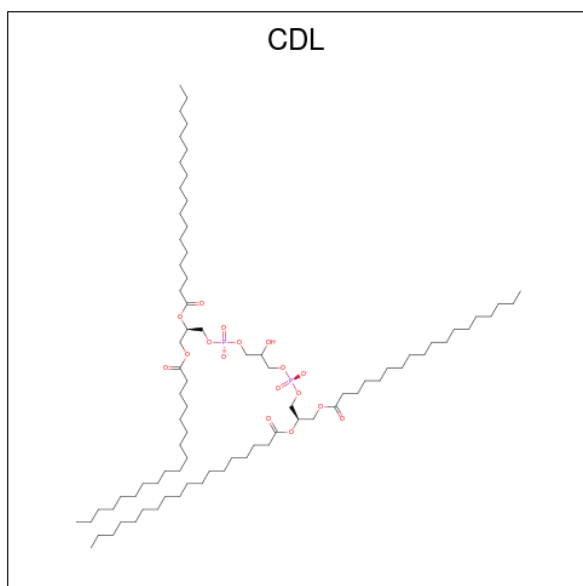
Mol	Chain	Residues	Atoms			AltConf
51	1L	1	Total	C	O	0
			15	14	1	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: C₄₁H₈₂NO₈P).



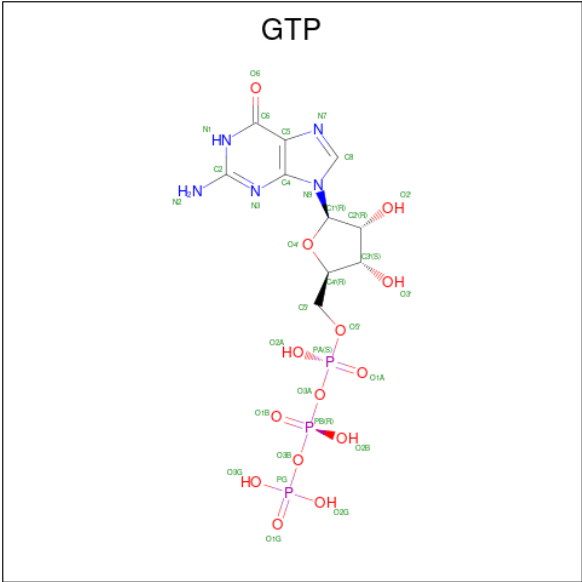
Mol	Chain	Residues	Atoms					AltConf
52	1M	1	Total	C	N	O	P	0
			38	28	1	8	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
53	1N	1	Total	C	O	P	0
			67	48	17	2	
53	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 54 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

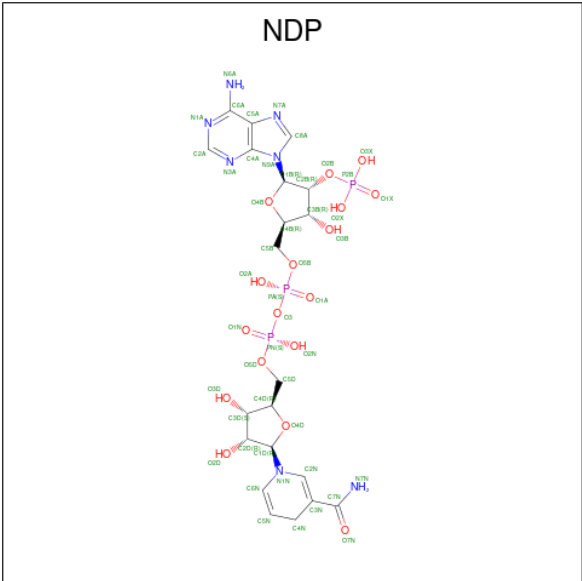


Mol	Chain	Residues	Atoms					AltConf
54	10	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

Mol	Chain	Residues	Atoms		AltConf
55	10	1	Total	Mg	0
			1	1	

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

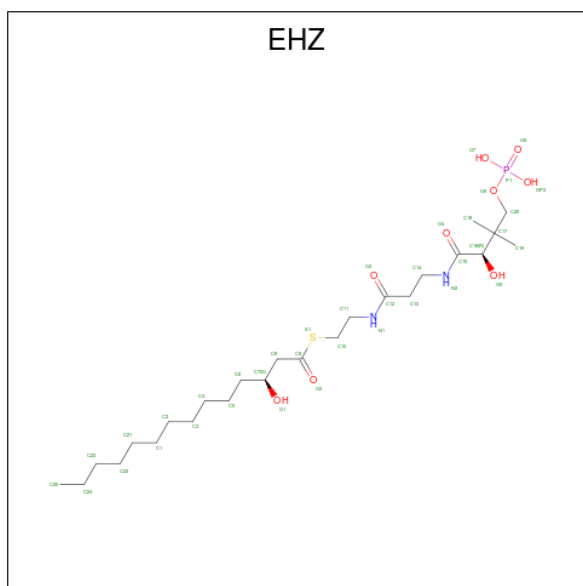


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

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

- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

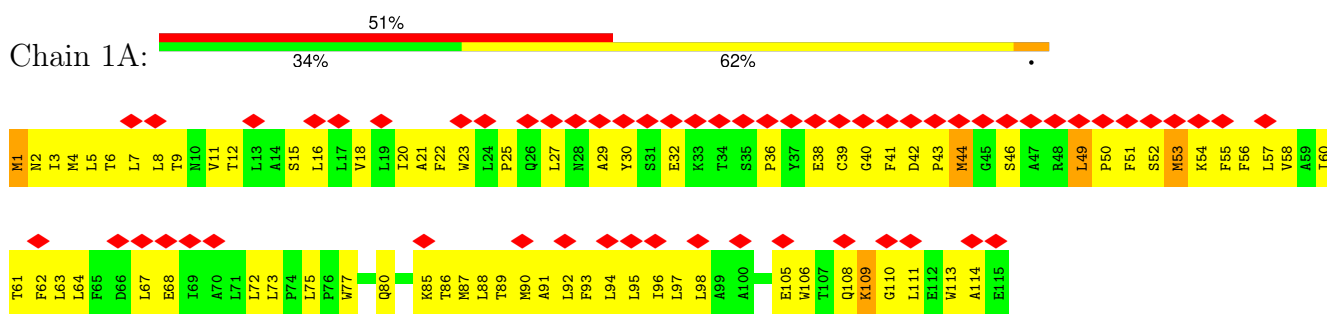


Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

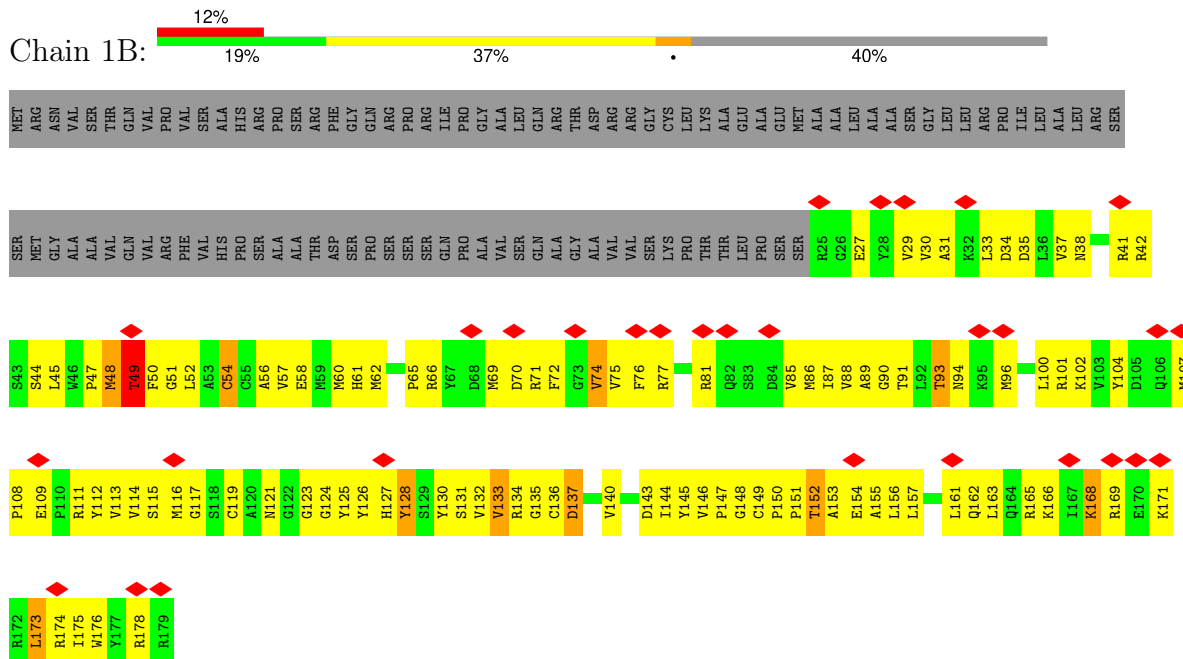
3 Residue-property plots

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

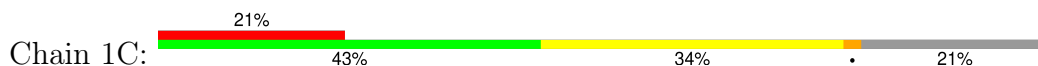
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

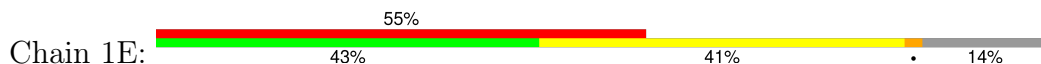


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

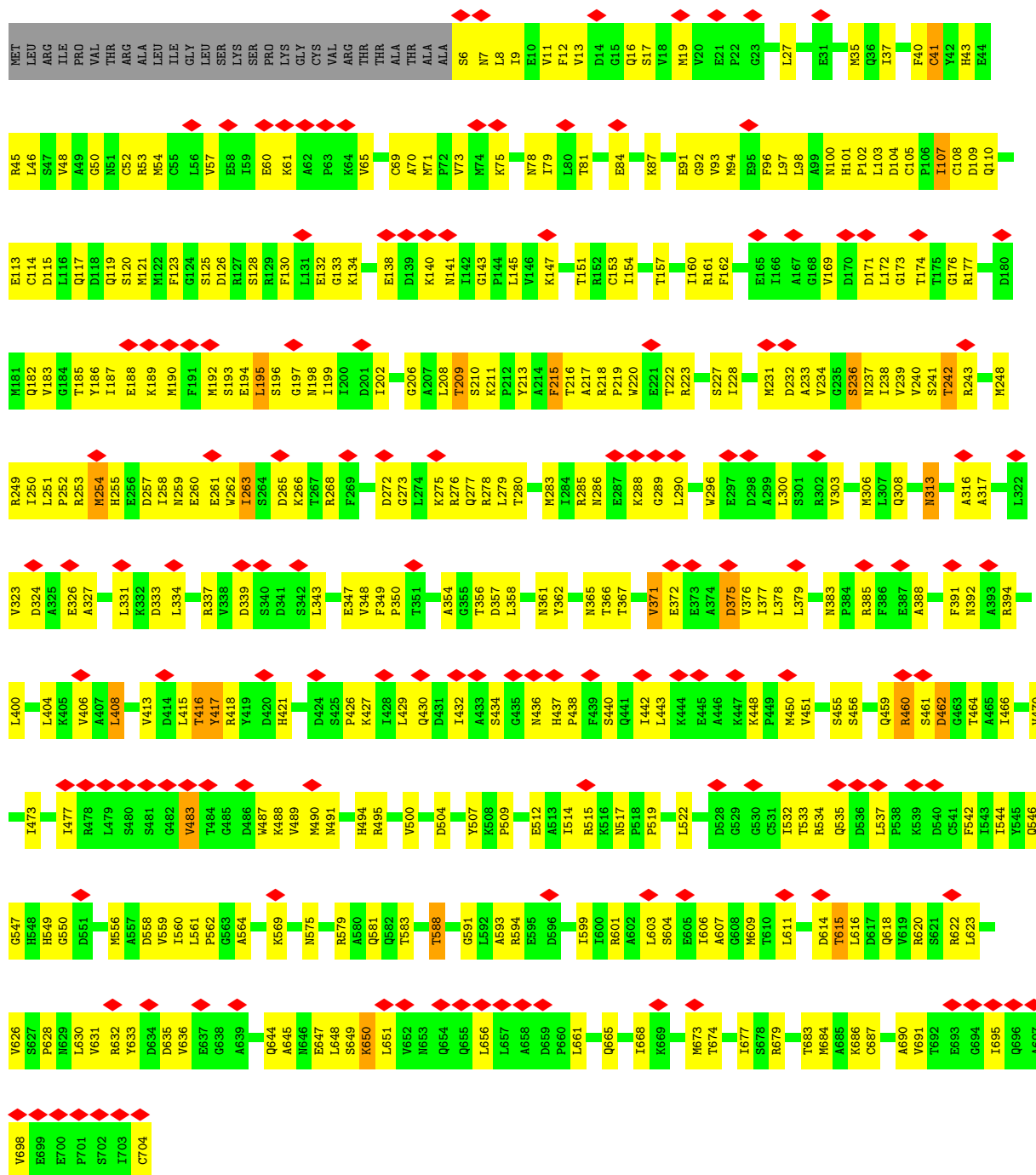


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

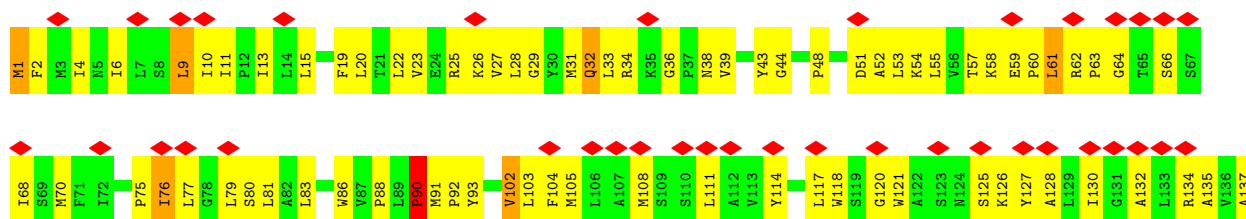


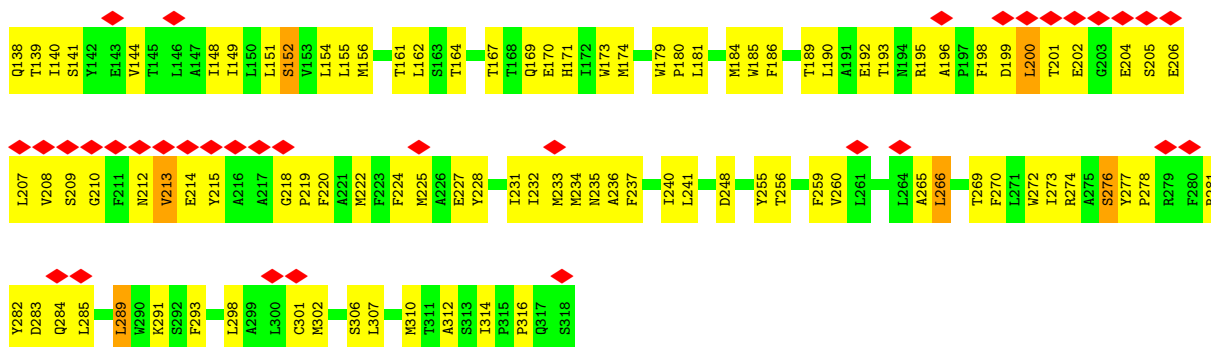






• Molecule 8: NADH-ubiquinone oxidoreductase chain 1





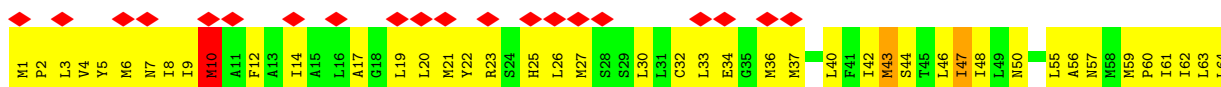
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

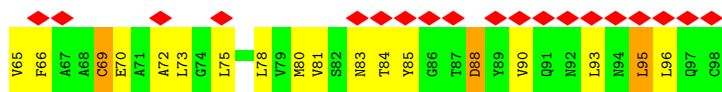


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

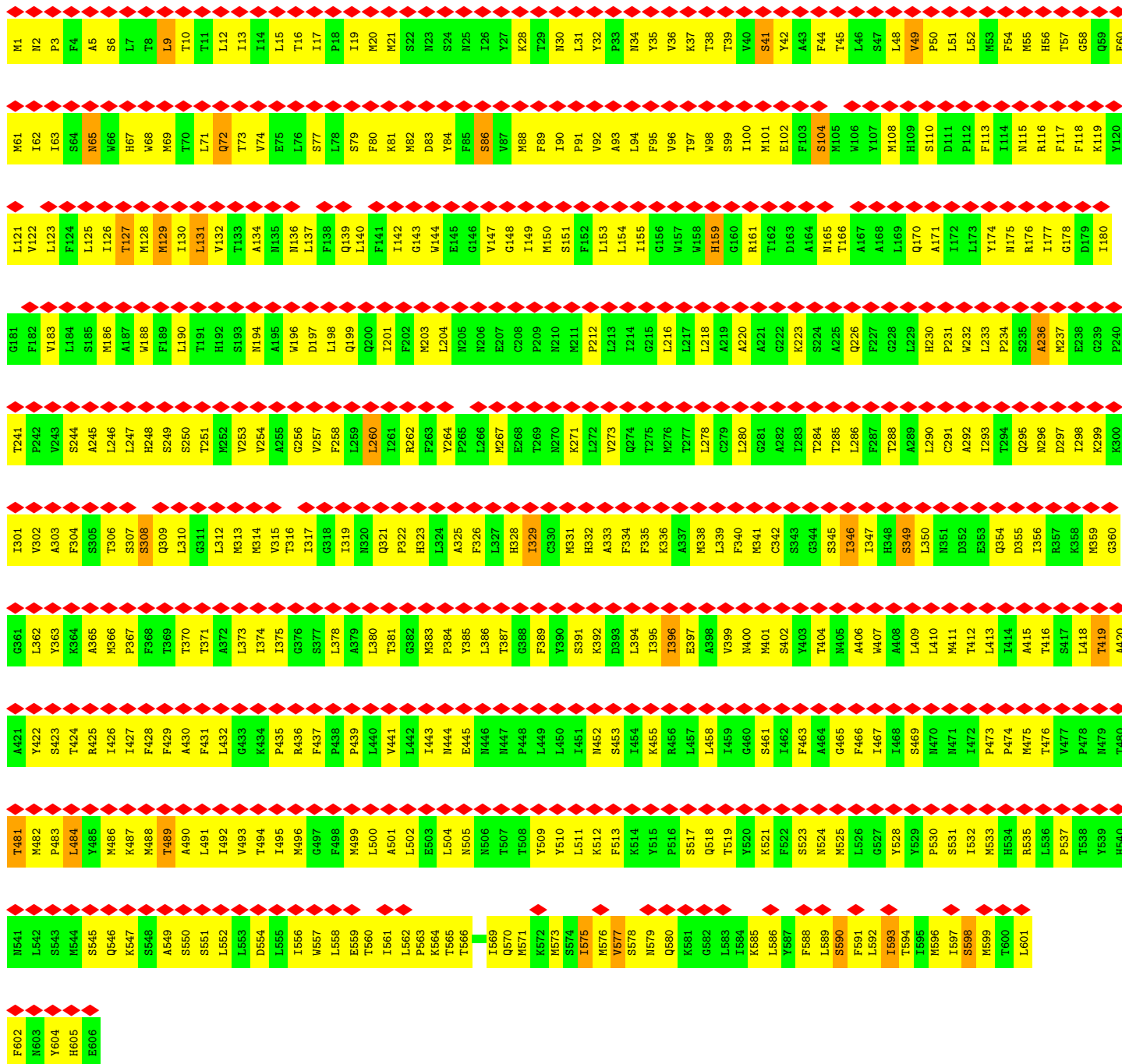


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



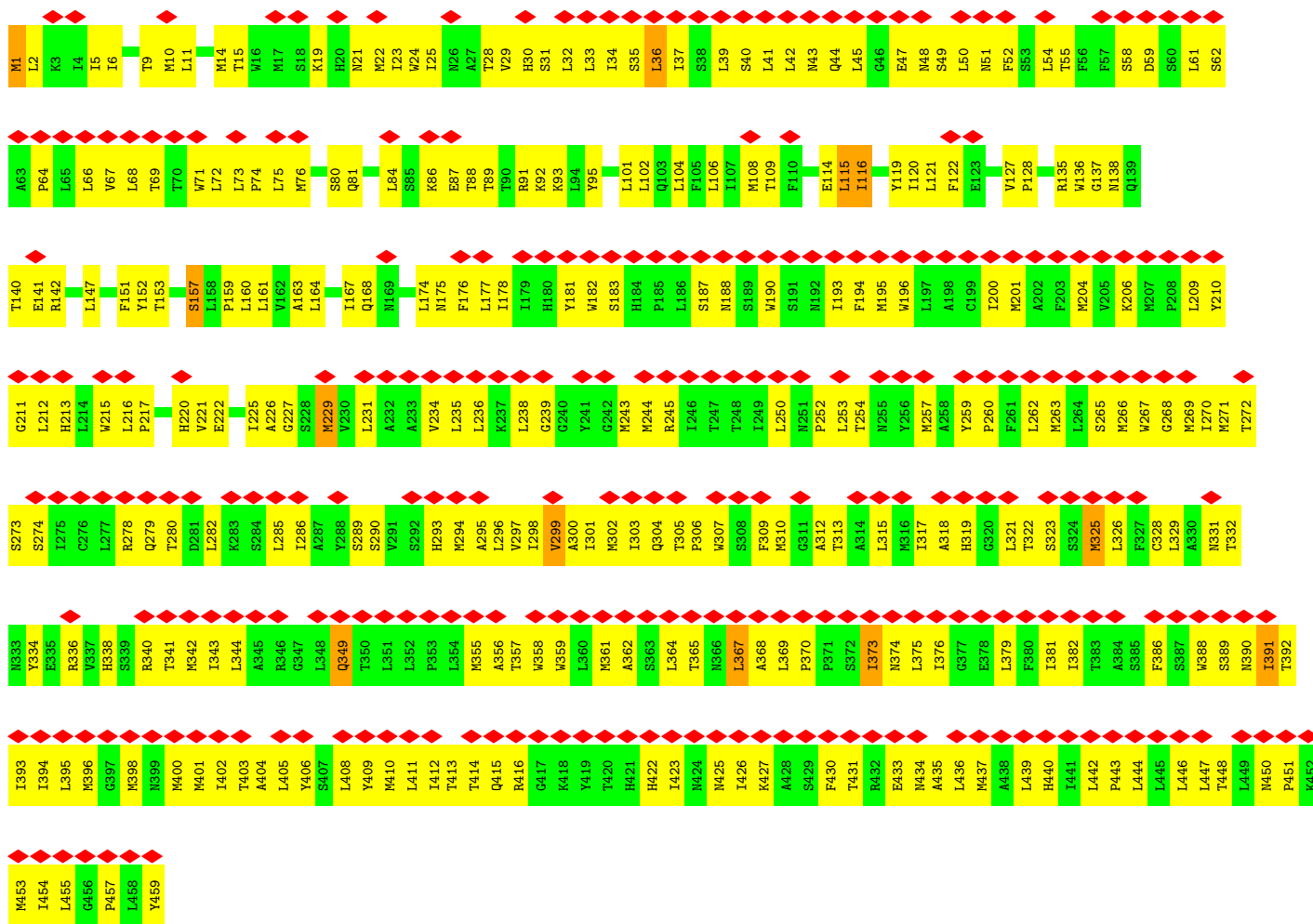


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

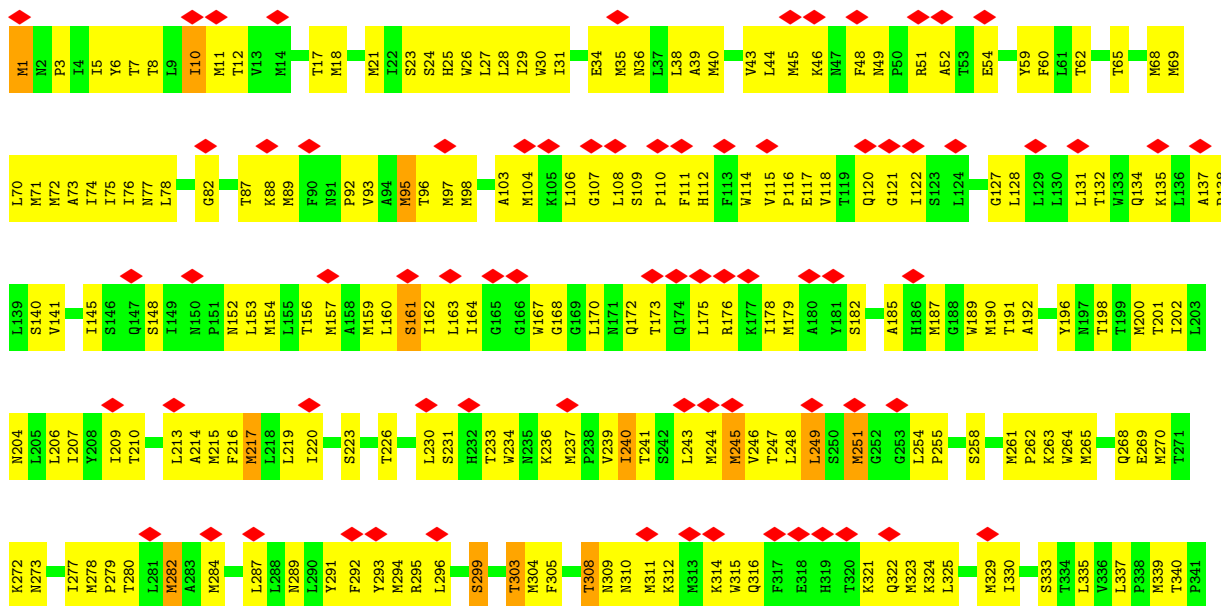


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



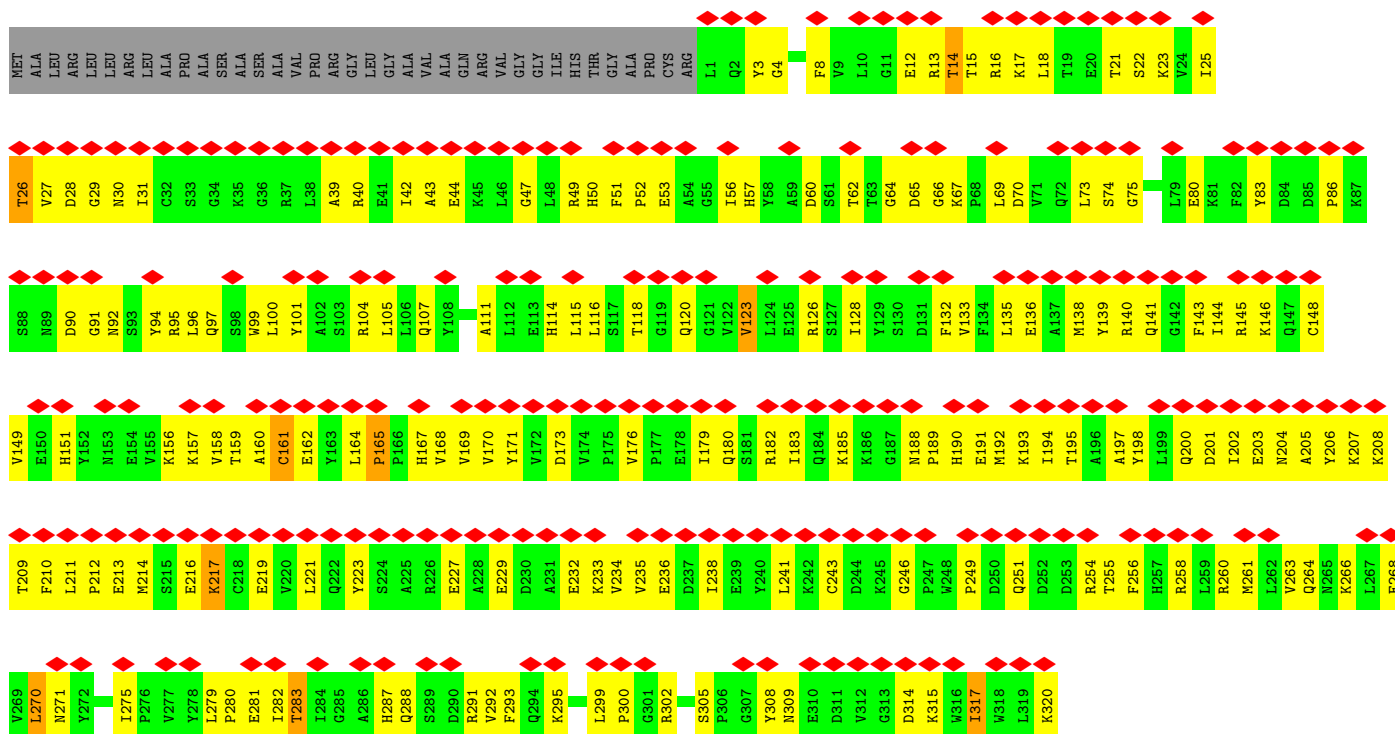


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

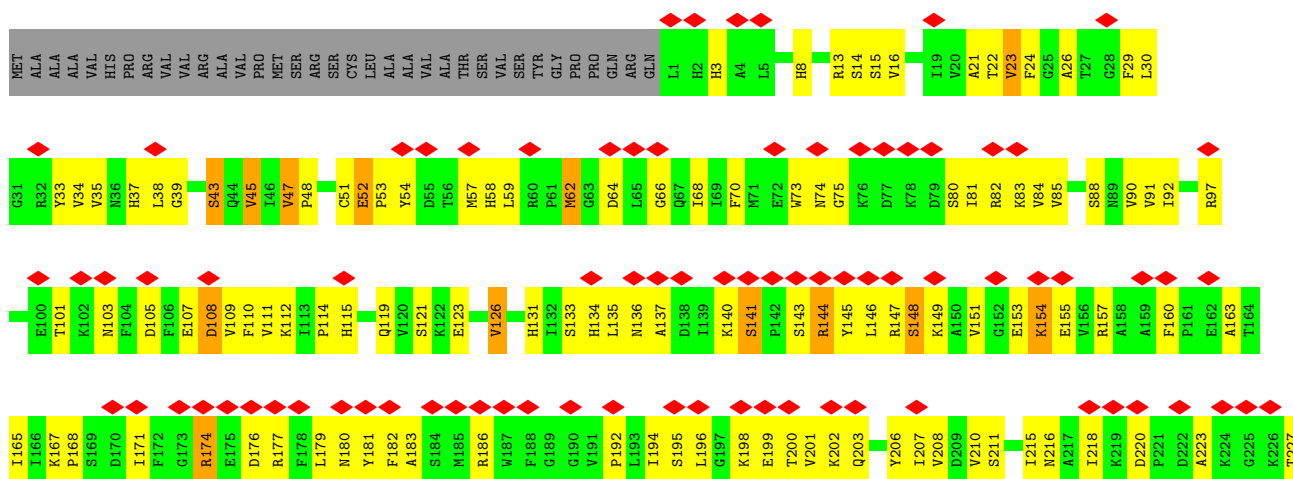
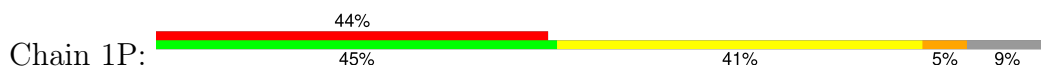


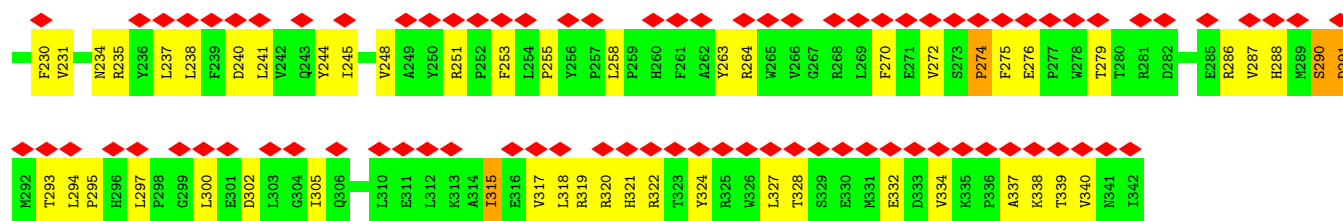


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

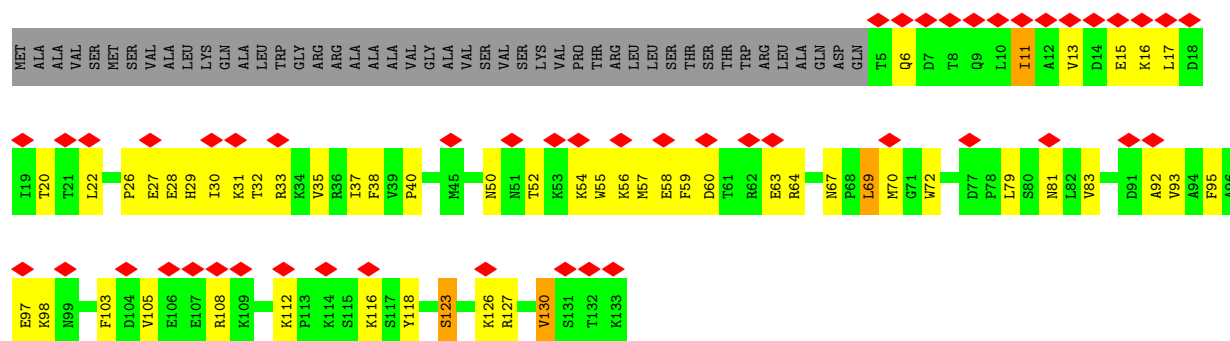
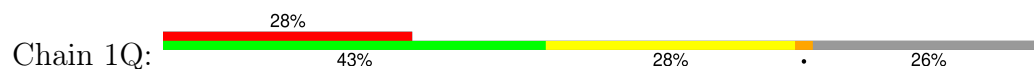


- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

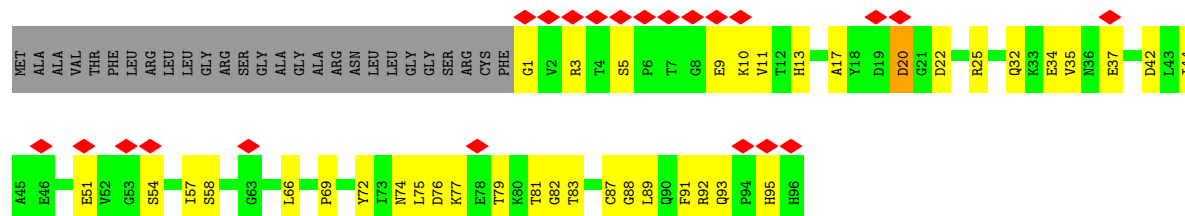




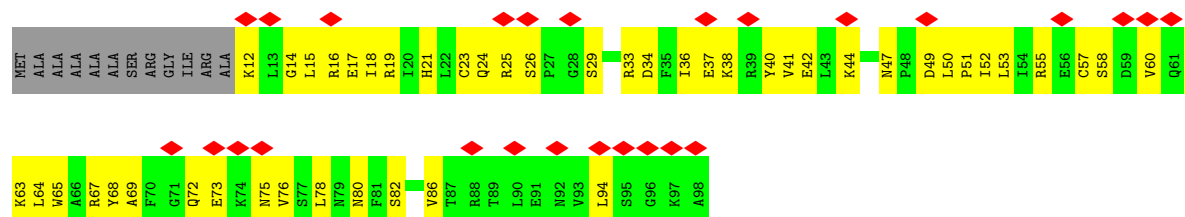
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



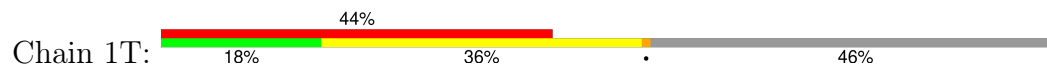
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

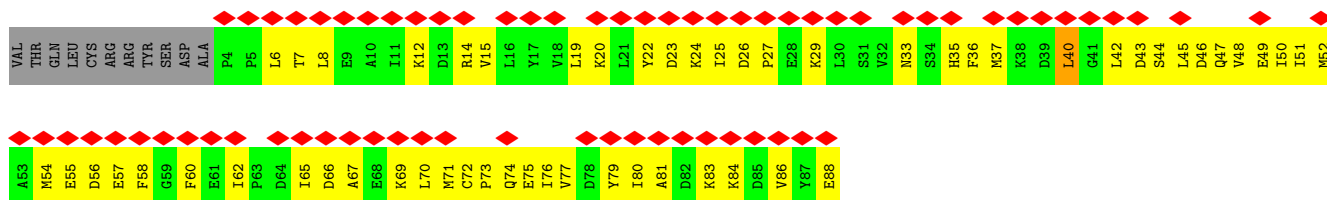


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

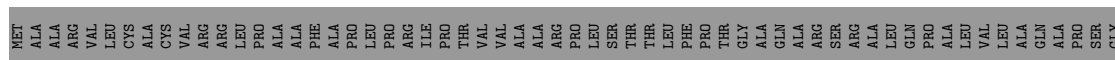
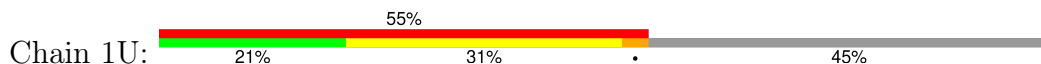


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

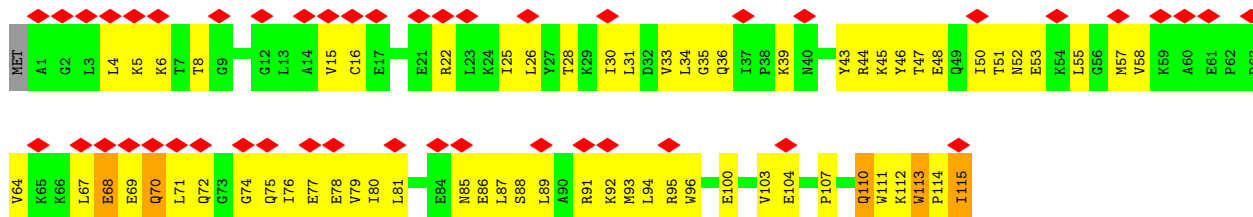
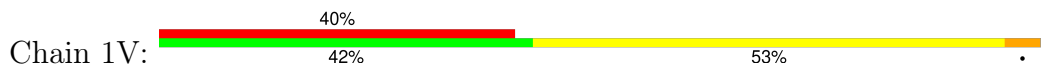




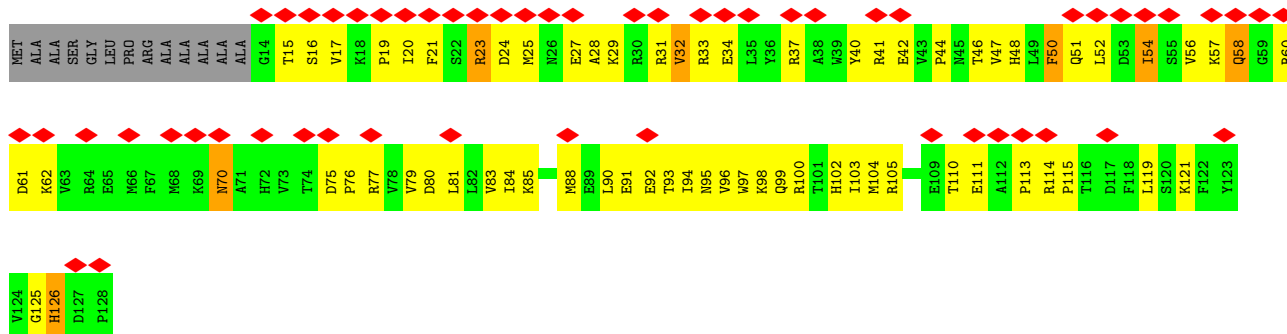
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



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

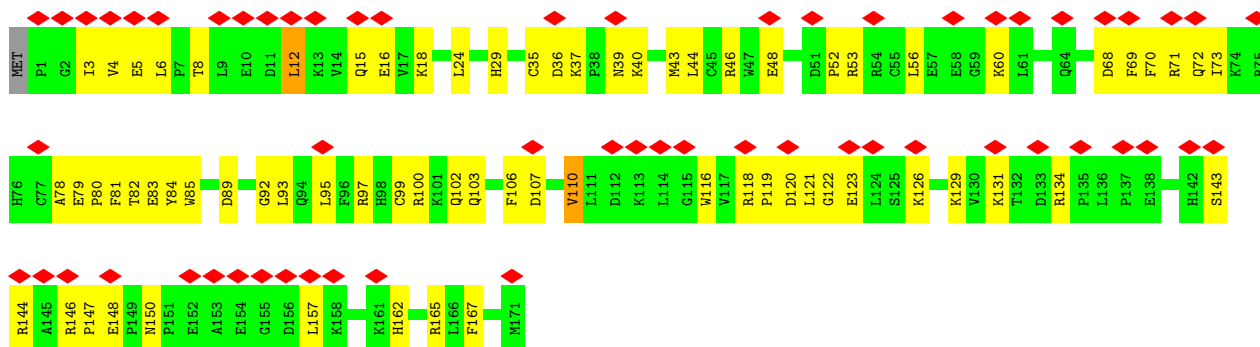


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

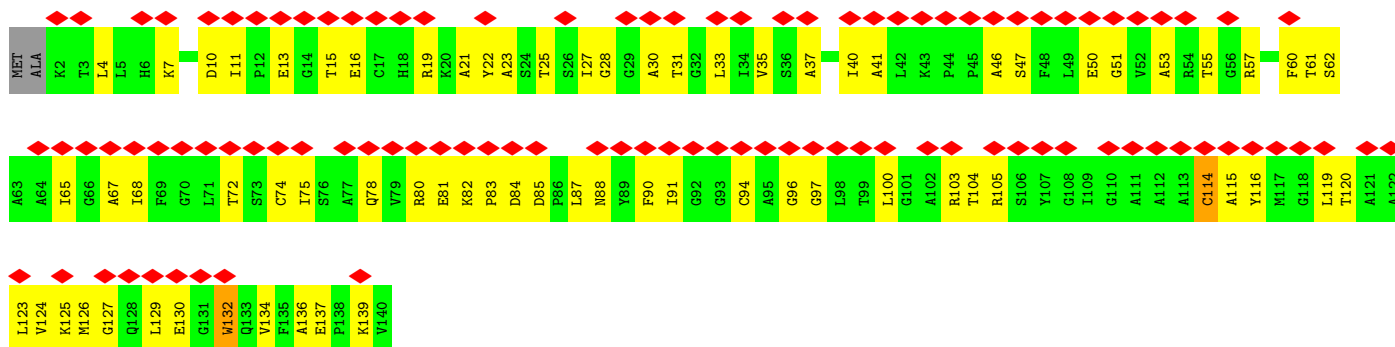


• Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

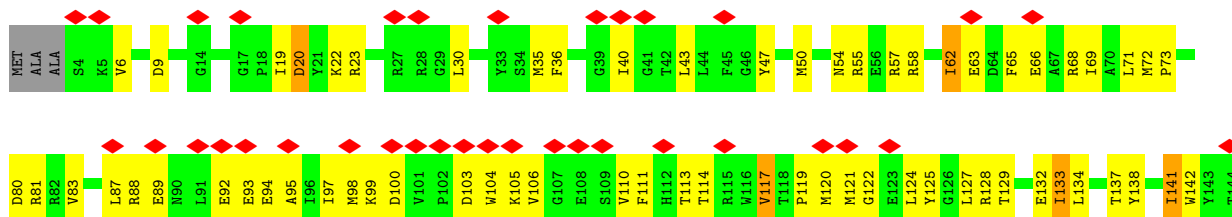




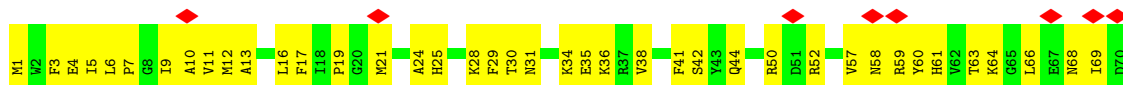
• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

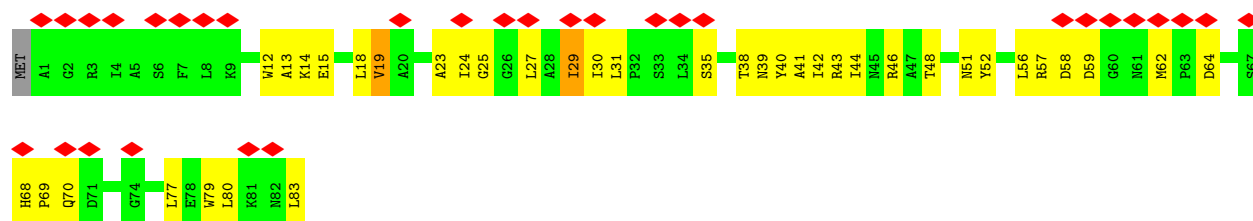


• Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

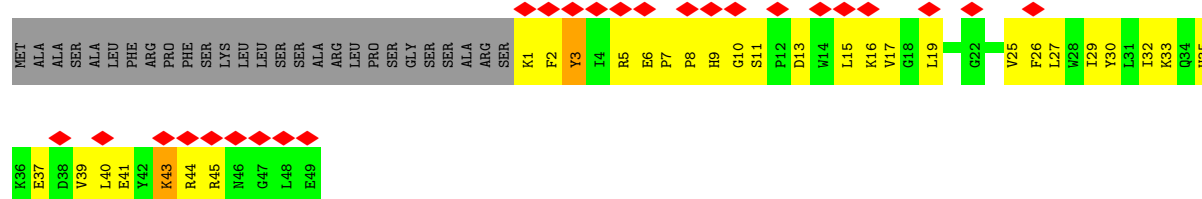
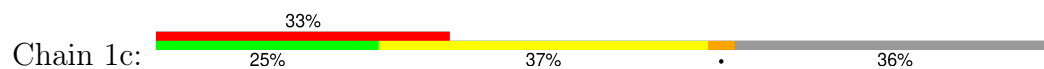


• Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

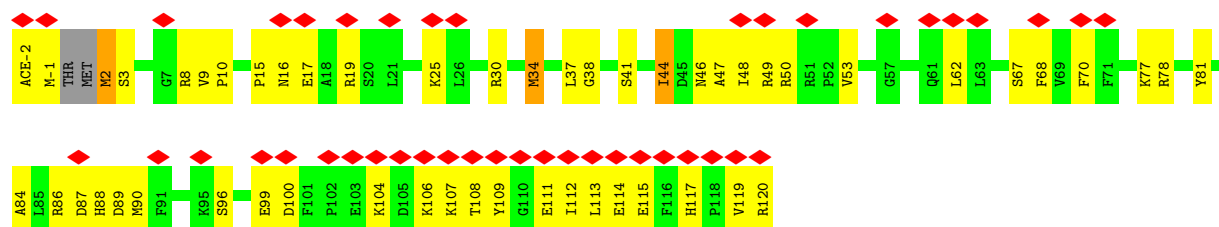




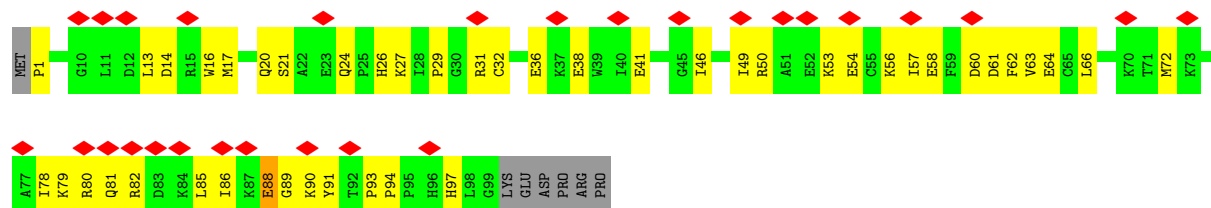
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



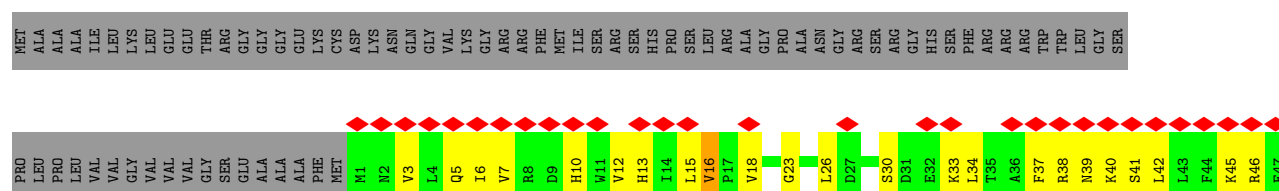
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



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

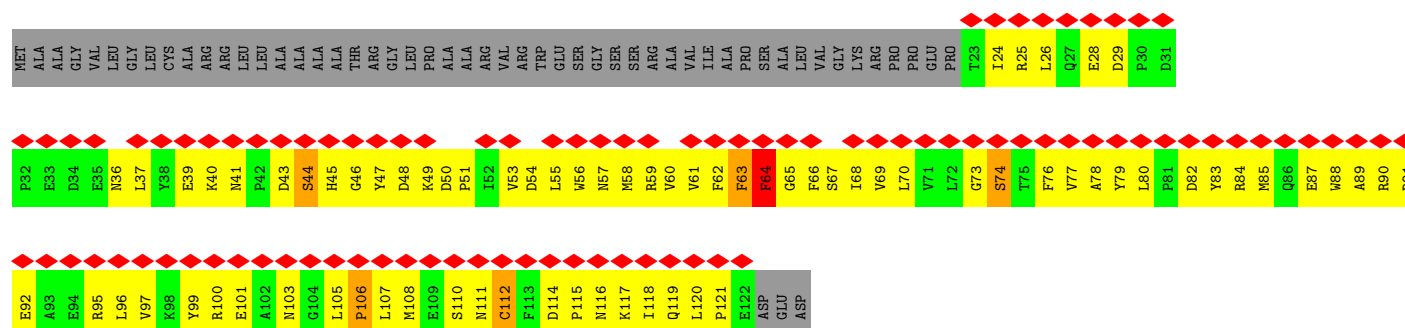
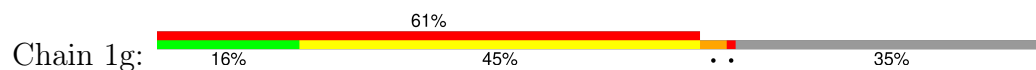


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

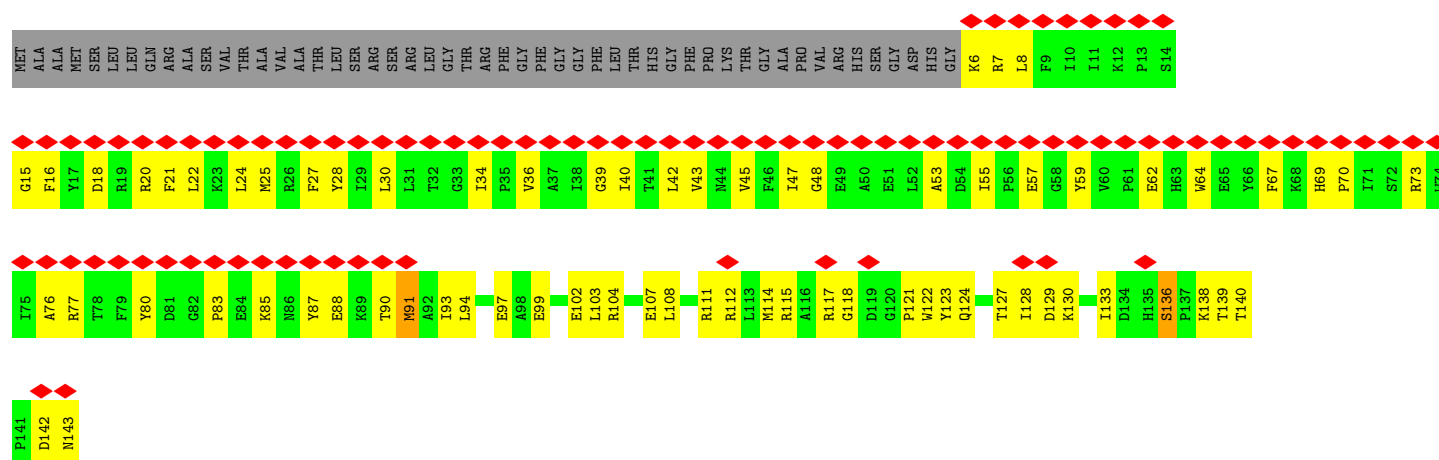




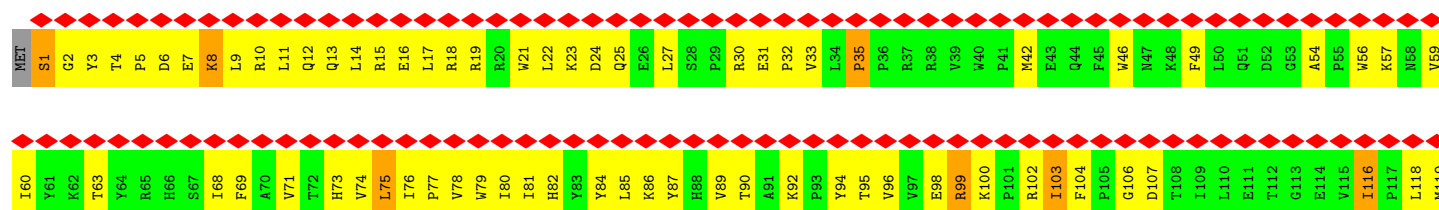
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



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

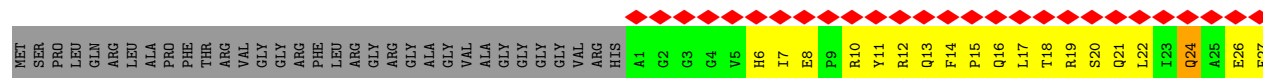
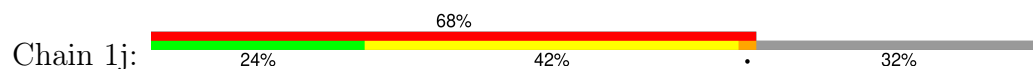


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

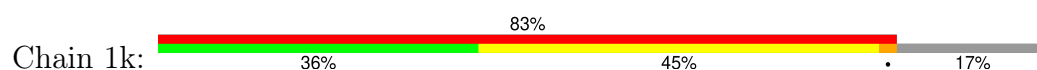




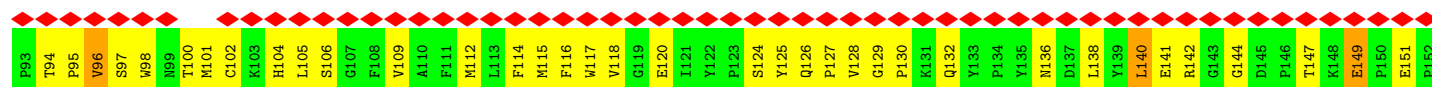
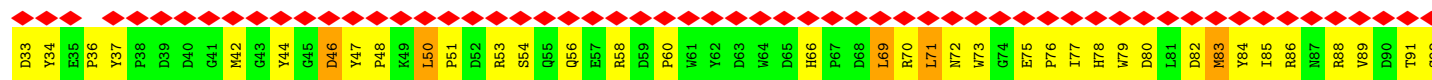
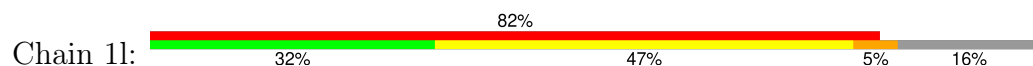
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



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



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

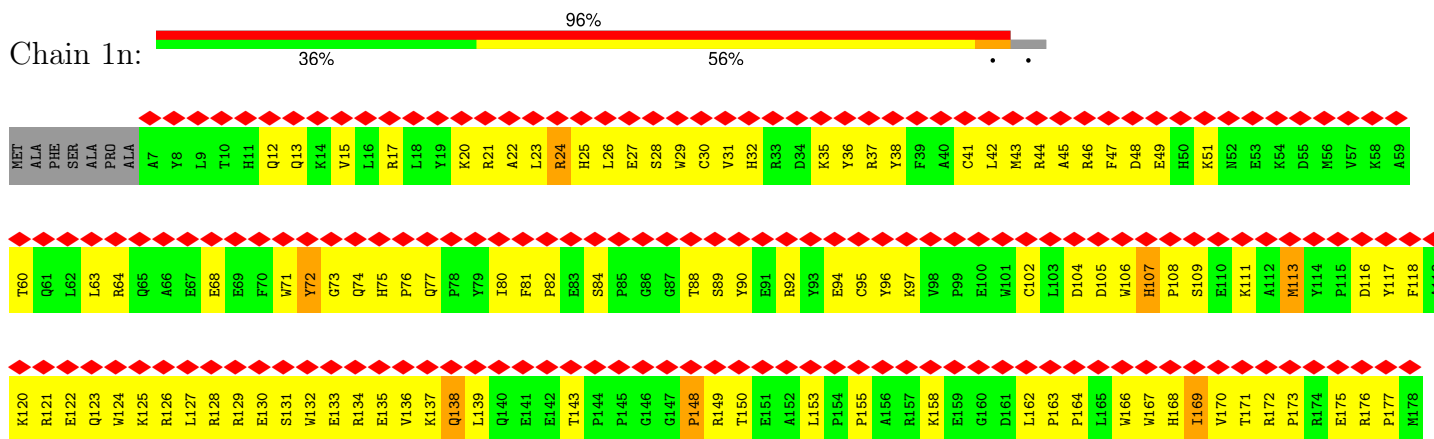


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

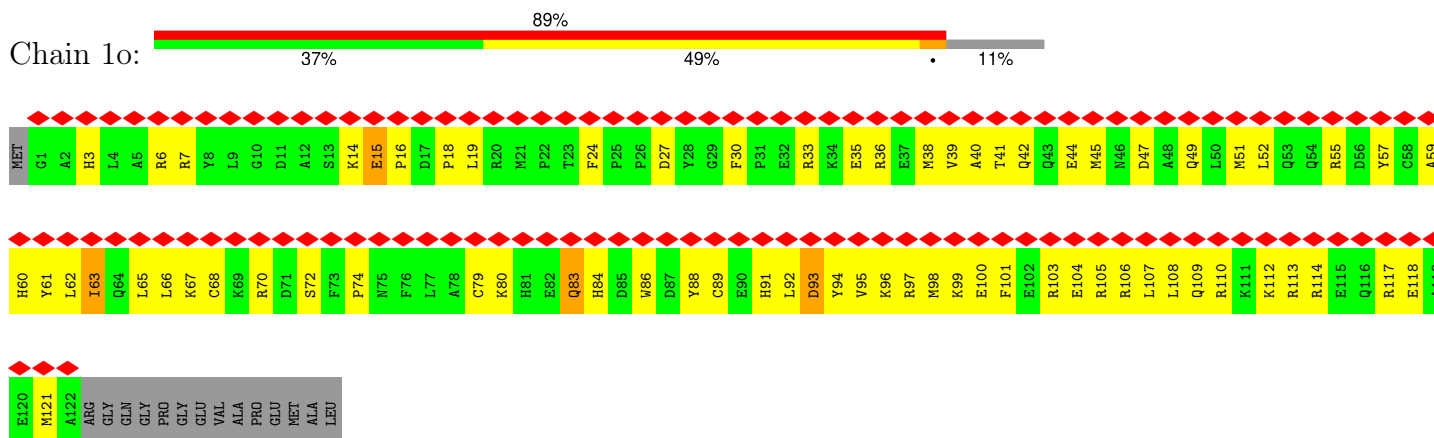




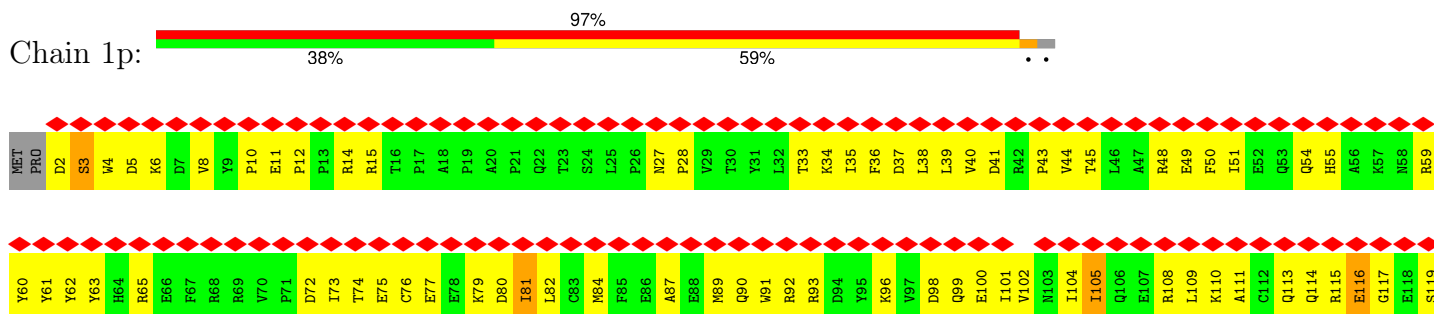
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



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

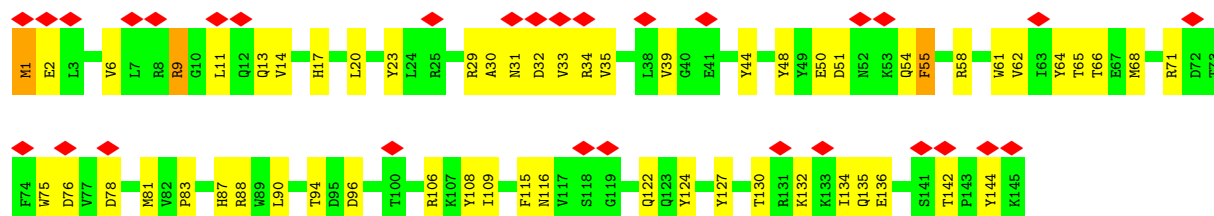


• Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

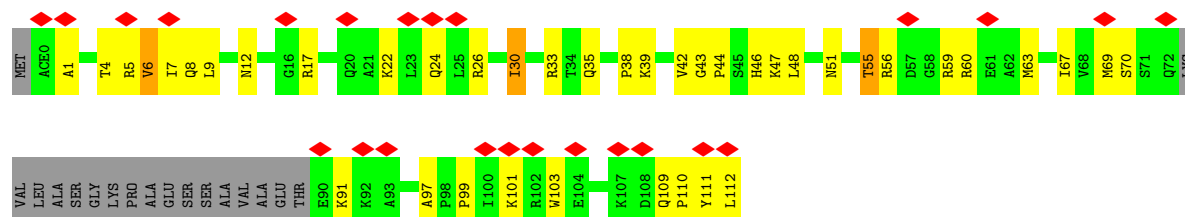




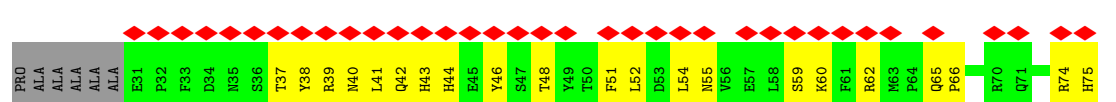
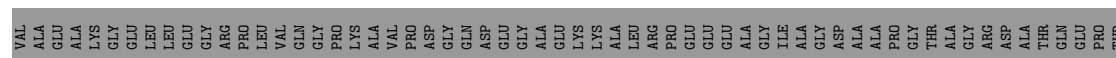
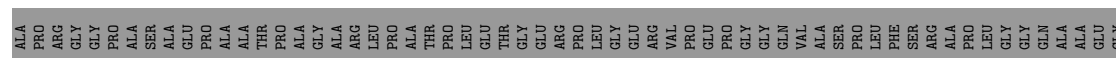
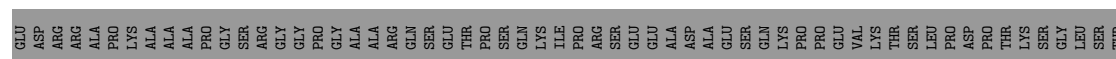
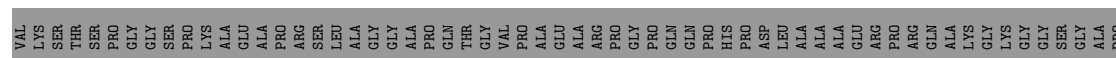
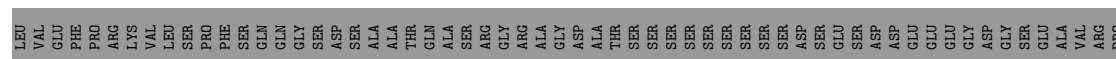
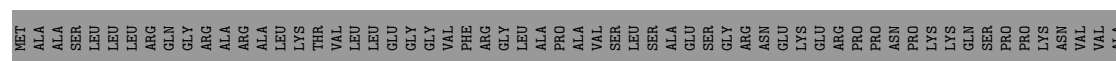
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.898	Depositor
Minimum map value	-0.238	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.020	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	444.8, 444.8, 444.8	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, CDL, MG, U10, MYR, K, ACE, FME, SAC, 3PE, EH2, ZN, SF4, FMN, FES, PC1, NDP

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	0.23	0/930	0.60	0/1271
2	1B	0.22	0/1273	0.50	1/1722 (0.1%)
3	1C	0.17	0/1791	0.41	0/2439
4	1D	0.22	0/3545	0.54	2/4806 (0.0%)
5	1E	0.15	0/1698	0.44	0/2311
6	1F	0.16	0/3401	0.40	0/4595
7	1G	0.16	0/5451	0.43	0/7387
8	1H	0.63	4/2566 (0.2%)	0.87	4/3509 (0.1%)
9	1I	0.19	0/1443	0.41	0/1952
10	1J	0.22	0/1364	0.55	0/1850
11	1K	0.31	0/751	0.73	1/1018 (0.1%)
12	1L	0.22	0/4939	0.61	2/6718 (0.0%)
13	1M	0.22	0/3713	0.60	1/5063 (0.0%)
14	1N	0.26	0/2765	0.67	4/3758 (0.1%)
15	1O	0.20	0/2650	0.48	1/3588 (0.0%)
16	1P	0.30	2/2828 (0.1%)	0.53	5/3834 (0.1%)
17	1Q	0.18	0/1070	0.45	0/1446
18	1R	0.13	0/755	0.39	0/1018
19	1S	0.17	0/711	0.42	0/956
20	1T	0.32	0/701	0.76	0/946
20	1U	0.24	0/706	0.69	1/954 (0.1%)
21	1V	0.21	0/946	0.56	0/1281
22	1W	0.26	0/995	0.69	2/1340 (0.1%)
23	1X	0.18	0/1436	0.46	0/1938
24	1Y	0.25	0/1037	0.59	0/1404
25	1Z	0.22	0/1199	0.45	0/1617
26	1a	0.13	0/577	0.34	0/777
27	1b	0.23	0/664	0.51	0/912
28	1c	0.22	0/430	0.72	0/581
29	1d	0.18	0/1024	0.41	0/1383
30	1e	0.18	0/836	0.55	0/1118
31	1f	0.21	0/499	0.55	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.49	1/858 (0.1%)	0.93	5/1165 (0.4%)
33	1h	0.21	0/1184	0.51	0/1603
34	1i	0.26	0/1131	0.70	1/1541 (0.1%)
35	1j	0.33	0/627	0.78	1/858 (0.1%)
36	1k	0.18	0/668	0.45	0/903
37	1l	0.20	0/1365	0.53	0/1867
38	1m	0.23	0/1092	0.59	1/1481 (0.1%)
39	1n	0.18	0/1549	0.67	3/2098 (0.1%)
40	1o	0.19	0/1069	0.49	0/1430
41	1p	0.19	0/1481	0.47	0/1997
42	1q	0.16	0/1253	0.38	1/1704 (0.1%)
43	1r	0.15	0/782	0.38	0/1057
44	1s	0.15	0/394	0.38	0/533
All	All	0.25	7/68147 (0.0%)	0.56	36/92402 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	1D	0	1
8	1H	0	1
21	1V	0	1
22	1W	0	1
34	1i	0	1
39	1n	0	1
All	All	0	6

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1H	90	PRO	CB-CG	21.70	2.58	1.49
8	1H	90	PRO	CG-CD	-16.04	0.96	1.50
32	1g	106	PRO	CG-CD	-9.89	1.17	1.50
16	1P	53	PRO	CG-CD	-8.49	1.21	1.50
8	1H	90	PRO	N-CD	8.00	1.58	1.47
8	1H	90	PRO	N-CA	-6.99	1.38	1.47
16	1P	274	PRO	CG-CD	-5.37	1.32	1.50

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1H	90	PRO	CB-CG-CD	-33.10	0.16	106.10
8	1H	90	PRO	CA-N-CD	-18.18	86.54	112.00
39	1n	24	ARG	CA-C-N	14.33	147.50	121.70
39	1n	24	ARG	C-N-CA	14.33	147.50	121.70
32	1g	106	PRO	CA-N-CD	-12.98	93.83	112.00
16	1P	274	PRO	CA-N-CD	-12.43	94.60	112.00
8	1H	90	PRO	CA-CB-CG	-11.85	81.99	104.50
35	1j	52	PRO	CA-N-CD	-11.68	95.65	112.00
16	1P	53	PRO	CA-N-CD	-11.50	95.89	112.00
34	1i	35	PRO	CA-N-CD	-11.11	96.45	112.00
32	1g	106	PRO	N-CD-CG	-9.71	88.63	103.20
8	1H	90	PRO	N-CA-CB	-9.04	93.75	103.25
16	1P	53	PRO	N-CD-CG	-8.97	89.75	103.20
15	1O	165	PRO	CA-N-CD	-8.57	100.00	112.00
12	1L	236	ALA	CA-C-N	-8.20	105.91	122.31
12	1L	236	ALA	C-N-CA	-8.20	105.91	122.31
20	1U	20	LYS	N-CA-C	-6.96	104.40	113.17
22	1W	54	ILE	CG1-CB-CG2	-6.90	90.00	110.70
16	1P	274	PRO	N-CD-CG	-6.84	92.94	103.20
32	1g	115	PRO	CA-N-CD	-6.63	102.72	112.00
16	1P	53	PRO	CA-CB-CG	-6.41	92.32	104.50
32	1g	106	PRO	CA-CB-CG	-6.36	92.42	104.50
14	1N	251	MET	CA-CB-CG	6.25	126.59	114.10
11	1K	10	MET	CA-CB-CG	5.75	125.61	114.10
14	1N	10	ILE	CB-CG1-CD1	5.57	125.51	113.80
38	1m	33	ALA	CB-CA-C	-5.46	109.29	115.79
39	1n	113	MET	CA-CB-CG	5.46	125.02	114.10
2	1B	48	MET	CB-CG-SD	5.39	128.86	112.70
42	1q	1	MET	CB-CG-SD	5.15	128.16	112.70
14	1N	10	ILE	CA-CB-CG1	5.13	119.13	110.40
13	1M	325	MET	CA-CB-CG	5.12	124.34	114.10
14	1N	245	MET	CB-CG-SD	5.09	127.98	112.70
4	1D	122	VAL	CA-C-N	-5.06	113.22	122.38
4	1D	122	VAL	C-N-CA	-5.06	113.22	122.38
22	1W	58	GLN	CA-CB-CG	5.04	124.18	114.10
32	1g	106	PRO	N-CA-CB	-5.02	97.98	103.25

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	1D	74	ARG	Sidechain
8	1H	90	PRO	Peptide

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Mol	Chain	Res	Type	Group
21	1V	113	TRP	Peptide
22	1W	23	ARG	Sidechain
34	1i	99	ARG	Sidechain
39	1n	42	LEU	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	916	0	950	81	0
2	1B	1242	0	1248	122	0
3	1C	1740	0	1691	83	0
4	1D	3452	0	3389	239	0
5	1E	1658	0	1662	106	0
6	1F	3325	0	3288	210	0
7	1G	5362	0	5388	257	0
8	1H	2504	0	2602	194	0
9	1I	1412	0	1366	94	0
10	1J	1339	0	1337	124	0
11	1K	750	0	798	90	0
12	1L	4818	0	4956	414	0
13	1M	3632	0	3836	303	0
14	1N	2712	0	2873	220	0
15	1O	2590	0	2556	171	0
16	1P	2751	0	2776	134	0
17	1Q	1047	0	1042	59	0
18	1R	741	0	704	30	0
19	1S	700	0	719	43	0
20	1T	689	0	687	65	0
20	1U	694	0	691	74	0
21	1V	927	0	972	64	0
22	1W	971	0	975	93	0
23	1X	1398	0	1378	66	0
24	1Y	1016	0	1020	65	0
25	1Z	1168	0	1161	77	0
26	1a	562	0	557	32	0
27	1b	643	0	645	37	0
28	1c	417	0	425	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
29	1d	996	0	989	48	0
30	1e	816	0	823	57	0
31	1f	487	0	498	34	0
32	1g	835	0	795	100	0
33	1h	1151	0	1164	77	0
34	1i	1100	0	1106	115	0
35	1j	601	0	546	55	0
36	1k	649	0	626	60	0
37	1l	1310	0	1204	101	0
38	1m	1062	0	1075	84	0
39	1n	1495	0	1434	110	0
40	1o	1045	0	1018	90	0
41	1p	1449	0	1416	136	0
42	1q	1212	0	1173	46	0
43	1r	767	0	791	42	0
44	1s	382	0	351	30	0
45	1B	8	0	0	1	0
45	1F	8	0	0	1	0
45	1G	16	0	0	2	0
45	1I	16	0	0	2	0
46	1B	34	0	42	4	0
46	1d	39	0	47	6	0
46	1q	48	0	70	2	0
47	1D	63	0	90	19	0
48	1E	4	0	0	1	0
48	1G	4	0	0	4	0
49	1F	31	0	19	1	0
50	1G	1	0	0	0	0
51	1L	15	0	27	2	0
52	1M	38	0	50	2	0
53	1N	67	0	76	8	0
53	1a	61	0	64	6	0
54	1O	32	0	12	3	0
55	1O	1	0	0	0	0
56	1P	48	0	26	6	0
57	1R	1	0	0	0	0
58	1W	37	0	0	1	0
58	1n	37	0	0	1	0
All	All	67142	0	67224	3999	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 30.

All (3999) 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)
7:1G:69:CYS:HB3	48:1G:803:FES:S2	1.92	1.08
13:1M:263:MET:HA	13:1M:266:MET:HE2	1.46	0.97
24:1Y:94:CYS:HB2	24:1Y:114:CYS:HA	1.46	0.96
32:1g:105:LEU:HD22	32:1g:106:PRO:HD3	1.49	0.94
14:1N:248:LEU:HA	14:1N:251:MET:HG2	1.47	0.94
34:1i:99:ARG:CZ	41:1p:117:GLY:HA2	1.98	0.94
32:1g:100:ARG:HD3	32:1g:107:LEU:HA	1.46	0.93
22:1W:52:LEU:HB3	22:1W:54:ILE:HG22	1.47	0.93
10:1J:103:MET:HE1	11:1K:6:MET:HE2	1.50	0.93
11:1K:43:MET:HE3	11:1K:47:ILE:HD11	1.53	0.89
2:1B:62:MET:HE3	2:1B:156:LEU:HD22	1.56	0.88
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.55	0.88
13:1M:68:LEU:HD23	13:1M:72:LEU:HD11	1.56	0.88
42:1q:75:TRP:HZ2	46:1q:201:PC1:H2	1.37	0.87
7:1G:376:VAL:O	7:1G:450:MET:HB2	1.74	0.87
39:1n:24:ARG:H	39:1n:25:HIS:HB2	1.37	0.87
12:1L:100:ILE:HD13	12:1L:246:LEU:HB2	1.57	0.87
4:1D:72:MET:O	4:1D:74:ARG:NH1	2.07	0.87
20:1T:6:LEU:HD13	20:1T:86:VAL:HG22	1.57	0.86
10:1J:118:LYS:HE3	10:1J:118:LYS:HA	1.56	0.86
20:1T:80:ILE:HA	20:1T:83:LYS:HG2	1.58	0.86
7:1G:275:LYS:HA	42:1q:134:ILE:HG13	1.57	0.85
12:1L:49:VAL:HG13	12:1L:50:PRO:HD3	1.58	0.85
4:1D:169:TRP:HE1	8:1H:32:GLN:HA	1.40	0.85
37:1l:30:ARG:NH1	38:1m:31:ALA:O	2.09	0.85
24:1Y:104:THR:O	24:1Y:105:ARG:NH1	2.11	0.84
2:1B:62:MET:HE2	2:1B:157:LEU:HD12	1.60	0.84
8:1H:281:ARG:NE	8:1H:284:GLN:OE1	2.10	0.84
20:1U:37:MET:HE3	20:1U:71:MET:HE3	1.60	0.83
1:1A:63:LEU:HD12	10:1J:66:VAL:HG21	1.60	0.83
7:1G:101:HIS:CD2	45:1G:801:SF4:S4	2.71	0.83
21:1V:67:LEU:O	21:1V:71:LEU:HB2	1.78	0.83
12:1L:203:MET:HB2	41:1p:113:GLN:HG3	1.60	0.83
6:1F:106:LYS:HB3	6:1F:257:ASN:HD21	1.44	0.83
1:1A:57:LEU:HD21	10:1J:169:MET:HE1	1.61	0.83
12:1L:380:LEU:HD13	12:1L:419:THR:HG22	1.61	0.82
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.60	0.82
23:1X:3:ILE:HG22	23:1X:4:VAL:HG13	1.61	0.82
14:1N:36:ASN:ND2	14:1N:134:GLN:OE1	2.12	0.82
13:1M:14:MET:HG3	31:1f:12:VAL:HB	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:114:ARG:HG3	40:1o:117:ARG:HH21	1.43	0.82
4:1D:65:VAL:HG21	22:1W:97:TRP:HE1	1.44	0.82
12:1L:286:LEU:HB2	12:1L:411:MET:HE2	1.61	0.81
13:1M:10:MET:HE1	31:1f:15:LEU:HB2	1.62	0.81
10:1J:127:ILE:HG13	11:1K:2:PRO:HG3	1.63	0.81
41:1p:116:GLU:O	41:1p:119:SER:OG	1.99	0.81
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.61	0.80
32:1g:82:ASP:H	33:1h:67:PHE:HE2	1.30	0.80
34:1i:22:LEU:HA	34:1i:25:GLN:HG2	1.63	0.80
16:1P:134:HIS:H	16:1P:149:LYS:HE3	1.44	0.80
20:1T:58:PHE:HB2	20:1T:60:PHE:HE2	1.47	0.79
14:1N:236:LYS:HB2	14:1N:311:MET:HE1	1.64	0.79
34:1i:85:LEU:HA	34:1i:89:VAL:HB	1.64	0.79
7:1G:27:LEU:HD13	7:1G:37:ILE:HB	1.62	0.79
29:1d:107:LYS:HA	29:1d:107:LYS:HE3	1.64	0.79
3:1C:93:VAL:HG12	3:1C:108:LYS:HG2	1.65	0.79
7:1G:243:ARG:HG2	7:1G:248:MET:HE2	1.63	0.79
14:1N:7:THR:HA	53:1N:401:CDL:H142	1.65	0.79
17:1Q:16:LYS:HE2	17:1Q:16:LYS:HA	1.64	0.78
1:1A:54:LYS:HZ1	4:1D:70:GLY:HA3	1.48	0.78
40:1o:59:ALA:HA	40:1o:62:LEU:HD13	1.65	0.78
14:1N:237:MET:HB3	14:1N:240:ILE:HB	1.66	0.78
23:1X:24:LEU:HB3	25:1Z:71:LEU:HD21	1.65	0.78
11:1K:70:GLU:OE1	14:1N:34:GLU:HG2	1.83	0.78
12:1L:15:LEU:HD11	12:1L:122:VAL:HG13	1.65	0.78
11:1K:96:LEU:HD12	14:1N:54:GLU:HB3	1.66	0.78
12:1L:338:MET:HE2	12:1L:458:LEU:HD12	1.64	0.78
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.66	0.78
34:1i:94:TYR:HE2	41:1p:108:ARG:HA	1.48	0.77
4:1D:281:VAL:HG11	4:1D:310:ILE:HG23	1.66	0.77
7:1G:615:THR:OG1	7:1G:616:LEU:N	2.16	0.77
20:1T:69:LYS:NZ	20:1T:69:LYS:O	2.17	0.77
34:1i:9:LEU:HA	34:1i:12:GLN:HE21	1.47	0.77
20:1T:58:PHE:HB2	20:1T:60:PHE:CE2	2.19	0.77
4:1D:413:ASP:OD1	8:1H:281:ARG:NH1	2.16	0.77
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.03	0.77
15:1O:62:THR:O	28:1c:5:ARG:NH1	2.18	0.77
20:1T:42:LEU:HB3	20:1T:46:ASP:HB2	1.64	0.77
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.67	0.77
12:1L:72:GLN:HG2	12:1L:73:THR:HG23	1.66	0.77
13:1M:14:MET:HB2	31:1f:15:LEU:HD11	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:35:CYS:O	23:1X:39:ASN:ND2	2.17	0.77
2:1B:71:ARG:HH12	9:1I:49:ASN:HA	1.48	0.77
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.66	0.77
15:1O:69:LEU:HB3	15:1O:73:LEU:HD23	1.67	0.77
20:1U:22:TYR:HA	36:1k:46:ARG:HH21	1.50	0.77
13:1M:433:GLU:HB3	13:1M:437:MET:HE1	1.67	0.76
19:1S:64:LEU:HB2	19:1S:78:LEU:HD11	1.67	0.76
2:1B:116:MET:HG3	2:1B:151:PRO:HG2	1.67	0.76
14:1N:315:TRP:HH2	15:1O:292:VAL:HG23	1.49	0.76
28:1c:40:LEU:HA	28:1c:43:LYS:NZ	2.00	0.75
38:1m:18:ASP:HB2	38:1m:21:GLU:HG3	1.66	0.75
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.50	0.75
6:1F:190:THR:HB	6:1F:204:ARG:HG2	1.68	0.75
14:1N:215:MET:HA	14:1N:215:MET:HE2	1.68	0.75
3:1C:120:SER:O	3:1C:122:THR:N	2.19	0.75
10:1J:18:VAL:HG11	10:1J:96:GLY:HA3	1.66	0.75
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.68	0.75
44:1s:37:THR:HG23	44:1s:39:ARG:HH22	1.52	0.75
13:1M:42:LEU:HD12	13:1M:453:MET:HB3	1.69	0.75
14:1N:159:MET:HA	14:1N:159:MET:HE2	1.67	0.75
28:1c:27:LEU:HD12	29:1d:70:PHE:HD1	1.50	0.75
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.66	0.75
14:1N:321:LYS:HG3	14:1N:323:MET:HG2	1.69	0.75
41:1p:109:LEU:HD11	41:1p:128:LEU:HA	1.66	0.75
3:1C:32:ILE:HG22	3:1C:33:LEU:HG	1.69	0.75
4:1D:148:LEU:HD23	4:1D:174:ARG:HG2	1.67	0.75
19:1S:15:LEU:HA	19:1S:68:TYR:HA	1.67	0.75
42:1q:58:ARG:HD3	43:1r:1:ALA:HA	1.68	0.75
5:1E:104:THR:HG23	6:1F:349:ARG:HE	1.52	0.74
18:1R:81:THR:HG22	18:1R:92:ARG:HD3	1.69	0.74
12:1L:82:MET:HE3	12:1L:82:MET:H	1.52	0.74
15:1O:138:MET:HG3	15:1O:143:PHE:HB2	1.69	0.74
40:1o:114:ARG:HA	40:1o:117:ARG:HE	1.50	0.74
7:1G:366:THR:HG22	7:1G:488:LYS:HB2	1.69	0.74
15:1O:139:TYR:HB3	15:1O:140:ARG:HH12	1.52	0.74
20:1U:37:MET:HE3	20:1U:37:MET:H	1.51	0.74
34:1i:42:MET:N	34:1i:42:MET:SD	2.61	0.74
39:1n:21:ARG:O	39:1n:25:HIS:ND1	2.20	0.74
2:1B:114:VAL:HG12	2:1B:144:ILE:HB	1.70	0.74
10:1J:172:THR:HA	11:1K:80:MET:HE2	1.69	0.74
3:1C:150:ARG:HH22	3:1C:155:TYR:HA	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:112:LYS:HG2	21:1V:114:PRO:HD2	1.70	0.74
8:1H:276:SER:HB3	9:1I:37:THR:HG21	1.67	0.73
12:1L:203:MET:HE2	41:1p:109:LEU:HD13	1.70	0.73
13:1M:379:LEU:HA	13:1M:382:ILE:HG12	1.69	0.73
12:1L:123:LEU:HB2	12:1L:150:MET:HE2	1.68	0.73
6:1F:175:VAL:O	44:1s:62:ARG:NH2	2.21	0.73
4:1D:111:MET:N	4:1D:111:MET:SD	2.61	0.73
6:1F:298:ILE:HG12	6:1F:335:ILE:HB	1.70	0.73
6:1F:365:CYS:HB2	45:1F:502:SF4:S2	2.27	0.73
1:1A:44:MET:HE1	8:1H:126:LYS:HZ2	1.54	0.73
7:1G:232:ASP:OD1	7:1G:234:VAL:N	2.21	0.73
14:1N:128:LEU:O	14:1N:132:THR:OG1	2.05	0.73
20:1T:46:ASP:HA	20:1T:49:GLU:HB2	1.70	0.73
39:1n:82:PRO:HA	39:1n:88:THR:H	1.53	0.73
20:1T:55:GLU:OE1	20:1T:55:GLU:N	2.20	0.73
38:1m:110:LYS:HA	38:1m:113:LYS:HZ2	1.53	0.73
36:1k:48:GLU:HG2	36:1k:51:ARG:HB2	1.71	0.73
16:1P:274:PRO:HD2	16:1P:275:PHE:HD2	1.54	0.72
4:1D:179:GLU:OE1	43:1r:26:ARG:NH1	2.22	0.72
20:1U:21:LEU:HA	36:1k:18:TYR:CE1	2.25	0.72
31:1f:5:GLN:N	31:1f:5:GLN:OE1	2.22	0.72
6:1F:81:PHE:O	6:1F:84:LYS:NZ	2.21	0.72
12:1L:171:ALA:HA	12:1L:232:TRP:HB2	1.71	0.72
34:1i:9:LEU:HA	34:1i:12:GLN:NE2	2.04	0.72
6:1F:247:ARG:NH1	6:1F:318:ASP:OD2	2.22	0.72
2:1B:162:GLN:NE2	9:1I:140:SER:O	2.22	0.72
4:1D:233:ARG:NH1	9:1I:24:THR:O	2.23	0.72
33:1h:70:PRO:HA	33:1h:73:ARG:HD2	1.72	0.72
34:1i:84:TYR:O	34:1i:89:VAL:N	2.21	0.72
3:1C:21:GLN:NE2	43:1r:97:ALA:HA	2.05	0.72
6:1F:272:MET:HE1	6:1F:318:ASP:HA	1.72	0.72
20:1T:26:ASP:HB3	20:1T:29:LYS:HE3	1.71	0.71
13:1M:80:SER:HB3	13:1M:84:LEU:HD23	1.72	0.71
16:1P:315:ILE:HD11	16:1P:319:ARG:HH21	1.54	0.71
33:1h:73:ARG:HH22	41:1p:62:TYR:HB3	1.55	0.71
11:1K:96:LEU:HB2	14:1N:54:GLU:HG2	1.72	0.71
21:1V:71:LEU:HD13	21:1V:79:VAL:HG11	1.73	0.71
32:1g:49:LYS:HA	32:1g:49:LYS:HE3	1.72	0.71
22:1W:24:ASP:OD1	22:1W:25:MET:N	2.22	0.71
27:1b:59:ASP:H	27:1b:62:MET:HE1	1.55	0.71
24:1Y:104:THR:C	24:1Y:105:ARG:HD3	2.16	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:362:TYR:OH	19:1S:55:ARG:NH1	2.24	0.71
16:1P:92:ILE:HD11	16:1P:218:ILE:HD11	1.72	0.71
4:1D:173:GLU:HA	4:1D:176:LYS:HD3	1.72	0.71
35:1j:54:PRO:HB2	35:1j:59:TRP:HZ2	1.54	0.71
6:1F:300:GLY:HA2	6:1F:333:ALA:H	1.56	0.71
15:1O:94:TYR:CD2	15:1O:282:ILE:HD11	2.26	0.71
21:1V:81:LEU:HD13	21:1V:85:ASN:HD21	1.56	0.71
32:1g:120:LEU:HD22	41:1p:162:MET:HE3	1.72	0.71
15:1O:176:VAL:HA	15:1O:179:ILE:HD12	1.73	0.70
32:1g:91:ARG:HH21	32:1g:92:GLU:HB3	1.56	0.70
2:1B:86:MET:HB2	2:1B:113:VAL:HG22	1.72	0.70
16:1P:171:ILE:HG13	56:1P:501:NDP:H42N	1.73	0.70
21:1V:75:GLN:OE1	21:1V:75:GLN:N	2.25	0.70
1:1A:97:LEU:HD21	10:1J:162:LEU:HB2	1.73	0.70
11:1K:59:MET:HG2	14:1N:27:LEU:HD22	1.74	0.70
14:1N:339:MET:HE3	29:1d:34:MET:HE2	1.72	0.70
32:1g:70:LEU:O	32:1g:74:SER:OG	2.10	0.70
7:1G:238:ILE:O	7:1G:253:ARG:NH1	2.23	0.70
5:1E:153:MET:HA	5:1E:164:LEU:HD23	1.74	0.70
13:1M:72:LEU:HB3	13:1M:76:MET:HE1	1.71	0.70
16:1P:183:ALA:O	16:1P:251:ARG:NH2	2.24	0.70
5:1E:82:GLU:OE1	6:1F:200:GLN:NE2	2.24	0.70
7:1G:13:VAL:HG23	7:1G:79:ILE:HB	1.73	0.70
7:1G:190:MET:HB2	7:1G:695:ILE:HG22	1.74	0.70
7:1G:379:LEU:HB2	7:1G:408:LEU:HB2	1.74	0.70
11:1K:10:MET:HE1	11:1K:14:ILE:HG23	1.73	0.70
13:1M:31:SER:HB3	13:1M:73:LEU:HD12	1.73	0.70
10:1J:169:MET:HE2	10:1J:169:MET:HA	1.74	0.70
11:1K:2:PRO:HD3	30:1e:72:MET:HE1	1.73	0.70
12:1L:360:GLY:HA2	12:1L:435:PRO:HA	1.74	0.70
23:1X:134:ARG:O	27:1b:57:ARG:NH2	2.24	0.70
41:1p:41:ASP:O	41:1p:45:THR:OG1	2.09	0.70
2:1B:48:MET:HE1	4:1D:54:GLN:HE21	1.57	0.70
4:1D:173:GLU:OE2	4:1D:221:ARG:NH1	2.25	0.70
12:1L:234:PRO:HA	12:1L:237:MET:HE1	1.74	0.70
23:1X:150:ASN:ND2	33:1h:124:GLN:OE1	2.25	0.70
40:1o:74:PRO:HD3	41:1p:28:PRO:HD3	1.73	0.70
34:1i:54:ALA:HB3	34:1i:57:LYS:HG3	1.74	0.70
42:1q:6:VAL:O	42:1q:9:ARG:NH2	2.25	0.70
32:1g:88:TRP:CD1	32:1g:91:ARG:HH22	2.10	0.69
14:1N:342:ALA:HB3	46:1d:201:PC1:H3D2	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:76:ILE:HD13	34:1i:79:TRP:HD1	1.57	0.69
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.73	0.69
8:1H:141:SER:HB2	8:1H:289:LEU:HD21	1.73	0.69
14:1N:26:TRP:HB3	14:1N:74:ILE:HD12	1.73	0.69
20:1T:12:LYS:HZ2	20:1T:74:GLN:HE22	1.37	0.69
20:1U:20:LYS:HG3	20:1U:30:LEU:HD11	1.72	0.69
34:1i:10:ARG:HE	39:1n:153:LEU:HD22	1.58	0.69
7:1G:434:SER:OG	7:1G:436:ASN:ND2	2.24	0.69
10:1J:173:ARG:HH22	15:1O:254:ARG:HG2	1.56	0.69
8:1H:144:VAL:O	8:1H:148:ILE:HD12	1.92	0.69
12:1L:535:ARG:HE	37:1l:98:TRP:HZ3	1.39	0.69
32:1g:114:ASP:OD2	32:1g:116:ASN:ND2	2.26	0.69
7:1G:684:MET:HA	7:1G:684:MET:HE3	1.73	0.69
13:1M:48:ASN:HD21	33:1h:90:THR:HG21	1.56	0.69
1:1A:90:MET:HE1	10:1J:151:THR:HA	1.74	0.69
4:1D:65:VAL:HG21	22:1W:97:TRP:NE1	2.07	0.69
37:1l:29:MET:HB3	37:1l:76:PRO:HG3	1.74	0.69
37:1l:112:MET:HB3	37:1l:116:PHE:HE2	1.58	0.69
21:1V:87:LEU:HD21	21:1V:91:ARG:HH21	1.58	0.69
28:1c:15:LEU:O	28:1c:19:LEU:HD12	1.92	0.69
4:1D:20:TYR:HB3	12:1L:571:MET:HE1	1.74	0.69
13:1M:23:ILE:HD11	13:1M:92:LYS:HD2	1.73	0.69
23:1X:5:GLU:HG3	23:1X:53:ARG:HD3	1.74	0.69
32:1g:96:LEU:HD23	32:1g:100:ARG:HD2	1.75	0.69
11:1K:40:LEU:HD21	14:1N:72:MET:HE2	1.76	0.68
13:1M:459:TYR:HB3	32:1g:84:ARG:HD2	1.75	0.68
15:1O:13:ARG:H	15:1O:16:ARG:HH21	1.39	0.68
2:1B:48:MET:HE3	2:1B:48:MET:O	1.92	0.68
3:1C:160:HIS:HB2	3:1C:163:ARG:HD2	1.72	0.68
20:1T:12:LYS:HE2	20:1T:77:VAL:HG11	1.74	0.68
21:1V:81:LEU:O	21:1V:85:ASN:ND2	2.26	0.68
5:1E:153:MET:HB2	5:1E:161:TYR:O	1.93	0.68
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.74	0.68
13:1M:393:ILE:HA	13:1M:396:MET:HG2	1.75	0.68
10:1J:46:ASN:HA	25:1Z:141:ILE:HG21	1.75	0.68
13:1M:76:MET:HB3	13:1M:229:MET:HE2	1.75	0.68
6:1F:89:ARG:NH2	6:1F:212:ASP:O	2.27	0.68
14:1N:44:LEU:HG	14:1N:122:ILE:HG21	1.75	0.68
35:1j:11:TYR:HB3	36:1k:16:PRO:HD3	1.74	0.68
8:1H:117:LEU:HD23	8:1H:118:TRP:H	1.58	0.68
15:1O:94:TYR:HD1	15:1O:144:ILE:HD13	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.11	0.68
3:1C:94:TYR:HB2	3:1C:107:VAL:HG22	1.74	0.68
12:1L:81:LYS:HB3	12:1L:262:ARG:HH22	1.58	0.68
15:1O:145:ARG:HH22	15:1O:280:PRO:HD2	1.58	0.68
38:1m:102:TYR:HA	38:1m:105:LYS:HE3	1.76	0.68
7:1G:648:LEU:HD21	19:1S:44:LYS:HG2	1.76	0.68
12:1L:113:PHE:HB3	12:1L:116:ARG:HB3	1.75	0.68
17:1Q:16:LYS:HD3	17:1Q:17:LEU:H	1.59	0.68
20:1U:18:VAL:HA	20:1U:21:LEU:HD23	1.76	0.68
1:1A:8:LEU:O	1:1A:12:THR:HG23	1.93	0.68
8:1H:76:ILE:O	8:1H:80:SER:OG	2.09	0.68
13:1M:263:MET:HE1	38:1m:97:LEU:HD13	1.74	0.67
15:1O:128:ILE:O	15:1O:156:LYS:NZ	2.26	0.67
32:1g:87:GLU:OE2	32:1g:87:GLU:N	2.25	0.67
2:1B:66:ARG:HG3	9:1I:48:ILE:HD13	1.76	0.67
15:1O:97:GLN:HG2	15:1O:135:LEU:HB2	1.76	0.67
23:1X:83:GLU:HG3	23:1X:102:GLN:HG2	1.76	0.67
25:1Z:127:LEU:HD23	30:1e:82:ARG:HD2	1.74	0.67
2:1B:69:MET:HE3	2:1B:76:PHE:HB2	1.76	0.67
4:1D:241:ASP:OD2	4:1D:290:ARG:NH1	2.26	0.67
7:1G:190:MET:HE2	7:1G:192:MET:SD	2.34	0.67
8:1H:209:SER:HB3	8:1H:213:VAL:HG13	1.77	0.67
22:1W:34:GLU:OE1	22:1W:34:GLU:N	2.27	0.67
23:1X:131:LYS:HG3	27:1b:58:ASP:HB3	1.76	0.67
1:1A:67:LEU:HD12	11:1K:65:VAL:HA	1.75	0.67
5:1E:82:GLU:HB3	6:1F:200:GLN:HE21	1.60	0.67
5:1E:87:TYR:HD1	6:1F:181:ALA:HB3	1.59	0.67
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	1.75	0.67
24:1Y:127:GLY:HA2	24:1Y:132:TRP:HB2	1.76	0.67
7:1G:533:THR:HA	7:1G:556:MET:HE1	1.76	0.67
26:1a:21:MET:N	26:1a:21:MET:SD	2.67	0.67
39:1n:45:ALA:O	39:1n:49:GLU:N	2.28	0.67
42:1q:122:GLN:OE1	42:1q:122:GLN:N	2.27	0.67
8:1H:33:LEU:HD11	43:1r:24:GLN:HE21	1.58	0.67
8:1H:102:VAL:HG11	8:1H:154:LEU:HD11	1.75	0.67
53:1N:401:CDL:H741	53:1N:401:CDL:H541	1.75	0.67
20:1T:20:LYS:HE2	20:1T:27:PRO:HG3	1.74	0.67
4:1D:239:THR:HG23	4:1D:293:CYS:HB3	1.77	0.67
14:1N:28:LEU:HA	14:1N:31:ILE:HD12	1.77	0.67
4:1D:303:GLU:O	4:1D:307:SER:OG	2.11	0.67
6:1F:20:ARG:HD3	6:1F:269:GLU:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:145:GLU:N	9:1I:145:GLU:OE2	2.26	0.67
13:1M:422:HIS:ND1	38:1m:59:ILE:O	2.28	0.67
12:1L:362:LEU:O	12:1L:366:MET:N	2.28	0.67
15:1O:280:PRO:HB3	32:1g:25:ARG:HA	1.76	0.67
7:1G:649:SER:O	7:1G:651:LEU:N	2.28	0.67
9:1I:152:GLU:HG2	18:1R:35:VAL:HA	1.76	0.67
13:1M:19:LYS:HD2	13:1M:22:MET:HE3	1.76	0.67
14:1N:243:LEU:HA	14:1N:246:VAL:HG12	1.77	0.67
25:1Z:125:TYR:HB3	25:1Z:133:ILE:HG22	1.76	0.67
10:1J:55:MET:HE2	10:1J:55:MET:HA	1.77	0.66
12:1L:331:MET:HA	12:1L:334:PHE:HD2	1.60	0.66
13:1M:231:LEU:HD12	13:1M:235:LEU:HD21	1.77	0.66
13:1M:270:ILE:O	13:1M:274:SER:N	2.26	0.66
35:1j:12:ARG:NH1	36:1k:47:ASN:O	2.28	0.66
39:1n:30:CYS:HB2	39:1n:35:LYS:HB3	1.77	0.66
4:1D:427:GLU:N	4:1D:427:GLU:OE1	2.27	0.66
5:1E:37:ASN:OD1	44:1s:62:ARG:NH1	2.28	0.66
12:1L:90:ILE:HD12	12:1L:91:PRO:HD3	1.77	0.66
16:1P:324:TYR:HA	16:1P:327:LEU:HB2	1.77	0.66
27:1b:51:ASN:HB3	33:1h:139:THR:HG22	1.77	0.66
5:1E:120:ILE:HD12	5:1E:173:ILE:HD11	1.76	0.66
7:1G:470:VAL:HG12	7:1G:490:MET:HE1	1.78	0.66
19:1S:72:GLN:OE1	19:1S:72:GLN:N	2.29	0.66
40:1o:95:VAL:O	40:1o:99:LYS:HB3	1.94	0.66
8:1H:88:PRO:O	8:1H:90:PRO:HG2	1.94	0.66
13:1M:76:MET:HB2	13:1M:226:ALA:HB1	1.78	0.66
13:1M:410:MET:HE1	13:1M:411:LEU:HD23	1.77	0.66
4:1D:14:PHE:HA	4:1D:19:MET:HB2	1.77	0.66
4:1D:398:HIS:HB3	4:1D:421:GLN:OE1	1.95	0.66
10:1J:23:LYS:HE3	10:1J:23:LYS:HA	1.76	0.66
15:1O:94:TYR:OH	15:1O:151:HIS:ND1	2.26	0.66
29:1d:99:GLU:OE2	29:1d:99:GLU:N	2.25	0.66
32:1g:62:PHE:HA	32:1g:66:PHE:HD1	1.61	0.66
32:1g:111:ASN:HA	41:1p:161:ARG:HH12	1.61	0.66
41:1p:125:ALA:O	41:1p:129:GLU:N	2.25	0.66
2:1B:107:MET:HG2	2:1B:111:ARG:HB3	1.76	0.66
6:1F:179:ARG:HD3	44:1s:51:PHE:HE1	1.60	0.66
7:1G:19:MET:HA	7:1G:19:MET:HE3	1.77	0.66
7:1G:192:MET:HA	7:1G:192:MET:HE3	1.78	0.66
8:1H:117:LEU:HD12	10:1J:68:PHE:CG	2.30	0.66
19:1S:18:ILE:HB	19:1S:52:ILE:HD13	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:13:ARG:HB2	15:1O:16:ARG:HE	1.59	0.66
37:1l:97:SER:O	37:1l:100:THR:OG1	2.12	0.66
40:1o:114:ARG:HA	40:1o:117:ARG:NE	2.10	0.66
4:1D:150:HIS:HB3	4:1D:304:MET:HE2	1.77	0.66
13:1M:356:ALA:HB2	13:1M:415:GLN:HE21	1.60	0.66
14:1N:251:MET:HB3	14:1N:293:TYR:CE1	2.31	0.66
41:1p:74:THR:OG1	41:1p:75:GLU:OE1	2.13	0.66
4:1D:300:ARG:NH2	4:1D:420:THR:O	2.29	0.66
12:1L:257:VAL:HG11	12:1L:313:MET:HB2	1.78	0.66
7:1G:16:GLN:OE1	7:1G:16:GLN:N	2.28	0.66
13:1M:342:MET:HE2	13:1M:413:THR:HG23	1.77	0.66
14:1N:73:ALA:HB1	14:1N:98:MET:HE2	1.78	0.66
14:1N:187:MET:HA	14:1N:190:MET:HE2	1.77	0.66
36:1k:58:ASN:ND2	36:1k:58:ASN:O	2.29	0.66
41:1p:131:PHE:HA	41:1p:134:VAL:HG12	1.76	0.66
8:1H:114:TYR:HA	8:1H:117:LEU:HD22	1.77	0.65
16:1P:13:ARG:HB3	16:1P:64:ASP:HB2	1.78	0.65
12:1L:437:PHE:HE2	12:1L:441:VAL:HA	1.57	0.65
53:1a:101:CDL:HA62	42:1q:9:ARG:HH22	1.60	0.65
34:1i:1:SAC:O	34:1i:2:GLY:N	2.28	0.65
38:1m:9:ARG:HE	38:1m:10:LEU:HG	1.60	0.65
8:1H:28:LEU:HD21	8:1H:274:ARG:HD2	1.78	0.65
13:1M:388:TRP:O	38:1m:111:LYS:NZ	2.27	0.65
16:1P:45:VAL:HG22	16:1P:68:ILE:HA	1.76	0.65
20:1U:87:TYR:HD1	34:1i:22:LEU:HG	1.59	0.65
14:1N:237:MET:HA	14:1N:237:MET:HE3	1.78	0.65
23:1X:120:ASP:OD2	23:1X:121:LEU:N	2.29	0.65
31:1f:39:ASN:ND2	31:1f:39:ASN:O	2.28	0.65
37:1l:140:LEU:O	41:1p:122:GLN:NE2	2.29	0.65
41:1p:37:ASP:HA	41:1p:41:ASP:HB2	1.78	0.65
1:1A:60:ILE:HD13	11:1K:75:LEU:HD11	1.78	0.65
1:1A:85:LYS:O	1:1A:89:THR:HG23	1.96	0.65
12:1L:86:SER:O	12:1L:90:ILE:HG13	1.97	0.65
37:1l:69:LEU:HD11	37:1l:86:ARG:H	1.60	0.65
15:1O:30:ASN:HD22	15:1O:203:GLU:HG2	1.61	0.65
34:1i:100:LYS:NZ	41:1p:116:GLU:O	2.28	0.65
37:1l:14:PRO:HB2	37:1l:20:ARG:HD2	1.78	0.65
6:1F:138:ILE:HG21	6:1F:146:ALA:HB2	1.79	0.65
6:1F:146:ALA:HA	6:1F:149:LEU:HG	1.79	0.65
6:1F:215:VAL:HG22	6:1F:220:THR:HG21	1.79	0.65
7:1G:347:GLU:OE2	7:1G:495:ARG:NH1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:63:PRO:HB2	8:1H:66:SER:HB3	1.78	0.65
9:1I:106:THR:HG21	9:1I:109:TYR:HD1	1.62	0.65
14:1N:312:LYS:HA	14:1N:315:TRP:NE1	2.11	0.65
3:1C:199:LEU:HD13	4:1D:385:ARG:HE	1.62	0.65
6:1F:42:TRP:HE3	6:1F:45:THR:HG21	1.62	0.65
14:1N:309:ASN:ND2	15:1O:95:ARG:HG2	2.11	0.65
28:1c:40:LEU:HA	28:1c:43:LYS:HZ2	1.60	0.65
32:1g:95:ARG:NH1	32:1g:96:LEU:HB2	2.12	0.65
6:1F:41:ASP:HA	6:1F:236:ARG:HH12	1.61	0.65
12:1L:176:ARG:NE	13:1M:400:MET:O	2.30	0.65
26:1a:31:ASN:ND2	26:1a:60:TYR:OH	2.27	0.65
26:1a:52:ARG:NH1	26:1a:58:ASN:OD1	2.29	0.65
40:1o:110:ARG:HH22	40:1o:114:ARG:HD3	1.61	0.65
41:1p:6:LYS:HD2	41:1p:11:GLU:N	2.11	0.65
6:1F:426:LEU:O	6:1F:430:MET:HG3	1.96	0.65
7:1G:306:MET:SD	7:1G:542:PHE:HB2	2.37	0.65
10:1J:20:PHE:CZ	11:1K:32:CYS:HA	2.32	0.65
12:1L:303:ALA:O	12:1L:306:THR:OG1	2.15	0.65
14:1N:239:VAL:HG11	29:1d:47:ALA:HB1	1.79	0.65
34:1i:35:PRO:O	34:1i:35:PRO:HD2	1.97	0.65
39:1n:25:HIS:CD2	39:1n:74:GLN:HB2	2.31	0.65
4:1D:338:MET:HE1	4:1D:348:HIS:CD2	2.32	0.64
5:1E:120:ILE:HD13	5:1E:169:ILE:HD13	1.79	0.64
6:1F:398:GLN:HE21	7:1G:92:GLY:HA3	1.62	0.64
12:1L:295:GLN:HG3	12:1L:304:PHE:HE2	1.62	0.64
12:1L:415:ALA:O	12:1L:419:THR:OG1	2.15	0.64
17:1Q:127:ARG:NE	44:1s:75:HIS:O	2.30	0.64
35:1j:16:GLN:HE22	35:1j:18:THR:HG22	1.61	0.64
40:1o:113:ARG:O	40:1o:117:ARG:HG3	1.96	0.64
4:1D:410:MET:HE2	4:1D:410:MET:N	2.13	0.64
6:1F:32:ARG:NH1	44:1s:42:GLN:OE1	2.29	0.64
6:1F:348:ALA:HB2	6:1F:380:VAL:HG21	1.78	0.64
7:1G:6:SER:OG	7:1G:7:ASN:N	2.24	0.64
7:1G:623:LEU:HD21	7:1G:630:LEU:HB3	1.79	0.64
14:1N:65:THR:O	14:1N:69:MET:HG3	1.97	0.64
14:1N:244:MET:O	14:1N:248:LEU:HD23	1.98	0.64
39:1n:135:GLU:HB2	39:1n:164:PRO:HA	1.79	0.64
5:1E:113:SER:HA	5:1E:116:ILE:HD13	1.79	0.64
16:1P:54:TYR:O	16:1P:57:MET:HG2	1.97	0.64
32:1g:108:MET:HG3	41:1p:134:VAL:HA	1.78	0.64
34:1i:68:ILE:HA	34:1i:71:VAL:HG12	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:418:ILE:HA	4:1D:421:GLN:HB3	1.78	0.64
37:1l:9:PHE:O	37:1l:26:LYS:NZ	2.28	0.64
38:1m:102:TYR:O	38:1m:106:THR:OG1	2.11	0.64
41:1p:6:LYS:HD2	41:1p:11:GLU:H	1.62	0.64
6:1F:300:GLY:HA2	6:1F:333:ALA:N	2.13	0.64
8:1H:105:MET:HA	8:1H:108:MET:HE3	1.79	0.64
13:1M:355:MET:HE1	13:1M:437:MET:HE2	1.80	0.64
36:1k:42:ASP:O	36:1k:46:ARG:NH1	2.31	0.64
39:1n:25:HIS:O	39:1n:28:SER:N	2.30	0.64
4:1D:159:LEU:HD12	47:1D:501:U10:H8	1.79	0.64
6:1F:391:SER:HB3	43:1r:48:LEU:HD13	1.80	0.64
7:1G:276:ARG:HE	7:1G:277:GLN:HG2	1.63	0.64
7:1G:615:THR:N	7:1G:618:GLN:OE1	2.24	0.64
12:1L:90:ILE:HD12	12:1L:91:PRO:CD	2.27	0.64
15:1O:308:TYR:HA	15:1O:317:ILE:HD11	1.80	0.64
32:1g:66:PHE:HA	32:1g:70:LEU:HD23	1.79	0.64
37:1l:5:THR:OG1	37:1l:6:LYS:N	2.28	0.64
5:1E:34:ILE:HD13	5:1E:49:PRO:HB2	1.79	0.64
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.30	0.64
10:1J:59:ILE:HD13	11:1K:64:LEU:HD11	1.80	0.64
14:1N:97:MET:HA	14:1N:97:MET:HE2	1.80	0.64
15:1O:168:VAL:HG12	15:1O:219:GLU:HB2	1.80	0.64
17:1Q:11:ILE:HG12	22:1W:23:ARG:NH2	2.12	0.64
23:1X:103:GLN:NE2	23:1X:107:ASP:OD2	2.30	0.64
25:1Z:98:MET:HE2	25:1Z:98:MET:HA	1.79	0.64
29:1d:17:GLU:OE2	29:1d:17:GLU:N	2.25	0.64
1:1A:80:GLN:OE1	25:1Z:58:ARG:NH1	2.31	0.64
7:1G:426:PRO:HB2	7:1G:656:LEU:HD13	1.78	0.64
12:1L:349:SER:HB2	12:1L:443:ILE:HA	1.79	0.64
13:1M:190:TRP:CD2	24:1Y:126:MET:HE1	2.33	0.64
14:1N:17:THR:HG22	14:1N:21:MET:HE2	1.80	0.64
30:1e:36:GLU:HB2	30:1e:62:PHE:CE1	2.33	0.64
10:1J:174:GLY:HA2	14:1N:48:PHE:HE2	1.61	0.64
13:1M:45:LEU:HD21	33:1h:83:PRO:HB3	1.80	0.64
20:1T:79:TYR:HD1	20:1T:80:ILE:HD12	1.62	0.64
39:1n:128:ARG:HD3	39:1n:129:ARG:HH21	1.62	0.64
7:1G:649:SER:OG	7:1G:650:LYS:N	2.31	0.64
13:1M:153:THR:O	13:1M:157:SER:OG	2.15	0.64
15:1O:168:VAL:HG11	15:1O:241:LEU:HD13	1.79	0.64
28:1c:1:LYS:HD2	28:1c:2:PHE:HB2	1.80	0.64
29:1d:120:ARG:O	38:1m:108:ARG:NH1	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:48:LEU:HD11	31:1f:53:GLU:HA	1.78	0.64
36:1k:28:LEU:HD11	39:1n:37:ARG:HG3	1.78	0.64
37:1l:30:ARG:HG3	37:1l:33:ASP:OD2	1.98	0.64
39:1n:167:TRP:O	39:1n:171:THR:OG1	2.14	0.64
4:1D:170:MET:HE3	4:1D:225:LEU:HD12	1.79	0.63
11:1K:12:PHE:HD2	14:1N:72:MET:HE3	1.61	0.63
12:1L:3:PRO:HG2	41:1p:33:THR:HG22	1.80	0.63
13:1M:49:SER:O	13:1M:51:ASN:ND2	2.32	0.63
13:1M:84:LEU:O	13:1M:92:LYS:NZ	2.29	0.63
14:1N:152:ASN:O	14:1N:156:THR:HG22	1.97	0.63
16:1P:168:PRO:HA	16:1P:230:PHE:HB2	1.80	0.63
16:1P:194:ILE:HG13	16:1P:263:TYR:HD2	1.63	0.63
16:1P:328:THR:HB	22:1W:48:HIS:HE1	1.63	0.63
20:1U:14:ARG:NH1	35:1j:11:TYR:OH	2.29	0.63
20:1U:88:GLU:O	33:1h:6:LYS:NZ	2.32	0.63
34:1i:77:PRO:O	34:1i:81:ILE:HG22	1.98	0.63
37:1l:95:PRO:O	39:1n:71:TRP:NE1	2.24	0.63
4:1D:405:MET:HE2	4:1D:417:ILE:HG12	1.80	0.63
10:1J:60:TYR:OH	11:1K:34:GLU:O	2.15	0.63
12:1L:55:MET:HE1	12:1L:473:PRO:HD3	1.81	0.63
31:1f:45:LYS:HD3	31:1f:45:LYS:H	1.63	0.63
36:1k:41:ARG:NH2	36:1k:42:ASP:O	2.31	0.63
1:1A:113:TRP:NE1	8:1H:283:ASP:OD1	2.32	0.63
13:1M:334:TYR:O	13:1M:338:HIS:N	2.28	0.63
2:1B:27:GLU:OE2	2:1B:178:ARG:NH1	2.30	0.63
7:1G:609:MET:SD	7:1G:609:MET:N	2.70	0.63
14:1N:6:TYR:CE2	53:1N:401:CDL:H111	2.34	0.63
35:1j:38:TRP:CZ3	35:1j:39:ARG:HD2	2.33	0.63
1:1A:39:CYS:HG	8:1H:127:TYR:HH	1.42	0.63
3:1C:118:GLU:OE2	3:1C:144:ASN:ND2	2.25	0.63
6:1F:179:ARG:HD3	44:1s:51:PHE:CE1	2.34	0.63
8:1H:62:ARG:HH21	8:1H:64:GLY:HA2	1.63	0.63
12:1L:149:ILE:O	12:1L:153:LEU:HD12	1.98	0.63
12:1L:237:MET:H	12:1L:237:MET:HE3	1.63	0.63
12:1L:391:SER:OG	12:1L:392:LYS:N	2.31	0.63
36:1k:76:ALA:HA	36:1k:79:VAL:HG22	1.79	0.63
38:1m:110:LYS:HD3	38:1m:113:LYS:HZ1	1.63	0.63
2:1B:125:TYR:HB2	9:1I:117:ILE:HG21	1.80	0.63
6:1F:248:GLU:HG2	6:1F:249:ARG:HE	1.64	0.63
7:1G:415:LEU:O	7:1G:417:TYR:N	2.32	0.63
12:1L:342:CYS:O	12:1L:346:ILE:HG22	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:291:ARG:NE	32:1g:29:ASP:OD2	2.31	0.63
17:1Q:69:LEU:HB3	17:1Q:70:MET:SD	2.39	0.63
35:1j:64:LEU:HG	40:1o:103:ARG:HA	1.80	0.63
40:1o:42:GLN:HA	40:1o:45:MET:HE3	1.80	0.63
40:1o:67:LYS:HZ2	40:1o:70:ARG:HH22	1.46	0.63
4:1D:69:SER:H	4:1D:74:ARG:HH11	1.47	0.63
6:1F:46:LYS:NZ	6:1F:167:CYS:O	2.32	0.63
8:1H:20:LEU:HA	8:1H:23:VAL:HG22	1.80	0.63
12:1L:290:LEU:HA	12:1L:293:ILE:HG12	1.79	0.63
12:1L:363:TYR:HD2	12:1L:370:THR:HG21	1.64	0.63
19:1S:64:LEU:HB3	19:1S:76:VAL:HG13	1.81	0.63
20:1T:52:MET:HG3	22:1W:37:ARG:HD3	1.81	0.63
32:1g:112:CYS:HB3	41:1p:141:ARG:HH21	1.64	0.63
35:1j:65:GLY:HA3	40:1o:30:PHE:HE1	1.62	0.63
37:1l:97:SER:HB2	38:1m:6:LYS:HG2	1.80	0.63
3:1C:41:GLN:HB2	43:1r:67:ILE:HA	1.81	0.63
10:1J:3:MET:HE3	10:1J:3:MET:O	1.98	0.63
12:1L:373:LEU:HD22	12:1L:431:PHE:HE2	1.64	0.63
12:1L:532:ILE:HG13	37:1l:105:LEU:HD23	1.81	0.63
13:1M:115:LEU:HB2	13:1M:174:LEU:HB3	1.81	0.63
38:1m:49:GLN:HB2	38:1m:55:ARG:HD3	1.81	0.63
38:1m:95:GLY:O	38:1m:99:PHE:HB3	1.99	0.63
10:1J:127:ILE:HG22	11:1K:50:ASN:HD21	1.64	0.63
10:1J:156:VAL:O	10:1J:160:SER:OG	2.17	0.63
12:1L:32:TYR:HE2	12:1L:119:LYS:HB3	1.63	0.63
12:1L:90:ILE:O	12:1L:94:LEU:HD12	1.97	0.63
13:1M:386:PHE:HB2	13:1M:393:ILE:HD11	1.81	0.63
15:1O:52:PRO:O	15:1O:107:GLN:NE2	2.32	0.63
31:1f:40:LYS:HA	31:1f:40:LYS:HE3	1.79	0.63
38:1m:13:LEU:HD11	38:1m:17:LEU:HB2	1.81	0.63
2:1B:109:GLU:N	8:1H:59:GLU:OE1	2.32	0.62
4:1D:342:MET:HE2	7:1G:103:LEU:HD13	1.81	0.62
7:1G:377:ILE:HG13	7:1G:404:LEU:HD21	1.81	0.62
12:1L:335:PHE:O	12:1L:339:LEU:HD12	1.98	0.62
12:1L:341:MET:HA	12:1L:341:MET:HE3	1.79	0.62
13:1M:236:LEU:HD23	13:1M:294:MET:HG3	1.80	0.62
14:1N:216:PHE:HA	14:1N:219:LEU:HD23	1.80	0.62
16:1P:186:ARG:HB3	16:1P:251:ARG:HH21	1.63	0.62
37:1l:154:VAL:HB	40:1o:35:GLU:HG2	1.80	0.62
42:1q:135:GLN:NE2	42:1q:136:GLU:O	2.32	0.62
13:1M:435:ALA:O	13:1M:439:LEU:HD12	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:136:GLU:O	15:1O:140:ARG:NH1	2.32	0.62
20:1T:12:LYS:NZ	20:1T:74:GLN:HE22	1.95	0.62
20:1T:33:ASN:HA	20:1T:72:CYS:SG	2.38	0.62
20:1U:23:ASP:OD1	36:1k:41:ARG:NH2	2.29	0.62
39:1n:117:TYR:O	39:1n:120:LYS:HG3	1.99	0.62
14:1N:72:MET:SD	14:1N:76:ILE:HG12	2.39	0.62
14:1N:272:LYS:HZ2	33:1h:108:LEU:HD21	1.63	0.62
17:1Q:22:LEU:HD11	22:1W:81:LEU:HD12	1.82	0.62
42:1q:106:ARG:HG3	42:1q:109:ILE:HG13	1.81	0.62
12:1L:131:LEU:HB2	12:1L:143:GLY:HA3	1.82	0.62
12:1L:313:MET:HB3	12:1L:325:ALA:HB1	1.82	0.62
13:1M:389:SER:O	13:1M:391:ILE:N	2.32	0.62
23:1X:123:GLU:O	23:1X:126:LYS:NZ	2.31	0.62
1:1A:46:SER:HB2	8:1H:126:LYS:HD3	1.81	0.62
6:1F:43:TYR:HD2	6:1F:44:LYS:N	1.97	0.62
6:1F:344:VAL:HG12	6:1F:380:VAL:HG22	1.82	0.62
10:1J:23:LYS:HG3	11:1K:23:ARG:HB2	1.81	0.62
10:1J:114:GLU:HA	10:1J:118:LYS:NZ	2.13	0.62
13:1M:72:LEU:O	13:1M:75:LEU:N	2.29	0.62
24:1Y:125:LYS:O	24:1Y:129:LEU:HG	1.99	0.62
25:1Z:65:PHE:O	25:1Z:69:ILE:HD12	2.00	0.62
37:1l:138:LEU:O	37:1l:142:ARG:HG2	1.99	0.62
38:1m:122:GLN:HE21	41:1p:139:GLN:HG2	1.64	0.62
2:1B:51:GLY:HA2	2:1B:89:ALA:HB3	1.80	0.62
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.81	0.62
12:1L:89:PHE:HB2	12:1L:326:PHE:HE1	1.64	0.62
12:1L:366:MET:O	12:1L:370:THR:OG1	2.18	0.62
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.35	0.62
15:1O:317:ILE:HA	15:1O:320:LYS:HB2	1.82	0.62
22:1W:50:PHE:HE1	22:1W:96:VAL:HG13	1.64	0.62
37:1l:105:LEU:O	37:1l:109:VAL:HG22	1.98	0.62
1:1A:105:GLU:HB3	1:1A:111:LEU:HD23	1.81	0.62
4:1D:223:ASP:OD2	4:1D:224:GLU:N	2.32	0.62
7:1G:69:CYS:CB	48:1G:803:FES:S2	2.69	0.62
12:1L:194:ASN:ND2	38:1m:124:PHE:O	2.33	0.62
12:1L:370:THR:O	12:1L:374:ILE:HG12	2.00	0.62
13:1M:278:ARG:HH22	37:1l:80:ASP:HA	1.64	0.62
14:1N:241:THR:O	14:1N:244:MET:HB3	2.00	0.62
15:1O:133:VAL:HG13	15:1O:205:ALA:HB3	1.81	0.62
16:1P:216:ASN:O	16:1P:220:ASP:N	2.33	0.62
17:1Q:37:ILE:HD11	17:1Q:105:VAL:HG22	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:47:GLN:NE2	20:1T:67:ALA:O	2.33	0.62
23:1X:150:ASN:OD1	30:1e:50:ARG:NH1	2.32	0.62
35:1j:6:HIS:CD2	35:1j:7:ILE:HD13	2.33	0.62
36:1k:18:TYR:OH	36:1k:46:ARG:HG3	2.00	0.62
37:1l:70:ARG:HG3	37:1l:86:ARG:HH22	1.64	0.62
6:1F:26:TYR:O	6:1F:28:ARG:NH1	2.32	0.62
14:1N:108:LEU:HD11	14:1N:191:THR:HG21	1.81	0.62
16:1P:327:LEU:O	22:1W:51:GLN:NE2	2.32	0.62
19:1S:17:GLU:OE2	19:1S:67:ARG:NH1	2.32	0.62
20:1U:37:MET:SD	20:1U:38:LYS:HG3	2.39	0.62
35:1j:54:PRO:HB2	35:1j:59:TRP:CZ2	2.32	0.62
47:1D:501:U10:H48	8:1H:52:ALA:CB	2.30	0.62
6:1F:199:LYS:NZ	17:1Q:130:VAL:O	2.32	0.62
8:1H:20:LEU:HD22	8:1H:232:ILE:HD11	1.81	0.62
14:1N:312:LYS:HD2	15:1O:75:GLY:H	1.64	0.62
17:1Q:58:GLU:HB3	17:1Q:83:VAL:HG12	1.81	0.62
37:1l:30:ARG:HD2	37:1l:32:GLU:OE2	2.00	0.62
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.32	0.62
2:1B:45:LEU:HD12	2:1B:85:VAL:HG11	1.82	0.61
8:1H:6:ILE:HG22	8:1H:10:ILE:HD11	1.81	0.61
12:1L:176:ARG:NH1	13:1M:401:MET:O	2.33	0.61
12:1L:288:THR:HB	12:1L:304:PHE:HB3	1.82	0.61
13:1M:163:ALA:O	13:1M:167:ILE:HG12	1.99	0.61
16:1P:29:PHE:CZ	16:1P:176:ASP:HA	2.34	0.61
20:1U:47:GLN:HE21	20:1U:71:MET:HA	1.65	0.61
4:1D:81:GLY:N	4:1D:429:ASP:OD2	2.17	0.61
5:1E:95:VAL:HB	5:1E:138:THR:HG21	1.81	0.61
5:1E:190:ARG:HH12	6:1F:266:CYS:HA	1.65	0.61
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.65	0.61
8:1H:195:ARG:HD3	8:1H:231:ILE:HD11	1.83	0.61
13:1M:137:GLY:HA3	13:1M:142:ARG:HD3	1.82	0.61
14:1N:312:LYS:HA	14:1N:315:TRP:CD1	2.35	0.61
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.25	0.61
38:1m:110:LYS:HD3	38:1m:113:LYS:NZ	2.14	0.61
4:1D:74:ARG:HH11	4:1D:74:ARG:HG2	1.64	0.61
6:1F:93:LEU:HD12	6:1F:129:MET:HG3	1.82	0.61
10:1J:71:THR:HA	10:1J:75:ALA:HB3	1.80	0.61
11:1K:12:PHE:HE2	14:1N:72:MET:HB2	1.65	0.61
12:1L:203:MET:HE2	41:1p:109:LEU:HB3	1.81	0.61
13:1M:68:LEU:O	13:1M:72:LEU:HD12	1.99	0.61
14:1N:135:LYS:NZ	14:1N:187:MET:SD	2.73	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:125:LYS:HE2	24:1Y:129:LEU:HD21	1.81	0.61
39:1n:126:ARG:HH21	39:1n:127:LEU:HG	1.66	0.61
8:1H:204:GLU:OE1	8:1H:204:GLU:N	2.33	0.61
10:1J:81:GLU:OE2	11:1K:25:HIS:NE2	2.32	0.61
32:1g:97:VAL:HG13	32:1g:107:LEU:HG	1.83	0.61
43:1r:8:GLN:OE1	43:1r:12:ASN:ND2	2.34	0.61
7:1G:365:ASN:ND2	7:1G:490:MET:O	2.34	0.61
10:1J:64:MET:HA	10:1J:67:VAL:HG22	1.83	0.61
10:1J:117:PHE:HB2	10:1J:119:PHE:CZ	2.36	0.61
13:1M:102:LEU:HD13	13:1M:106:LEU:HD23	1.82	0.61
16:1P:145:TYR:HE1	16:1P:149:LYS:HE2	1.65	0.61
16:1P:201:VAL:N	16:1P:290:SER:OG	2.33	0.61
20:1U:35:HIS:ND1	20:1U:72:CYS:SG	2.74	0.61
24:1Y:13:GLU:HB2	24:1Y:83:PRO:HB3	1.82	0.61
32:1g:83:TYR:CD1	32:1g:84:ARG:HG3	2.36	0.61
32:1g:100:ARG:NE	32:1g:106:PRO:O	2.24	0.61
34:1i:6:ASP:HA	39:1n:155:PRO:HG3	1.82	0.61
39:1n:22:ALA:O	39:1n:26:LEU:HD23	2.00	0.61
6:1F:178:VAL:HG21	6:1F:196:ILE:HD11	1.82	0.61
12:1L:161:ARG:O	12:1L:165:ASN:ND2	2.34	0.61
15:1O:104:ARG:HH21	15:1O:126:ARG:HD2	1.66	0.61
56:1P:501:NDP:H8A	56:1P:501:NDP:H51A	1.82	0.61
7:1G:196:SER:OG	7:1G:265:ASP:OD2	2.16	0.61
9:1I:132:VAL:HG11	9:1I:165:ILE:HG21	1.83	0.61
12:1L:302:VAL:O	12:1L:306:THR:HG23	2.01	0.61
13:1M:87:GLU:OE1	13:1M:92:LYS:NZ	2.32	0.61
32:1g:37:LEU:H	32:1g:37:LEU:HD12	1.65	0.61
6:1F:54:ASP:N	6:1F:54:ASP:OD1	2.32	0.61
8:1H:6:ILE:O	8:1H:10:ILE:HD12	2.00	0.61
10:1J:10:SER:O	10:1J:13:PHE:HB3	2.01	0.61
13:1M:312:ALA:O	13:1M:315:LEU:N	2.32	0.61
15:1O:182:ARG:HA	15:1O:185:LYS:HD2	1.81	0.61
40:1o:14:LYS:HA	40:1o:112:LYS:HE2	1.83	0.61
4:1D:158:ALA:HB1	4:1D:163:ALA:HB3	1.80	0.61
11:1K:42:ILE:O	11:1K:46:LEU:HD23	2.00	0.61
12:1L:10:THR:HG22	34:1i:81:ILE:HG21	1.83	0.61
20:1T:43:ASP:OD2	20:1T:45:LEU:N	2.34	0.61
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.36	0.61
1:1A:91:ALA:O	1:1A:95:LEU:HD22	2.01	0.61
6:1F:24:ASN:HB2	6:1F:39:ARG:HH12	1.64	0.61
7:1G:285:ARG:NH1	7:1G:289:GLY:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:153:GLU:OE1	16:1P:167:LYS:NZ	2.34	0.61
33:1h:87:TYR:CE2	33:1h:91:MET:HE1	2.36	0.61
38:1m:34:GLU:OE1	38:1m:37:ALA:HB2	2.01	0.61
4:1D:354:GLU:O	4:1D:384:SER:OG	2.19	0.60
5:1E:129:GLY:N	5:1E:139:LEU:O	2.31	0.60
6:1F:357:GLU:HA	7:1G:177:ARG:HH21	1.66	0.60
7:1G:190:MET:HG3	7:1G:192:MET:HG2	1.83	0.60
7:1G:228:ILE:HB	7:1G:583:THR:HG22	1.83	0.60
8:1H:111:LEU:HD21	10:1J:61:LEU:HD23	1.83	0.60
13:1M:2:LEU:HA	13:1M:5:ILE:HG22	1.83	0.60
15:1O:279:LEU:O	15:1O:283:THR:OG1	2.17	0.60
16:1P:35:VAL:O	16:1P:39:GLY:N	2.28	0.60
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	1.81	0.60
23:1X:68:ASP:OD1	23:1X:71:ARG:NH1	2.34	0.60
7:1G:53:ARG:N	48:1G:803:FES:S1	2.73	0.60
10:1J:70:TYR:HA	10:1J:73:ALA:HB3	1.83	0.60
14:1N:77:ASN:ND2	14:1N:89:MET:SD	2.73	0.60
15:1O:176:VAL:HG21	15:1O:200:GLN:HB2	1.83	0.60
41:1p:45:THR:O	41:1p:49:GLU:HG2	2.02	0.60
4:1D:149:ASN:HD21	4:1D:371:LYS:HG2	1.66	0.60
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.33	0.60
13:1M:269:MET:HB3	13:1M:295:ALA:HB3	1.82	0.60
14:1N:294:MET:HE2	14:1N:294:MET:HA	1.83	0.60
14:1N:309:ASN:OD1	14:1N:310:ASN:N	2.33	0.60
32:1g:40:LYS:N	32:1g:40:LYS:HE2	2.15	0.60
35:1j:52:PRO:HD2	35:1j:52:PRO:O	1.99	0.60
2:1B:166:LYS:HG2	2:1B:169:ARG:HH22	1.65	0.60
6:1F:109:GLU:O	6:1F:113:HIS:ND1	2.33	0.60
6:1F:207:PRO:HD2	7:1G:71:MET:HE1	1.83	0.60
53:1N:401:CDL:H812	53:1N:401:CDL:H622	1.83	0.60
17:1Q:11:ILE:HG12	22:1W:23:ARG:CZ	2.32	0.60
20:1T:20:LYS:HA	20:1T:20:LYS:HE3	1.82	0.60
23:1X:146:ARG:NH2	30:1e:38:GLU:OE1	2.35	0.60
35:1j:20:SER:O	35:1j:24:GLN:HG2	2.00	0.60
14:1N:196:TYR:HD1	14:1N:273:ASN:HD22	1.49	0.60
15:1O:12:GLU:OE2	15:1O:17:LYS:NZ	2.33	0.60
22:1W:75:ASP:OD2	22:1W:77:ARG:NH2	2.35	0.60
33:1h:34:ILE:H	33:1h:34:ILE:HD12	1.67	0.60
34:1i:106:GLY:HA3	34:1i:118:LEU:HD23	1.84	0.60
6:1F:191:ALA:HB2	6:1F:203:PRO:HG3	1.84	0.60
6:1F:318:ASP:N	6:1F:318:ASP:OD1	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:357:THR:HG22	13:1M:361:MET:HE1	1.81	0.60
15:1O:145:ARG:HH12	15:1O:280:PRO:HG2	1.67	0.60
17:1Q:15:GLU:N	17:1Q:15:GLU:OE2	2.34	0.60
20:1U:34:SER:HB2	20:1U:40:LEU:HD21	1.82	0.60
22:1W:52:LEU:HD13	22:1W:104:MET:HE1	1.84	0.60
38:1m:122:GLN:OE1	38:1m:125:ASN:HB2	2.02	0.60
5:1E:116:ILE:H	5:1E:116:ILE:HD12	1.66	0.60
7:1G:213:TYR:OH	7:1G:217:ALA:O	2.18	0.60
7:1G:371:VAL:HG11	7:1G:391:PHE:HE1	1.66	0.60
8:1H:130:ILE:O	8:1H:134:ARG:HG2	2.01	0.60
12:1L:61:MET:HG3	34:1i:98:GLU:HA	1.84	0.60
16:1P:319:ARG:NH1	16:1P:327:LEU:O	2.35	0.60
21:1V:22:ARG:HH21	21:1V:26:LEU:HD21	1.66	0.60
1:1A:54:LYS:HB3	1:1A:114:ALA:HB3	1.82	0.60
1:1A:105:GLU:HG3	1:1A:111:LEU:HB3	1.84	0.60
7:1G:308:GLN:NE2	7:1G:607:ALA:O	2.35	0.60
7:1G:462:ASP:OD1	7:1G:462:ASP:N	2.33	0.60
8:1H:31:MET:HE1	8:1H:272:TRP:CD1	2.36	0.60
12:1L:231:PRO:HB3	12:1L:530:PRO:HG3	1.83	0.60
13:1M:306:PRO:O	13:1M:310:MET:HG2	2.01	0.60
14:1N:339:MET:HE1	29:1d:30:ARG:HB3	1.83	0.60
18:1R:34:GLU:HG3	42:1q:124:TYR:HD1	1.67	0.60
37:1l:80:ASP:HB3	37:1l:83:MET:HB2	1.84	0.60
40:1o:94:TYR:CD1	40:1o:98:MET:HE2	2.37	0.60
8:1H:63:PRO:HG3	8:1H:214:GLU:HG2	1.83	0.60
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.36	0.60
15:1O:25:ILE:O	15:1O:123:VAL:HA	2.00	0.60
16:1P:108:ASP:HA	16:1P:112:LYS:HG3	1.83	0.60
40:1o:100:GLU:OE2	40:1o:103:ARG:NH1	2.35	0.60
2:1B:137:ASP:OD1	2:1B:137:ASP:N	2.35	0.60
3:1C:207:PRO:HB3	3:1C:210:ARG:HH22	1.66	0.60
8:1H:277:TYR:OH	9:1I:30:LEU:HB3	2.02	0.60
10:1J:5:ILE:HA	10:1J:8:ILE:HG12	1.84	0.60
12:1L:586:LEU:HD23	24:1Y:41:ALA:O	2.02	0.60
13:1M:297:VAL:O	13:1M:301:ILE:HG12	2.02	0.60
15:1O:157:LYS:HE2	15:1O:157:LYS:N	2.16	0.60
16:1P:30:LEU:CA	16:1P:207:ILE:HD11	2.32	0.60
25:1Z:133:ILE:O	25:1Z:137:THR:HG23	2.01	0.60
41:1p:102:VAL:HG11	41:1p:138:PHE:HD2	1.66	0.60
10:1J:114:GLU:HA	10:1J:118:LYS:HZ1	1.65	0.59
11:1K:93:LEU:HG	14:1N:54:GLU:OE1	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:14:MET:HE1	13:1M:30:HIS:CG	2.37	0.59
13:1M:221:VAL:O	13:1M:340:ARG:NH1	2.35	0.59
15:1O:83:TYR:OH	54:1O:401:GTP:O3'	2.20	0.59
22:1W:27:GLU:N	22:1W:27:GLU:OE1	2.34	0.59
24:1Y:61:THR:O	24:1Y:65:ILE:HD12	2.02	0.59
35:1j:65:GLY:HA3	40:1o:30:PHE:CE1	2.36	0.59
38:1m:34:GLU:OE1	39:1n:149:ARG:NH2	2.35	0.59
39:1n:169:ILE:O	39:1n:172:ARG:NH1	2.34	0.59
4:1D:109:VAL:HG11	4:1D:152:MET:HG2	1.83	0.59
6:1F:189:GLU:O	6:1F:193:ILE:HG12	2.02	0.59
9:1I:11:SER:O	9:1I:20:ARG:NH2	2.35	0.59
12:1L:332:HIS:HA	12:1L:335:PHE:CE1	2.36	0.59
13:1M:2:LEU:HD13	31:1f:26:LEU:HB3	1.84	0.59
13:1M:394:ILE:O	13:1M:398:MET:HG2	2.02	0.59
34:1i:5:PRO:HA	34:1i:8:LYS:HE2	1.83	0.59
37:1l:136:ASN:HA	37:1l:153:VAL:HG23	1.83	0.59
1:1A:3:ILE:O	1:1A:7:LEU:HD12	2.01	0.59
8:1H:62:ARG:HD3	8:1H:68:ILE:HG22	1.83	0.59
12:1L:410:LEU:HA	12:1L:413:LEU:HD21	1.84	0.59
14:1N:315:TRP:CD1	14:1N:315:TRP:H	2.20	0.59
25:1Z:80:ASP:N	25:1Z:80:ASP:OD1	2.35	0.59
40:1o:61:TYR:HD2	40:1o:89:CYS:HB2	1.67	0.59
1:1A:75:LEU:HD12	8:1H:151:LEU:HD21	1.83	0.59
4:1D:149:ASN:ND2	4:1D:370:PRO:HB2	2.17	0.59
5:1E:50:VAL:HG11	5:1E:73:LEU:HD21	1.84	0.59
9:1I:164:GLU:OE2	42:1q:88:ARG:N	2.35	0.59
12:1L:5:ALA:HA	12:1L:61:MET:HE1	1.84	0.59
12:1L:483:PRO:HA	35:1j:53:TYR:CG	2.37	0.59
13:1M:368:ALA:O	13:1M:375:LEU:HD23	2.01	0.59
21:1V:30:ILE:O	21:1V:34:LEU:HG	2.02	0.59
27:1b:12:TRP:HA	27:1b:19:VAL:HG11	1.85	0.59
41:1p:167:LYS:HA	41:1p:170:LYS:HE3	1.84	0.59
4:1D:62:LEU:HD12	4:1D:425:PHE:CZ	2.37	0.59
4:1D:410:MET:HE2	4:1D:410:MET:H	1.68	0.59
7:1G:94:MET:HE3	7:1G:120:SER:HA	1.84	0.59
7:1G:237:ASN:OD1	7:1G:253:ARG:NH2	2.36	0.59
10:1J:95:SER:HA	10:1J:98:MET:SD	2.42	0.59
12:1L:465:GLY:O	12:1L:469:SER:OG	2.20	0.59
13:1M:122:PHE:CZ	13:1M:206:LYS:HD2	2.37	0.59
13:1M:444:LEU:O	13:1M:448:THR:OG1	2.18	0.59
14:1N:40:MET:HE1	14:1N:134:GLN:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:19:ARG:NH2	19:1S:73:GLU:OE1	2.36	0.59
20:1U:87:TYR:CE1	34:1i:18:ARG:HG2	2.37	0.59
22:1W:56:VAL:O	22:1W:60:ARG:HG2	2.01	0.59
37:1l:85:ILE:HG13	37:1l:88:ARG:H	1.67	0.59
43:1r:8:GLN:O	43:1r:12:ASN:ND2	2.35	0.59
3:1C:193:GLU:OE1	17:1Q:64:ARG:NH1	2.36	0.59
6:1F:326:GLN:OE1	6:1F:420:ARG:NH1	2.35	0.59
11:1K:19:LEU:HD23	11:1K:36:MET:HE1	1.84	0.59
12:1L:102:GLU:HB2	12:1L:453:SER:HB3	1.85	0.59
20:1T:56:ASP:N	20:1T:56:ASP:OD1	2.31	0.59
24:1Y:137:GLU:OE2	24:1Y:137:GLU:N	2.17	0.59
40:1o:80:LYS:HA	40:1o:83:GLN:HG2	1.84	0.59
7:1G:45:ARG:HD2	7:1G:261:GLU:HG2	1.83	0.59
8:1H:169:GLN:O	8:1H:171:HIS:N	2.35	0.59
8:1H:281:ARG:O	8:1H:285:LEU:N	2.32	0.59
11:1K:50:ASN:OD1	30:1e:31:ARG:NH1	2.34	0.59
13:1M:410:MET:O	13:1M:414:THR:OG1	2.13	0.59
14:1N:217:MET:HA	14:1N:220:ILE:HD11	1.84	0.59
15:1O:216:GLU:HG2	15:1O:217:LYS:HG3	1.83	0.59
18:1R:20:ASP:N	18:1R:20:ASP:OD1	2.34	0.59
21:1V:93:MET:HB3	21:1V:96:TRP:HE3	1.67	0.59
23:1X:129:LYS:NZ	27:1b:62:MET:O	2.36	0.59
5:1E:99:HIS:O	5:1E:101:GLN:NE2	2.35	0.59
6:1F:189:GLU:HB2	6:1F:222:VAL:HG11	1.85	0.59
7:1G:348:VAL:O	7:1G:459:GLN:NE2	2.35	0.59
12:1L:44:PHE:O	12:1L:48:LEU:HD22	2.02	0.59
12:1L:82:MET:HA	12:1L:86:SER:HB2	1.84	0.59
13:1M:325:MET:HE2	13:1M:362:ALA:HB2	1.83	0.59
15:1O:101:TYR:HE1	15:1O:128:ILE:HG23	1.66	0.59
31:1f:30:SER:HA	31:1f:33:LYS:HD3	1.83	0.59
32:1g:73:GLY:O	32:1g:77:VAL:HG12	2.02	0.59
3:1C:199:LEU:HD23	4:1D:354:GLU:HA	1.84	0.59
4:1D:19:MET:HE1	14:1N:172:GLN:N	2.18	0.59
4:1D:72:MET:HB2	4:1D:74:ARG:NH2	2.18	0.59
6:1F:178:VAL:HG11	6:1F:196:ILE:HG13	1.84	0.59
6:1F:360:GLY:HA2	6:1F:366:ARG:HB2	1.83	0.59
7:1G:575:ASN:HD21	7:1G:579:ARG:HB3	1.67	0.59
12:1L:119:LYS:O	12:1L:123:LEU:HD22	2.03	0.59
12:1L:373:LEU:HD21	12:1L:426:ILE:HG23	1.84	0.59
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.31	0.59
16:1P:82:ARG:NH2	16:1P:123:GLU:OE1	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:120:THR:O	24:1Y:124:VAL:HG13	2.02	0.59
34:1i:68:ILE:HD12	34:1i:69:PHE:N	2.17	0.59
37:1l:96:VAL:HB	37:1l:101:MET:HE1	1.85	0.59
39:1n:48:ASP:HA	39:1n:51:LYS:HD3	1.83	0.59
42:1q:75:TRP:CZ2	46:1q:201:PC1:H2	2.27	0.59
7:1G:110:GLN:HG3	7:1G:114:CYS:HA	1.85	0.59
12:1L:12:LEU:O	12:1L:16:THR:HG23	2.02	0.59
20:1T:23:ASP:OD2	20:1T:24:LYS:N	2.36	0.59
25:1Z:20:ASP:N	25:1Z:20:ASP:OD1	2.36	0.59
32:1g:37:LEU:HD13	32:1g:46:GLY:HA2	1.84	0.59
34:1i:81:ILE:O	34:1i:85:LEU:HB2	2.03	0.59
34:1i:104:PHE:CZ	40:1o:67:LYS:HB2	2.37	0.59
37:1l:54:SER:HB2	37:1l:91:THR:H	1.68	0.59
12:1L:116:ARG:HA	12:1L:119:LYS:CD	2.32	0.58
12:1L:332:HIS:HA	12:1L:335:PHE:CD1	2.38	0.58
12:1L:444:ASN:ND2	35:1j:7:ILE:HG12	2.18	0.58
13:1M:453:MET:SD	13:1M:453:MET:N	2.75	0.58
20:1U:12:LYS:O	20:1U:16:LEU:HD22	2.02	0.58
25:1Z:97:ILE:O	30:1e:81:GLN:NE2	2.36	0.58
43:1r:5:ARG:HA	43:1r:8:GLN:HB3	1.83	0.58
4:1D:110:SER:HA	4:1D:145:THR:HG22	1.85	0.58
8:1H:51:ASP:OD2	8:1H:52:ALA:N	2.35	0.58
12:1L:528:TYR:OH	37:1l:104:HIS:ND1	2.29	0.58
18:1R:87:CYS:SG	18:1R:88:GLY:N	2.76	0.58
21:1V:35:GLY:HA2	21:1V:44:ARG:HH22	1.68	0.58
33:1h:87:TYR:CZ	33:1h:91:MET:HE1	2.38	0.58
1:1A:7:LEU:O	1:1A:11:VAL:HG22	2.02	0.58
1:1A:62:PHE:CE2	8:1H:140:ILE:HB	2.38	0.58
2:1B:47:PRO:HD3	2:1B:74:VAL:HG12	1.84	0.58
4:1D:209:ASP:N	4:1D:209:ASP:OD1	2.36	0.58
6:1F:287:VAL:HG11	6:1F:294:LEU:HB2	1.85	0.58
6:1F:291:TRP:O	6:1F:309:LYS:NZ	2.32	0.58
8:1H:140:ILE:HG21	10:1J:65:LEU:HD11	1.86	0.58
8:1H:195:ARG:O	8:1H:199:ASP:N	2.36	0.58
12:1L:278:LEU:HD22	12:1L:315:VAL:HG13	1.84	0.58
14:1N:156:THR:O	14:1N:160:LEU:HD22	2.03	0.58
14:1N:308:THR:HG22	14:1N:311:MET:H	1.67	0.58
16:1P:38:LEU:O	16:1P:43:SER:OG	2.21	0.58
20:1T:29:LYS:NZ	20:1T:40:LEU:HD12	2.18	0.58
23:1X:6:LEU:O	25:1Z:88:ARG:NH2	2.36	0.58
23:1X:48:GLU:OE1	23:1X:134:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:127:GLU:O	41:1p:130:GLN:HG2	2.02	0.58
4:1D:413:ASP:CG	8:1H:281:ARG:NH1	2.60	0.58
5:1E:217:LEU:HD21	6:1F:44:LYS:HG2	1.85	0.58
6:1F:368:GLY:HA3	6:1F:399:ILE:HD11	1.85	0.58
10:1J:100:GLU:N	10:1J:100:GLU:OE2	2.34	0.58
12:1L:65:ASN:OD1	12:1L:65:ASN:N	2.31	0.58
16:1P:192:PRO:HB2	16:1P:258:LEU:HD22	1.85	0.58
27:1b:14:LYS:HE2	27:1b:14:LYS:N	2.17	0.58
38:1m:1:SER:OG	38:1m:2:PHE:N	2.33	0.58
41:1p:59:ARG:NH2	41:1p:60:TYR:O	2.36	0.58
5:1E:103:CYS:SG	5:1E:105:THR:OG1	2.62	0.58
5:1E:217:LEU:HD12	6:1F:55:TRP:HH2	1.69	0.58
6:1F:82:MET:HB2	6:1F:129:MET:HE3	1.85	0.58
10:1J:25:SER:HB3	10:1J:28:TYR:HD2	1.67	0.58
14:1N:346:LEU:HD21	46:1d:201:PC1:H3A2	1.85	0.58
15:1O:139:TYR:CD2	15:1O:149:VAL:HG21	2.39	0.58
21:1V:5:LYS:NZ	21:1V:77:GLU:OE2	2.31	0.58
22:1W:84:ILE:HD12	22:1W:85:LYS:N	2.18	0.58
23:1X:3:ILE:HG23	25:1Z:105:LYS:HZ3	1.69	0.58
6:1F:149:LEU:HD12	6:1F:150:GLN:N	2.19	0.58
13:1M:91:ARG:HD2	52:1M:501:3PE:H321	1.85	0.58
13:1M:349:GLN:OE1	13:1M:356:ALA:HB3	2.04	0.58
13:1M:367:LEU:HD11	13:1M:408:LEU:HD21	1.84	0.58
14:1N:304:MET:N	14:1N:304:MET:HE2	2.19	0.58
34:1i:82:HIS:NE2	41:1p:41:ASP:OD1	2.36	0.58
34:1i:118:LEU:HD21	40:1o:67:LYS:HE2	1.85	0.58
35:1j:8:GLU:HB3	36:1k:11:SER:HB3	1.86	0.58
4:1D:283:PHE:HA	4:1D:309:ARG:HH11	1.68	0.58
8:1H:189:THR:HG22	8:1H:270:PHE:HZ	1.68	0.58
12:1L:57:THR:O	34:1i:102:ARG:NH1	2.33	0.58
13:1M:266:MET:HG3	13:1M:299:VAL:HG11	1.84	0.58
24:1Y:97:GLY:HA2	24:1Y:100:LEU:HD23	1.85	0.58
37:1l:4:VAL:HG11	37:1l:9:PHE:CZ	2.38	0.58
2:1B:70:ASP:OD2	8:1H:34:ARG:NH2	2.35	0.58
4:1D:79:HIS:HE2	22:1W:97:TRP:CD1	2.22	0.58
23:1X:126:LYS:NZ	27:1b:69:PRO:O	2.37	0.58
37:1l:136:ASN:HA	37:1l:153:VAL:H	1.68	0.58
41:1p:35:ILE:O	41:1p:39:LEU:HD23	2.04	0.58
6:1F:92:TYR:HB2	6:1F:220:THR:HG22	1.85	0.58
6:1F:101:GLU:O	6:1F:104:THR:OG1	2.17	0.58
12:1L:413:LEU:HD23	12:1L:413:LEU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:159:MET:HE3	14:1N:278:MET:HE1	1.84	0.58
34:1i:95:THR:HG23	34:1i:96:VAL:HG22	1.86	0.58
42:1q:32:ASP:OD1	42:1q:33:VAL:N	2.36	0.58
3:1C:65:ARG:HD2	3:1C:66:ASP:OD2	2.04	0.58
6:1F:29:HIS:CD2	6:1F:39:ARG:HD2	2.39	0.58
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.39	0.58
15:1O:221:LEU:HD22	15:1O:238:ILE:HD12	1.85	0.58
35:1j:33:TRP:HZ2	36:1k:67:LEU:HA	1.68	0.58
40:1o:72:SER:OG	40:1o:79:CYS:SG	2.53	0.58
12:1L:147:VAL:HG23	12:1L:223:LYS:HE2	1.85	0.57
20:1T:54:MET:HA	20:1T:54:MET:HE2	1.86	0.57
42:1q:94:THR:HG23	42:1q:96:ASP:H	1.69	0.57
6:1F:125:GLY:O	6:1F:129:MET:HG2	2.04	0.57
15:1O:188:ASN:ND2	15:1O:191:GLU:OE2	2.38	0.57
20:1T:35:HIS:HE1	20:1T:37:MET:HG2	1.69	0.57
20:1U:44:SER:O	20:1U:47:GLN:HB3	2.03	0.57
1:1A:85:LYS:HG3	1:1A:86:THR:N	2.19	0.57
12:1L:54:PHE:O	12:1L:58:GLY:N	2.37	0.57
20:1U:8:LEU:O	20:1U:12:LYS:HB2	2.04	0.57
20:1U:21:LEU:HA	36:1k:18:TYR:CZ	2.39	0.57
22:1W:42:GLU:OE1	22:1W:46:THR:HB	2.04	0.57
23:1X:78:ALA:O	23:1X:82:THR:N	2.33	0.57
25:1Z:103:ASP:N	25:1Z:103:ASP:OD2	2.36	0.57
34:1i:21:TRP:O	34:1i:25:GLN:NE2	2.31	0.57
1:1A:44:MET:SD	1:1A:44:MET:N	2.78	0.57
4:1D:334:LYS:HD3	4:1D:336:ALA:H	1.69	0.57
6:1F:139:ARG:HD3	6:1F:141:GLU:HB2	1.87	0.57
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	1.86	0.57
12:1L:176:ARG:HH22	13:1M:403:THR:N	2.02	0.57
12:1L:599:MET:HA	12:1L:599:MET:HE3	1.86	0.57
13:1M:64:PRO:HB3	13:1M:454:ILE:HG22	1.86	0.57
14:1N:243:LEU:O	14:1N:247:THR:HG22	2.04	0.57
20:1U:72:CYS:H	20:1U:75:GLU:HG3	1.70	0.57
22:1W:25:MET:HA	22:1W:25:MET:HE3	1.86	0.57
24:1Y:116:TYR:O	24:1Y:119:LEU:HD12	2.05	0.57
30:1e:29:PRO:HB3	33:1h:138:LYS:HG2	1.87	0.57
4:1D:405:MET:HE3	4:1D:405:MET:O	2.04	0.57
7:1G:286:ASN:HD21	7:1G:290:LEU:HB2	1.69	0.57
8:1H:256:THR:O	8:1H:260:VAL:HG22	2.03	0.57
34:1i:13:GLN:O	34:1i:17:LEU:HG	2.04	0.57
34:1i:100:LYS:HB2	41:1p:14:ARG:HH22	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:85:ILE:HD11	37:1l:88:ARG:HG2	1.87	0.57
40:1o:110:ARG:NH2	40:1o:114:ARG:HD3	2.19	0.57
41:1p:105:ILE:HG21	41:1p:134:VAL:HG11	1.86	0.57
4:1D:72:MET:HB2	4:1D:74:ARG:HH22	1.69	0.57
4:1D:342:MET:HE1	7:1G:103:LEU:HA	1.87	0.57
7:1G:622:ARG:NH2	19:1S:73:GLU:OE2	2.35	0.57
8:1H:316:PRO:HG3	25:1Z:57:ARG:HB3	1.85	0.57
10:1J:55:MET:O	10:1J:59:ILE:HG13	2.05	0.57
13:1M:365:THR:O	13:1M:374:ASN:ND2	2.38	0.57
2:1B:75:VAL:O	2:1B:77:ARG:N	2.38	0.57
7:1G:683:THR:HA	7:1G:686:LYS:HD3	1.86	0.57
12:1L:605:HIS:HB2	14:1N:92:PRO:HB2	1.86	0.57
31:1f:3:VAL:O	31:1f:7:VAL:HG23	2.04	0.57
38:1m:13:LEU:HD12	38:1m:14:PRO:HD2	1.86	0.57
42:1q:29:ARG:NH2	42:1q:64:TYR:O	2.38	0.57
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.85	0.57
8:1H:231:ILE:O	8:1H:235:ASN:ND2	2.30	0.57
16:1P:171:ILE:H	56:1P:501:NDP:H71N	1.53	0.57
19:1S:63:LYS:HD3	19:1S:64:LEU:N	2.20	0.57
20:1T:12:LYS:HE2	20:1T:12:LYS:HA	1.87	0.57
20:1T:47:GLN:O	20:1T:51:ILE:HG12	2.05	0.57
30:1e:29:PRO:HG2	33:1h:143:ASN:HD22	1.70	0.57
38:1m:110:LYS:HA	38:1m:113:LYS:NZ	2.20	0.57
41:1p:102:VAL:HG11	41:1p:138:PHE:CD2	2.40	0.57
2:1B:42:ARG:HH21	2:1B:168:LYS:HA	1.70	0.57
7:1G:231:MET:N	7:1G:231:MET:HE2	2.19	0.57
9:1I:27:TRP:HB3	9:1I:30:LEU:HD13	1.86	0.57
11:1K:19:LEU:HD21	14:1N:65:THR:HG22	1.86	0.57
12:1L:39:THR:HA	12:1L:42:TYR:CD2	2.39	0.57
13:1M:402:ILE:HA	13:1M:405:LEU:HD12	1.86	0.57
13:1M:403:THR:HA	13:1M:406:TYR:CZ	2.40	0.57
19:1S:57:CYS:SG	19:1S:58:SER:N	2.76	0.57
20:1T:55:GLU:HB3	20:1T:62:ILE:HG12	1.86	0.57
22:1W:81:LEU:HD13	22:1W:84:ILE:HD11	1.87	0.57
23:1X:24:LEU:HB3	25:1Z:71:LEU:CD2	2.34	0.57
27:1b:64:ASP:OD2	27:1b:64:ASP:N	2.37	0.57
38:1m:63:ALA:HA	38:1m:66:ARG:HE	1.68	0.57
38:1m:126:ILE:HD13	41:1p:138:PHE:HB3	1.86	0.57
41:1p:6:LYS:NZ	41:1p:11:GLU:HB3	2.20	0.57
3:1C:61:LEU:HB3	3:1C:123:VAL:HG11	1.87	0.56
3:1C:174:LEU:HD22	22:1W:105:ARG:HH21	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:253:THR:HG22	6:1F:271:GLU:HA	1.87	0.56
7:1G:121:MET:HE2	7:1G:121:MET:HA	1.87	0.56
7:1G:326:GLU:N	7:1G:326:GLU:OE2	2.33	0.56
11:1K:44:SER:HB2	11:1K:59:MET:HE1	1.86	0.56
12:1L:176:ARG:NH2	13:1M:404:ALA:H	2.02	0.56
12:1L:496:MET:HE1	12:1L:500:LEU:HD12	1.86	0.56
34:1i:78:VAL:HA	34:1i:81:ILE:HG22	1.87	0.56
40:1o:40:ALA:HB1	40:1o:59:ALA:HB3	1.86	0.56
3:1C:149:ARG:NH1	4:1D:77:ASP:OD2	2.37	0.56
4:1D:72:MET:N	4:1D:72:MET:SD	2.78	0.56
6:1F:45:THR:O	6:1F:49:LEU:HD22	2.05	0.56
17:1Q:27:GLU:H	17:1Q:27:GLU:CD	2.12	0.56
17:1Q:81:ASN:O	17:1Q:81:ASN:ND2	2.38	0.56
2:1B:162:GLN:OE1	42:1q:116:ASN:ND2	2.37	0.56
4:1D:17:ALA:O	14:1N:173:THR:OG1	2.15	0.56
4:1D:338:MET:HE1	4:1D:348:HIS:CG	2.39	0.56
5:1E:181:ILE:HD12	5:1E:181:ILE:O	2.05	0.56
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.70	0.56
7:1G:376:VAL:HG11	7:1G:442:ILE:HG22	1.86	0.56
7:1G:620:ARG:NE	7:1G:633:TYR:OH	2.32	0.56
10:1J:126:VAL:HG12	10:1J:127:ILE:HD13	1.87	0.56
12:1L:28:LYS:HZ3	12:1L:31:LEU:N	2.03	0.56
12:1L:67:HIS:HA	12:1L:77:SER:HA	1.86	0.56
12:1L:116:ARG:HA	12:1L:119:LYS:HD3	1.86	0.56
13:1M:1:FME:HE2	13:1M:66:LEU:HD23	1.86	0.56
13:1M:141:GLU:N	13:1M:141:GLU:OE2	2.39	0.56
13:1M:235:LEU:HD12	13:1M:236:LEU:HD12	1.85	0.56
14:1N:289:ASN:HA	14:1N:292:PHE:CE1	2.40	0.56
18:1R:10:LYS:HD3	18:1R:10:LYS:H	1.70	0.56
18:1R:37:GLU:N	18:1R:37:GLU:OE2	2.38	0.56
22:1W:23:ARG:H	22:1W:27:GLU:HG3	1.71	0.56
28:1c:37:GLU:HA	28:1c:40:LEU:HG	1.87	0.56
30:1e:62:PHE:CE1	30:1e:66:LEU:HD21	2.39	0.56
30:1e:88:GLU:CD	30:1e:90:LYS:HD3	2.30	0.56
36:1k:22:LYS:HA	36:1k:22:LYS:HE3	1.85	0.56
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.05	0.56
42:1q:13:GLN:O	42:1q:17:HIS:ND1	2.38	0.56
5:1E:123:LYS:HG2	5:1E:173:ILE:HG21	1.88	0.56
7:1G:60:GLU:OE2	7:1G:78:ASN:N	2.36	0.56
8:1H:312:ALA:O	25:1Z:55:ARG:NH1	2.38	0.56
13:1M:61:LEU:HB2	13:1M:457:PRO:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:51:ILE:CG2	20:1T:62:ILE:HG21	2.35	0.56
32:1g:64:PHE:HD1	32:1g:68:ILE:HD11	1.70	0.56
37:1l:73:TRP:O	38:1m:39:ARG:NH1	2.26	0.56
38:1m:24:ILE:O	38:1m:24:ILE:HD12	2.05	0.56
41:1p:84:MET:HE2	41:1p:152:ARG:HD2	1.88	0.56
6:1F:208:PRO:HD2	17:1Q:118:TYR:HD2	1.70	0.56
7:1G:40:PHE:CZ	7:1G:119:GLN:HG3	2.41	0.56
12:1L:366:MET:HE1	12:1L:445:GLU:HB3	1.88	0.56
15:1O:23:LYS:HA	15:1O:167:HIS:ND1	2.21	0.56
15:1O:94:TYR:HD2	15:1O:282:ILE:HD11	1.71	0.56
21:1V:103:VAL:HG23	21:1V:104:GLU:OE1	2.05	0.56
22:1W:44:PRO:HD3	22:1W:60:ARG:NH1	2.20	0.56
41:1p:72:ASP:OD2	41:1p:90:GLN:NE2	2.39	0.56
5:1E:175:GLU:OE1	5:1E:180:LYS:NZ	2.38	0.56
8:1H:224:PHE:HE1	8:1H:228:TYR:CD2	2.24	0.56
9:1I:17:VAL:HG23	27:1b:13:ALA:HB2	1.88	0.56
10:1J:14:VAL:HG11	10:1J:100:GLU:HG3	1.87	0.56
10:1J:62:GLY:O	10:1J:66:VAL:HG22	2.05	0.56
10:1J:70:TYR:CE2	11:1K:75:LEU:HD13	2.41	0.56
11:1K:85:TYR:HE2	11:1K:93:LEU:HA	1.71	0.56
12:1L:151:SER:O	12:1L:155:ILE:HD12	2.05	0.56
13:1M:239:GLY:O	13:1M:243:MET:HG2	2.04	0.56
20:1T:55:GLU:HA	20:1T:60:PHE:CE2	2.40	0.56
2:1B:47:PRO:HA	2:1B:85:VAL:HG13	1.87	0.56
2:1B:65:PRO:HD3	4:1D:168:PHE:HB3	1.87	0.56
4:1D:180:PHE:O	4:1D:184:VAL:HG22	2.06	0.56
4:1D:284:ASP:N	4:1D:284:ASP:OD1	2.39	0.56
7:1G:169:VAL:HG21	7:1G:193:SER:HB2	1.88	0.56
10:1J:127:ILE:HA	25:1Z:120:MET:HE1	1.87	0.56
12:1L:387:THR:O	12:1L:391:SER:HB3	2.05	0.56
12:1L:496:MET:HE3	12:1L:496:MET:C	2.31	0.56
14:1N:244:MET:HE2	14:1N:244:MET:HA	1.86	0.56
22:1W:93:THR:HG22	22:1W:103:ILE:HD11	1.88	0.56
24:1Y:94:CYS:HB2	24:1Y:114:CYS:CA	2.26	0.56
38:1m:34:GLU:CD	38:1m:37:ALA:HB2	2.30	0.56
4:1D:110:SER:O	4:1D:114:ASN:ND2	2.38	0.56
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.24	0.56
4:1D:233:ARG:HG3	9:1I:30:LEU:HD11	1.87	0.56
4:1D:371:LYS:NZ	4:1D:422:ASP:HB2	2.20	0.56
5:1E:123:LYS:NZ	5:1E:170:GLU:O	2.38	0.56
13:1M:298:ILE:O	13:1M:302:MET:HG2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:223:SER:OG	15:1O:271:ASN:ND2	2.39	0.56
16:1P:237:LEU:HB3	16:1P:240:ASP:OD1	2.05	0.56
20:1U:47:GLN:OE1	20:1U:50:ILE:HD11	2.05	0.56
22:1W:23:ARG:CZ	22:1W:23:ARG:HA	2.35	0.56
24:1Y:25:THR:HG22	24:1Y:67:ALA:HB2	1.88	0.56
28:1c:7:PRO:HG2	28:1c:10:GLY:HA3	1.85	0.56
41:1p:159:LYS:HD2	41:1p:162:MET:SD	2.45	0.56
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.86	0.56
11:1K:4:VAL:O	11:1K:8:ILE:HG13	2.06	0.56
12:1L:359:MET:N	12:1L:359:MET:SD	2.79	0.56
14:1N:12:THR:HG23	14:1N:39:ALA:HB1	1.88	0.56
16:1P:177:ARG:NH2	56:1P:501:NDP:O2N	2.39	0.56
18:1R:32:GLN:NE2	18:1R:34:GLU:OE2	2.39	0.56
20:1T:29:LYS:HZ2	20:1T:40:LEU:HD12	1.70	0.56
37:1l:80:ASP:O	37:1l:83:MET:HB2	2.06	0.56
5:1E:116:ILE:HG23	5:1E:169:ILE:HG21	1.87	0.56
6:1F:20:ARG:NE	6:1F:269:GLU:O	2.38	0.56
7:1G:303:VAL:HG11	7:1G:603:LEU:HD11	1.87	0.56
13:1M:422:HIS:CE1	13:1M:423:ILE:HG23	2.41	0.56
16:1P:241:LEU:O	16:1P:245:ILE:HG23	2.06	0.56
29:1d:78:ARG:HH12	46:1d:201:PC1:H221	1.70	0.56
37:1l:42:MET:HA	37:1l:42:MET:HE3	1.87	0.56
2:1B:126:TYR:CD1	4:1D:85:ARG:HG2	2.41	0.55
4:1D:184:VAL:HB	4:1D:193:TYR:CE2	2.41	0.55
6:1F:22:PHE:HE2	6:1F:255:LEU:HB2	1.70	0.55
6:1F:44:LYS:HG3	6:1F:47:GLU:HB2	1.89	0.55
7:1G:564:ALA:O	7:1G:569:LYS:NZ	2.36	0.55
12:1L:63:ILE:HG22	34:1i:96:VAL:HG12	1.87	0.55
12:1L:123:LEU:HD23	12:1L:150:MET:HE1	1.89	0.55
13:1M:22:MET:HE2	13:1M:22:MET:N	2.21	0.55
15:1O:3:TYR:CD2	15:1O:260:ARG:HG2	2.41	0.55
18:1R:51:GLU:OE1	18:1R:92:ARG:NH2	2.38	0.55
23:1X:12:LEU:HB2	25:1Z:81:ARG:HG2	1.89	0.55
27:1b:43:ARG:HA	27:1b:46:ARG:HG2	1.87	0.55
29:1d:108:THR:OG1	29:1d:111:GLU:OE1	2.18	0.55
2:1B:173:LEU:HD22	2:1B:176:TRP:HE3	1.72	0.55
4:1D:159:LEU:HD11	47:1D:501:U10:H112	1.88	0.55
5:1E:36:LYS:HZ3	44:1s:59:SER:HA	1.71	0.55
6:1F:108:ARG:O	6:1F:112:ARG:HG2	2.06	0.55
21:1V:58:VAL:HA	21:1V:67:LEU:HD11	1.87	0.55
32:1g:95:ARG:HH12	32:1g:96:LEU:HB2	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:103:ILE:HG21	41:1p:15:ARG:HG3	1.89	0.55
38:1m:26:PRO:HA	38:1m:29:ARG:HG3	1.88	0.55
4:1D:61:VAL:HG21	4:1D:83:LEU:HB2	1.88	0.55
6:1F:295:LEU:HB2	6:1F:339:ARG:HD2	1.89	0.55
7:1G:647:GLU:HA	7:1G:650:LYS:HE3	1.89	0.55
12:1L:297:ASP:HA	12:1L:355:ASP:HA	1.89	0.55
12:1L:406:ALA:HA	37:1l:124:SER:HB3	1.87	0.55
13:1M:193:ILE:HD12	13:1M:194:PHE:N	2.21	0.55
22:1W:90:LEU:HD13	22:1W:94:ILE:HD13	1.88	0.55
24:1Y:61:THR:OG1	24:1Y:103:ARG:NH1	2.39	0.55
37:1l:37:TYR:HB2	37:1l:44:TYR:CG	2.42	0.55
4:1D:342:MET:HG3	7:1G:98:LEU:HG	1.87	0.55
6:1F:233:THR:HA	6:1F:236:ARG:HE	1.72	0.55
12:1L:38:THR:HB	12:1L:42:TYR:CZ	2.42	0.55
13:1M:119:TYR:CD1	13:1M:160:LEU:HD12	2.41	0.55
15:1O:169:VAL:HG11	15:1O:210:PHE:HZ	1.69	0.55
24:1Y:28:GLY:O	24:1Y:62:SER:OG	2.15	0.55
32:1g:68:ILE:HD12	32:1g:69:VAL:H	1.71	0.55
37:1l:112:MET:O	37:1l:116:PHE:HD2	1.88	0.55
1:1A:38:GLU:N	1:1A:41:PHE:O	2.35	0.55
6:1F:147:SER:O	6:1F:151:VAL:HG12	2.07	0.55
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.35	0.55
8:1H:162:LEU:HD11	8:1H:237:PHE:HE2	1.71	0.55
12:1L:597:ILE:HA	12:1L:601:LEU:HB2	1.89	0.55
13:1M:44:GLN:NE2	13:1M:48:ASN:O	2.40	0.55
13:1M:76:MET:HE3	13:1M:76:MET:H	1.71	0.55
14:1N:277:ILE:HD11	24:1Y:132:TRP:CE3	2.42	0.55
24:1Y:31:THR:O	24:1Y:35:VAL:HG12	2.05	0.55
25:1Z:58:ARG:O	25:1Z:62:ILE:HG22	2.06	0.55
25:1Z:113:THR:HG23	30:1e:61:ASP:OD2	2.06	0.55
37:1l:13:TYR:OH	37:1l:37:TYR:O	2.23	0.55
43:1r:110:PRO:C	43:1r:111:TYR:HD1	2.14	0.55
6:1F:263:ASN:ND2	6:1F:286:GLY:O	2.39	0.55
12:1L:21:MET:HA	12:1L:21:MET:HE3	1.88	0.55
12:1L:73:THR:HG22	41:1p:102:VAL:HG21	1.87	0.55
12:1L:363:TYR:HB2	12:1L:431:PHE:HB3	1.89	0.55
12:1L:406:ALA:O	12:1L:410:LEU:HD12	2.06	0.55
13:1M:116:ILE:O	13:1M:120:ILE:HG13	2.07	0.55
20:1U:18:VAL:HG21	20:1U:58:PHE:HZ	1.72	0.55
22:1W:52:LEU:HD21	22:1W:103:ILE:HG21	1.89	0.55
32:1g:85:MET:O	32:1g:89:ALA:N	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:88:TRP:CD1	41:1p:65:ARG:HB3	2.41	0.55
32:1g:110:SER:O	41:1p:161:ARG:NH1	2.39	0.55
39:1n:29:TRP:NE1	39:1n:73:GLY:O	2.40	0.55
6:1F:24:ASN:OD1	6:1F:29:HIS:N	2.37	0.55
6:1F:194:GLU:OE2	6:1F:204:ARG:NH2	2.30	0.55
6:1F:276:LEU:HA	6:1F:279:LEU:HD12	1.88	0.55
7:1G:35:MET:HE1	7:1G:37:ILE:HD12	1.88	0.55
9:1I:150:ASN:ND2	42:1q:127:TYR:O	2.40	0.55
12:1L:292:ALA:HB2	12:1L:304:PHE:HD2	1.72	0.55
12:1L:512:LYS:HG2	12:1L:513:PHE:H	1.71	0.55
12:1L:576:MET:SD	12:1L:577:VAL:HG23	2.47	0.55
13:1M:227:GLY:O	13:1M:231:LEU:HD22	2.05	0.55
13:1M:317:ILE:HD13	13:1M:454:ILE:HB	1.89	0.55
14:1N:8:THR:HA	14:1N:11:MET:HE2	1.87	0.55
14:1N:27:LEU:HG	14:1N:31:ILE:HD11	1.87	0.55
24:1Y:22:TYR:O	24:1Y:25:THR:OG1	2.22	0.55
24:1Y:68:ILE:HD11	24:1Y:96:GLY:N	2.21	0.55
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.07	0.55
36:1k:74:PHE:O	36:1k:77:PHE:HB2	2.06	0.55
4:1D:46:ASN:HB2	4:1D:67:GLU:OE1	2.07	0.55
4:1D:69:SER:H	4:1D:74:ARG:NH1	2.03	0.55
47:1D:501:U10:H262	8:1H:274:ARG:HH22	1.70	0.55
5:1E:190:ARG:HG3	5:1E:194:GLU:O	2.06	0.55
8:1H:86:TRP:NE1	8:1H:233:MET:HB2	2.21	0.55
12:1L:71:LEU:HG	12:1L:74:VAL:HB	1.88	0.55
12:1L:378:LEU:HD12	12:1L:383:MET:HE3	1.87	0.55
13:1M:175:ASN:HB3	13:1M:178:ILE:HG22	1.88	0.55
14:1N:30:TRP:CD2	14:1N:71:MET:HE2	2.41	0.55
29:1d:16:ASN:OD1	29:1d:19:ARG:NH2	2.39	0.55
32:1g:96:LEU:CD2	32:1g:100:ARG:HD2	2.36	0.55
36:1k:29:GLU:HA	36:1k:32:GLN:HB3	1.88	0.55
37:1l:128:VAL:HA	40:1o:98:MET:HA	1.89	0.55
2:1B:101:ARG:HG3	3:1C:183:VAL:HG23	1.89	0.55
2:1B:123:GLY:HA3	2:1B:127:HIS:ND1	2.22	0.55
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.89	0.55
7:1G:240:VAL:HG12	7:1G:242:THR:HG22	1.88	0.55
8:1H:117:LEU:HB2	10:1J:68:PHE:CZ	2.42	0.55
9:1I:8:ARG:NH2	43:1r:111:TYR:HB2	2.22	0.55
9:1I:29:GLU:N	9:1I:29:GLU:OE1	2.40	0.55
9:1I:164:GLU:OE1	9:1I:164:GLU:HA	2.07	0.55
12:1L:37:LYS:O	12:1L:41:SER:OG	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:267:MET:HE1	12:1L:273:VAL:HB	1.89	0.55
12:1L:401:MET:O	37:1L:126:GLN:NE2	2.40	0.55
15:1O:200:GLN:NE2	15:1O:204:ASN:HD21	2.04	0.55
15:1O:204:ASN:HD22	15:1O:208:LYS:HZ3	1.54	0.55
17:1Q:33:ARG:NH2	17:1Q:60:ASP:O	2.40	0.55
25:1Z:127:LEU:H	25:1Z:127:LEU:HD12	1.71	0.55
36:1k:83:ALA:HA	36:1k:86:TYR:CE2	2.42	0.55
4:1D:27:HIS:HA	4:1D:29:LYS:NZ	2.22	0.55
4:1D:170:MET:HE2	4:1D:170:MET:N	2.22	0.55
8:1H:10:ILE:HD12	8:1H:10:ILE:H	1.72	0.55
8:1H:91:MET:H	8:1H:91:MET:HE2	1.71	0.55
8:1H:306:SER:O	8:1H:310:MET:HG2	2.07	0.55
10:1J:111:GLU:HB3	10:1J:120:ASN:OD1	2.07	0.55
12:1L:521:LYS:O	12:1L:525:MET:HG2	2.07	0.55
13:1M:425:ASN:HB3	38:1m:57:GLY:HA2	1.90	0.55
17:1Q:11:ILE:HD12	22:1W:17:VAL:O	2.08	0.55
24:1Y:16:GLU:HG3	24:1Y:19:ARG:HB2	1.89	0.55
24:1Y:51:GLY:O	24:1Y:55:THR:HG23	2.07	0.55
38:1m:51:ASN:HA	39:1n:128:ARG:HH21	1.72	0.55
5:1E:36:LYS:HZ2	44:1s:62:ARG:HH11	1.55	0.54
5:1E:155:GLN:OE1	5:1E:159:ASN:N	2.39	0.54
10:1J:33:LEU:HD11	10:1J:60:TYR:HE2	1.72	0.54
12:1L:267:MET:O	12:1L:267:MET:HE3	2.07	0.54
12:1L:425:ARG:HA	12:1L:428:PHE:CE1	2.41	0.54
12:1L:481:THR:HG23	35:1j:51:PHE:HB2	1.88	0.54
13:1M:325:MET:O	13:1M:325:MET:HE3	2.07	0.54
13:1M:341:THR:HB	13:1M:344:LEU:HB2	1.89	0.54
13:1M:451:PRO:O	13:1M:455:LEU:HB2	2.07	0.54
20:1U:15:VAL:HG11	20:1U:77:VAL:HG13	1.89	0.54
34:1i:94:TYR:CE2	41:1p:108:ARG:HA	2.37	0.54
40:1o:52:LEU:HD23	40:1o:55:ARG:HD2	1.89	0.54
5:1E:27:ASN:OD1	5:1E:30:ARG:NH1	2.41	0.54
6:1F:91:LYS:HG2	6:1F:219:PRO:HB2	1.89	0.54
9:1I:97:GLU:HG2	9:1I:107:THR:OG1	2.07	0.54
13:1M:225:ILE:HD13	13:1M:331:ASN:ND2	2.23	0.54
14:1N:279:PRO:HA	14:1N:282:MET:SD	2.47	0.54
20:1T:72:CYS:HB3	20:1T:75:GLU:CD	2.33	0.54
31:1f:39:ASN:C	31:1f:39:ASN:HD22	2.16	0.54
33:1h:94:LEU:HD12	41:1p:81:ILE:HG13	1.87	0.54
2:1B:51:GLY:O	4:1D:60:GLY:HA3	2.07	0.54
3:1C:32:ILE:HG21	3:1C:63:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:41:CYS:N	7:1G:52:CYS:SG	2.81	0.54
8:1H:199:ASP:OD1	8:1H:200:LEU:N	2.40	0.54
10:1J:141:MET:HE1	30:1e:26:HIS:CG	2.43	0.54
11:1K:47:ILE:H	11:1K:47:ILE:HD12	1.72	0.54
12:1L:511:LEU:HD11	39:1n:38:TYR:CE2	2.42	0.54
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.40	0.54
14:1N:115:VAL:HA	14:1N:118:VAL:HG22	1.89	0.54
14:1N:209:ILE:O	14:1N:213:LEU:HD22	2.07	0.54
14:1N:277:ILE:HD11	24:1Y:132:TRP:CZ3	2.42	0.54
15:1O:169:VAL:HB	15:1O:214:MET:HE3	1.89	0.54
17:1Q:59:PHE:HE2	17:1Q:79:LEU:HD23	1.72	0.54
30:1e:90:LYS:HD2	30:1e:90:LYS:N	2.22	0.54
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.08	0.54
38:1m:15:ALA:O	38:1m:21:GLU:HG2	2.06	0.54
41:1p:139:GLN:HA	41:1p:143:SER:HB3	1.88	0.54
4:1D:62:LEU:HD21	4:1D:64:LEU:HG	1.90	0.54
6:1F:276:LEU:HD22	6:1F:312:CYS:HB2	1.89	0.54
7:1G:623:LEU:HD21	7:1G:630:LEU:CB	2.37	0.54
9:1I:92:ILE:HG13	9:1I:111:ILE:HG12	1.89	0.54
10:1J:18:VAL:O	10:1J:22:SER:N	2.40	0.54
12:1L:62:ILE:HG12	12:1L:81:LYS:HG3	1.90	0.54
12:1L:63:ILE:HG13	12:1L:80:PHE:HB2	1.89	0.54
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.07	0.54
16:1P:195:SER:OG	16:1P:199:GLU:OE2	2.24	0.54
20:1T:26:ASP:H	20:1T:29:LYS:HE3	1.72	0.54
20:1U:37:MET:SD	20:1U:38:LYS:N	2.80	0.54
21:1V:77:GLU:O	21:1V:80:ILE:HD12	2.08	0.54
22:1W:54:ILE:HD11	22:1W:58:GLN:C	2.32	0.54
29:1d:90:MET:HE1	33:1h:107:GLU:CA	2.37	0.54
2:1B:174:ARG:HB3	2:1B:178:ARG:NH2	2.22	0.54
4:1D:4:TRP:CE3	13:1M:140:THR:HA	2.43	0.54
4:1D:411:LEU:O	4:1D:414:VAL:HG12	2.08	0.54
8:1H:10:ILE:HG23	8:1H:83:LEU:HD22	1.88	0.54
10:1J:133:SER:N	26:1a:42:SER:OG	2.38	0.54
12:1L:424:THR:OG1	12:1L:501:ALA:HB1	2.08	0.54
12:1L:488:MET:HB3	12:1L:491:LEU:HB2	1.90	0.54
12:1L:528:TYR:HH	37:1l:104:HIS:HD1	1.37	0.54
13:1M:5:ILE:O	13:1M:9:THR:HG23	2.08	0.54
14:1N:189:TRP:CZ2	14:1N:263:LYS:HG2	2.43	0.54
16:1P:74:ASN:OD1	16:1P:75:GLY:N	2.40	0.54
16:1P:141:SER:O	16:1P:147:ARG:NH2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:69:LYS:HB2	34:1i:1:SAC:H	1.72	0.54
21:1V:107:PRO:HD2	21:1V:110:GLN:HG3	1.88	0.54
24:1Y:87:LEU:O	24:1Y:91:ILE:HG12	2.07	0.54
37:1l:30:ARG:HH22	38:1m:32:GLN:HA	1.73	0.54
7:1G:232:ASP:OD1	7:1G:233:ALA:N	2.40	0.54
7:1G:392:ASN:HD21	7:1G:415:LEU:HD22	1.73	0.54
13:1M:21:ASN:N	13:1M:21:ASN:OD1	2.39	0.54
14:1N:127:GLY:O	14:1N:131:LEU:HD12	2.06	0.54
15:1O:40:ARG:HH22	15:1O:44:GLU:HB2	1.73	0.54
15:1O:101:TYR:OH	15:1O:159:THR:OG1	2.18	0.54
29:1d:-2:ACE:O	29:1d:2:MET:N	2.39	0.54
32:1g:48:ASP:N	32:1g:54:ASP:OD1	2.40	0.54
33:1h:73:ARG:NH2	41:1p:62:TYR:HB3	2.21	0.54
39:1n:126:ARG:O	39:1n:130:GLU:HG2	2.07	0.54
15:1O:104:ARG:NH2	54:1O:401:GTP:N7	2.56	0.54
16:1P:293:THR:HG22	16:1P:295:PRO:HD3	1.90	0.54
17:1Q:93:VAL:O	17:1Q:97:GLU:HG3	2.08	0.54
18:1R:20:ASP:O	18:1R:25:ARG:NH1	2.37	0.54
23:1X:15:GLN:NE2	23:1X:16:GLU:O	2.41	0.54
33:1h:15:GLY:HA2	39:1n:107:HIS:NE2	2.21	0.54
38:1m:119:LYS:C	38:1m:119:LYS:HD3	2.33	0.54
41:1p:105:ILE:HD11	41:1p:130:GLN:HG3	1.90	0.54
2:1B:166:LYS:HA	2:1B:169:ARG:NH1	2.22	0.54
7:1G:280:THR:HB	7:1G:591:GLY:HA3	1.90	0.54
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	1.89	0.54
9:1I:69:ARG:HD2	42:1q:108:TYR:CG	2.42	0.54
12:1L:309:GLN:HE22	12:1L:332:HIS:HB2	1.73	0.54
13:1M:181:TYR:O	41:1p:152:ARG:NH1	2.34	0.54
14:1N:157:MET:O	14:1N:161:SER:OG	2.23	0.54
14:1N:178:ILE:HD12	14:1N:179:MET:N	2.23	0.54
15:1O:204:ASN:HD22	15:1O:208:LYS:NZ	2.06	0.54
21:1V:43:TYR:CZ	21:1V:47:THR:HG21	2.43	0.54
1:1A:27:LEU:HG	1:1A:29:ALA:H	1.71	0.54
4:1D:152:MET:HE1	4:1D:171:PHE:CZ	2.43	0.54
5:1E:116:ILE:CG2	5:1E:169:ILE:HG21	2.38	0.54
6:1F:349:ARG:NH1	6:1F:349:ARG:O	2.40	0.54
7:1G:375:ASP:OD2	7:1G:448:LYS:N	2.30	0.54
8:1H:22:LEU:HB2	8:1H:48:PRO:HG3	1.89	0.54
12:1L:482:MET:HG3	12:1L:486:MET:HE1	1.90	0.54
20:1T:65:ILE:HD12	20:1T:66:ASP:N	2.23	0.54
20:1T:75:GLU:OE1	20:1T:75:GLU:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:75:LEU:HB3	8:1H:155:LEU:HD21	1.90	0.54
6:1F:24:ASN:HB2	6:1F:39:ARG:NH1	2.23	0.54
6:1F:151:VAL:HG23	6:1F:154:ARG:HH21	1.71	0.54
6:1F:247:ARG:NH2	6:1F:248:GLU:OE2	2.41	0.54
7:1G:46:LEU:O	17:1Q:116:LYS:NZ	2.38	0.54
7:1G:185:THR:O	7:1G:187:ILE:N	2.41	0.54
8:1H:190:LEU:HD21	8:1H:273:ILE:HG21	1.90	0.54
12:1L:293:ILE:HD11	12:1L:418:LEU:HG	1.89	0.54
12:1L:486:MET:O	12:1L:486:MET:HE2	2.08	0.54
12:1L:578:SER:HB3	14:1N:168:GLY:HA2	1.89	0.54
15:1O:299:LEU:HD22	15:1O:300:PRO:HD2	1.89	0.54
16:1P:294:LEU:HB3	16:1P:297:LEU:HD23	1.90	0.54
23:1X:84:TYR:HD2	23:1X:102:GLN:HB2	1.73	0.54
32:1g:43:ASP:OD1	33:1h:20:ARG:NH1	2.40	0.54
37:1l:156:TYR:CZ	37:1l:158:ILE:HG23	2.43	0.54
38:1m:64:LEU:O	38:1m:68:THR:HG23	2.07	0.54
4:1D:66:MET:HE1	4:1D:414:VAL:HG11	1.89	0.53
4:1D:68:LEU:HD22	4:1D:411:LEU:HD11	1.89	0.53
4:1D:263:SER:HA	4:1D:291:GLY:HA2	1.90	0.53
5:1E:98:TYR:CE2	5:1E:176:LEU:HD12	2.43	0.53
7:1G:143:GLY:HA2	7:1G:190:MET:HE1	1.88	0.53
7:1G:514:ILE:HG13	7:1G:519:PRO:HG3	1.90	0.53
8:1H:11:ILE:O	8:1H:15:LEU:HD22	2.09	0.53
10:1J:59:ILE:HD12	10:1J:60:TYR:N	2.22	0.53
12:1L:385:TYR:O	35:1j:35:TRP:NE1	2.41	0.53
13:1M:69:THR:HG22	13:1M:234:VAL:HG11	1.90	0.53
13:1M:209:LEU:HD21	13:1M:212:LEU:HD12	1.89	0.53
16:1P:121:SER:HB3	16:1P:126:VAL:HG11	1.89	0.53
19:1S:50:LEU:HD22	19:1S:51:PRO:HD2	1.89	0.53
21:1V:5:LYS:HZ3	21:1V:15:VAL:HG12	1.73	0.53
4:1D:212:TYR:CZ	4:1D:216:LYS:HD2	2.43	0.53
6:1F:37:GLN:OE1	6:1F:42:TRP:HD1	1.91	0.53
8:1H:117:LEU:HD23	8:1H:118:TRP:N	2.22	0.53
12:1L:117:PHE:O	12:1L:121:LEU:HD22	2.08	0.53
12:1L:466:PHE:HB3	35:1j:35:TRP:HZ2	1.74	0.53
13:1M:294:MET:N	13:1M:294:MET:SD	2.81	0.53
14:1N:153:LEU:HD23	14:1N:157:MET:HG3	1.89	0.53
17:1Q:67:ASN:OD1	17:1Q:72:TRP:N	2.30	0.53
20:1U:34:SER:OG	20:1U:36:PHE:HE2	1.91	0.53
24:1Y:65:ILE:HD12	24:1Y:65:ILE:H	1.73	0.53
33:1h:129:ASP:OD2	33:1h:130:LYS:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:335:ARG:HH12	9:1I:124:GLU:HA	1.73	0.53
7:1G:367:THR:HG22	7:1G:636:VAL:HG11	1.89	0.53
7:1G:544:ILE:HG23	7:1G:559:VAL:HG13	1.89	0.53
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.41	0.53
9:1I:4:PHE:HB3	9:1I:7:MET:HG2	1.91	0.53
9:1I:108:ARG:HH21	42:1q:130:THR:HG21	1.74	0.53
12:1L:79:SER:HB2	12:1L:136:ASN:HD22	1.74	0.53
13:1M:450:ASN:HD21	32:1g:78:ALA:HA	1.74	0.53
14:1N:190:MET:HG2	14:1N:204:ASN:HB3	1.90	0.53
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.40	0.53
21:1V:113:TRP:CG	21:1V:113:TRP:O	2.61	0.53
3:1C:32:ILE:HD11	21:1V:46:TYR:CD2	2.43	0.53
4:1D:51:PHE:HE1	8:1H:206:GLU:HA	1.73	0.53
5:1E:78:MET:HE1	7:1G:185:THR:C	2.34	0.53
6:1F:148:ASN:ND2	44:1s:40:ASN:OD1	2.42	0.53
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.90	0.53
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.90	0.53
13:1M:43:ASN:HD22	33:1h:80:TYR:HE2	1.55	0.53
13:1M:391:ILE:O	13:1M:394:ILE:HG22	2.08	0.53
14:1N:187:MET:HA	14:1N:190:MET:CE	2.38	0.53
15:1O:30:ASN:OD1	15:1O:31:ILE:N	2.42	0.53
16:1P:203:GLN:N	16:1P:291:ASP:OD1	2.37	0.53
20:1U:21:LEU:O	36:1k:46:ARG:NE	2.32	0.53
20:1U:88:GLU:O	34:1i:23:LYS:NZ	2.41	0.53
27:1b:40:TYR:O	27:1b:44:ILE:HG12	2.08	0.53
29:1d:2:MET:HE1	33:1h:122:TRP:CE3	2.44	0.53
31:1f:42:LEU:HA	31:1f:45:LYS:HD2	1.90	0.53
32:1g:64:PHE:HB3	32:1g:69:VAL:HG23	1.91	0.53
35:1j:11:TYR:O	35:1j:13:GLN:NE2	2.41	0.53
38:1m:90:ALA:O	38:1m:94:ILE:HG13	2.08	0.53
13:1M:28:THR:O	13:1M:31:SER:OG	2.24	0.53
22:1W:27:GLU:O	22:1W:31:ARG:HG2	2.08	0.53
25:1Z:88:ARG:O	25:1Z:92:GLU:HG2	2.08	0.53
32:1g:68:ILE:O	32:1g:73:GLY:N	2.40	0.53
34:1i:59:VAL:O	34:1i:63:THR:HG22	2.08	0.53
5:1E:45:ALA:HA	6:1F:198:GLY:HA3	1.90	0.53
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	1.91	0.53
8:1H:88:PRO:O	8:1H:90:PRO:CG	2.56	0.53
16:1P:21:ALA:HA	16:1P:90:VAL:HG23	1.90	0.53
33:1h:67:PHE:O	33:1h:73:ARG:NH2	2.42	0.53
43:1r:55:THR:O	43:1r:55:THR:OG1	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:48:LEU:HD22	3:1C:105:ILE:HD11	1.90	0.53
7:1G:104:ASP:O	7:1G:108:CYS:N	2.42	0.53
7:1G:650:LYS:HG2	7:1G:650:LYS:O	2.08	0.53
13:1M:178:ILE:HD11	13:1M:182:TRP:CD2	2.43	0.53
13:1M:373:ILE:HA	13:1M:376:ILE:HG12	1.91	0.53
14:1N:25:HIS:N	30:1e:14:ASP:OD2	2.22	0.53
30:1e:56:LYS:C	30:1e:56:LYS:HD3	2.34	0.53
34:1i:89:VAL:O	34:1i:95:THR:HG21	2.09	0.53
38:1m:70:ALA:HA	38:1m:74:ASN:HB3	1.89	0.53
43:1r:101:LYS:H	43:1r:101:LYS:HZ3	1.57	0.53
2:1B:49:THR:OG1	2:1B:50:PHE:N	2.39	0.53
5:1E:98:TYR:HD2	5:1E:157:ASN:HD21	1.57	0.53
11:1K:10:MET:HE1	11:1K:14:ILE:CG2	2.37	0.53
13:1M:270:ILE:HG13	13:1M:395:LEU:HD12	1.91	0.53
13:1M:459:TYR:O	41:1p:96:LYS:NZ	2.42	0.53
14:1N:309:ASN:ND2	15:1O:282:ILE:HA	2.24	0.53
15:1O:8:PHE:O	15:1O:13:ARG:NH1	2.41	0.53
15:1O:193:LYS:HD3	15:1O:193:LYS:H	1.73	0.53
22:1W:70:ASN:ND2	58:1W:201:EHZ:O1	2.42	0.53
24:1Y:21:ALA:O	24:1Y:25:THR:HG23	2.09	0.53
29:1d:90:MET:HE1	33:1h:107:GLU:HA	1.91	0.53
30:1e:49:ILE:HD11	33:1h:118:GLY:HA3	1.90	0.53
32:1g:62:PHE:HA	32:1g:66:PHE:CD1	2.43	0.53
32:1g:97:VAL:O	32:1g:101:GLU:HG3	2.09	0.53
37:1l:8:MET:O	37:1l:8:MET:HE2	2.09	0.53
2:1B:72:PHE:CE1	2:1B:157:LEU:HD11	2.44	0.53
7:1G:385:ARG:N	7:1G:392:ASN:HD22	2.07	0.53
7:1G:418:ARG:HD3	44:1s:75:HIS:CG	2.44	0.53
7:1G:562:PRO:HB2	7:1G:593:ALA:HB2	1.90	0.53
8:1H:2:PHE:O	8:1H:6:ILE:HG13	2.09	0.53
8:1H:149:ILE:HG23	8:1H:181:LEU:HG	1.91	0.53
8:1H:215:TYR:C	8:1H:220:PHE:HB2	2.34	0.53
9:1I:123:GLN:OE1	9:1I:133:GLU:N	2.42	0.53
12:1L:6:SER:O	12:1L:10:THR:HG23	2.08	0.53
12:1L:319:ILE:CD1	12:1L:321:GLN:HB2	2.38	0.53
13:1M:262:LEU:HD23	13:1M:299:VAL:HG12	1.91	0.53
15:1O:190:HIS:HA	15:1O:193:LYS:HZ3	1.72	0.53
16:1P:136:ASN:HD21	16:1P:291:ASP:HA	1.74	0.53
16:1P:200:THR:O	16:1P:238:LEU:N	2.41	0.53
17:1Q:11:ILE:O	22:1W:16:SER:HA	2.09	0.53
1:1A:12:THR:O	1:1A:16:LEU:HG	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:49:LEU:HD13	1:1A:50:PRO:HD2	1.91	0.53
4:1D:203:LEU:H	4:1D:203:LEU:HD12	1.73	0.53
7:1G:357:ASP:OD2	19:1S:44:LYS:NZ	2.37	0.53
12:1L:316:THR:HB	12:1L:325:ALA:HB2	1.90	0.53
14:1N:24:SER:HB3	30:1e:1:PRO:HG3	1.91	0.53
14:1N:200:MET:HE3	14:1N:265:MET:HB3	1.90	0.53
15:1O:180:GLN:O	15:1O:183:ILE:HG13	2.09	0.53
22:1W:40:TYR:O	22:1W:60:ARG:NH1	2.42	0.53
23:1X:148:GLU:OE2	30:1e:50:ARG:NH2	2.40	0.53
31:1f:49:ARG:NE	31:1f:52:GLU:OE1	2.37	0.53
33:1h:62:GLU:HG3	33:1h:64:TRP:CE2	2.45	0.53
2:1B:86:MET:HE1	2:1B:100:LEU:HD21	1.91	0.52
7:1G:606:ILE:HG12	22:1W:119:LEU:HD21	1.91	0.52
10:1J:12:ILE:HA	10:1J:15:ILE:HD11	1.91	0.52
12:1L:413:LEU:HB2	12:1L:493:VAL:HG11	1.92	0.52
12:1L:564:LYS:HG3	38:1m:76:TYR:CE2	2.44	0.52
15:1O:47:GLY:O	15:1O:120:GLN:NE2	2.38	0.52
31:1f:34:LEU:HD21	33:1h:93:ILE:HD11	1.91	0.52
34:1i:12:GLN:HB3	34:1i:15:ARG:NH2	2.24	0.52
47:1D:501:U10:H262	8:1H:274:ARG:NH2	2.24	0.52
8:1H:10:ILE:HG23	8:1H:83:LEU:CD2	2.38	0.52
13:1M:244:MET:HE3	13:1M:301:ILE:HD12	1.91	0.52
13:1M:245:ARG:HA	13:1M:245:ARG:HH11	1.73	0.52
13:1M:279:GLN:HB2	13:1M:285:LEU:HD13	1.90	0.52
16:1P:235:ARG:NH2	16:1P:293:THR:OG1	2.42	0.52
20:1U:35:HIS:HB3	20:1U:37:MET:HE1	1.91	0.52
22:1W:95:ASN:HB2	22:1W:97:TRP:CZ3	2.44	0.52
39:1n:125:LYS:O	39:1n:129:ARG:HG2	2.09	0.52
2:1B:51:GLY:HA3	2:1B:56:ALA:HB2	1.91	0.52
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.10	0.52
11:1K:8:ILE:HD12	11:1K:9:ILE:N	2.25	0.52
12:1L:322:PRO:HD2	12:1L:323:HIS:CE1	2.43	0.52
13:1M:24:TRP:NE1	13:1M:92:LYS:HD3	2.24	0.52
15:1O:135:LEU:HD21	15:1O:149:VAL:HG22	1.90	0.52
16:1P:300:LEU:HD22	16:1P:305:ILE:HD11	1.91	0.52
18:1R:57:ILE:HG21	18:1R:91:PHE:CD2	2.45	0.52
20:1T:36:PHE:CE1	20:1T:40:LEU:HD23	2.43	0.52
23:1X:43:MET:HA	23:1X:46:ARG:HB2	1.92	0.52
28:1c:40:LEU:HA	28:1c:43:LYS:HZ1	1.71	0.52
32:1g:83:TYR:CE1	32:1g:84:ARG:HG3	2.43	0.52
41:1p:124:CYS:O	41:1p:128:LEU:N	2.32	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:108:GLN:C	1:1A:109:LYS:HE2	2.34	0.52
6:1F:112:ARG:O	44:1s:40:ASN:ND2	2.42	0.52
10:1J:13:PHE:CE2	11:1K:8:ILE:HG22	2.45	0.52
11:1K:12:PHE:CE2	14:1N:72:MET:HB2	2.44	0.52
12:1L:28:LYS:HE2	12:1L:30:ASN:HB3	1.92	0.52
13:1M:28:THR:O	13:1M:32:LEU:HD22	2.10	0.52
20:1U:52:MET:CG	39:1n:24:ARG:HH21	2.22	0.52
21:1V:72:GLN:HG3	43:1r:99:PRO:HG2	1.92	0.52
32:1g:41:ASN:O	32:1g:44:SER:OG	2.14	0.52
32:1g:107:LEU:CD2	41:1p:108:ARG:HH12	2.22	0.52
37:1l:6:LYS:HE3	37:1l:6:LYS:HA	1.91	0.52
39:1n:138:GLN:HG3	39:1n:158:LYS:HZ1	1.75	0.52
39:1n:168:HIS:CE1	39:1n:169:ILE:HG13	2.44	0.52
41:1p:72:ASP:O	41:1p:76:CYS:N	2.42	0.52
2:1B:166:LYS:HA	2:1B:169:ARG:HH12	1.74	0.52
7:1G:385:ARG:HD3	7:1G:415:LEU:HA	1.92	0.52
9:1I:136:ASN:OD1	9:1I:138:GLU:N	2.42	0.52
12:1L:375:ILE:HD11	12:1L:458:LEU:HD11	1.89	0.52
14:1N:325:LEU:HG	53:1N:401:CDL:H781	1.91	0.52
15:1O:210:PHE:CD1	15:1O:211:LEU:HD13	2.44	0.52
16:1P:110:PHE:CD1	16:1P:149:LYS:HD3	2.45	0.52
22:1W:111:GLU:OE1	22:1W:111:GLU:N	2.37	0.52
35:1j:33:TRP:HA	35:1j:36:ILE:HG22	1.90	0.52
40:1o:108:LEU:HD22	40:1o:112:LYS:NZ	2.24	0.52
7:1G:107:ILE:HD13	9:1I:78:ILE:HB	1.91	0.52
12:1L:306:THR:HG22	12:1L:336:LYS:HG2	1.90	0.52
13:1M:278:ARG:O	38:1m:71:ARG:NH2	2.43	0.52
14:1N:278:MET:HG2	24:1Y:134:VAL:O	2.09	0.52
24:1Y:97:GLY:O	24:1Y:100:LEU:HG	2.09	0.52
26:1a:1:MET:HE2	26:1a:1:MET:N	2.25	0.52
26:1a:64:LYS:HB3	26:1a:68:ASN:HB2	1.91	0.52
28:1c:41:GLU:O	28:1c:45:ARG:HB2	2.10	0.52
36:1k:13:MET:HE2	36:1k:13:MET:HA	1.91	0.52
5:1E:43:LYS:NZ	5:1E:74:GLN:OE1	2.32	0.52
5:1E:156:ILE:HD12	5:1E:156:ILE:O	2.10	0.52
11:1K:81:VAL:O	11:1K:85:TYR:HB2	2.10	0.52
12:1L:125:LEU:HD13	12:1L:129:MET:SD	2.48	0.52
12:1L:347:ILE:HG12	12:1L:354:GLN:HG2	1.90	0.52
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.91	0.52
13:1M:151:PHE:CD1	14:1N:287:LEU:HD12	2.45	0.52
15:1O:305:SER:HA	29:1d:50:ARG:CZ	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:133:SER:O	16:1P:167:LYS:HA	2.09	0.52
22:1W:115:PRO:O	22:1W:121:LYS:NZ	2.40	0.52
31:1f:38:ARG:O	31:1f:40:LYS:HD2	2.09	0.52
32:1g:110:SER:OG	41:1p:161:ARG:NH2	2.43	0.52
40:1o:117:ARG:HD2	40:1o:118:GLU:N	2.25	0.52
1:1A:63:LEU:HD12	10:1J:66:VAL:CG2	2.37	0.52
4:1D:19:MET:HE2	14:1N:295:ARG:HH22	1.75	0.52
12:1L:573:MET:HA	12:1L:576:MET:HG3	1.92	0.52
12:1L:586:LEU:O	12:1L:590:SER:OG	2.28	0.52
13:1M:265:SER:O	13:1M:269:MET:N	2.37	0.52
14:1N:289:ASN:HA	14:1N:292:PHE:CZ	2.44	0.52
14:1N:311:MET:O	14:1N:314:LYS:HB2	2.10	0.52
16:1P:22:THR:HG21	16:1P:85:VAL:HG12	1.91	0.52
20:1U:50:ILE:HD12	20:1U:51:ILE:N	2.25	0.52
25:1Z:129:THR:HB	25:1Z:132:GLU:HG3	1.91	0.52
44:1s:40:ASN:HA	44:1s:42:GLN:HE22	1.75	0.52
6:1F:100:GLY:HA2	6:1F:139:ARG:HH12	1.75	0.52
7:1G:404:LEU:O	17:1Q:127:ARG:NH1	2.36	0.52
8:1H:77:LEU:HD22	8:1H:81:LEU:HD23	1.92	0.52
12:1L:188:TRP:CE3	12:1L:212:PRO:HG3	2.44	0.52
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.44	0.52
13:1M:342:MET:HE3	13:1M:342:MET:O	2.10	0.52
15:1O:221:LEU:HD21	15:1O:241:LEU:HD11	1.90	0.52
15:1O:282:ILE:HD12	15:1O:282:ILE:N	2.25	0.52
16:1P:328:THR:HA	22:1W:51:GLN:NE2	2.24	0.52
20:1U:6:LEU:O	20:1U:86:VAL:HG13	2.09	0.52
20:1U:19:LEU:HD22	20:1U:76:ILE:HG13	1.92	0.52
24:1Y:61:THR:HG23	24:1Y:103:ARG:HG3	1.92	0.52
40:1o:108:LEU:HD22	40:1o:112:LYS:HZ2	1.75	0.52
2:1B:108:PRO:HB2	8:1H:58:LYS:NZ	2.24	0.52
2:1B:115:SER:OG	2:1B:121:ASN:OD1	2.24	0.52
5:1E:87:TYR:CD1	6:1F:181:ALA:HB3	2.43	0.52
6:1F:15:LEU:HB2	6:1F:271:GLU:H	1.74	0.52
6:1F:42:TRP:HZ2	6:1F:119:VAL:HG23	1.74	0.52
11:1K:63:LEU:HD12	14:1N:71:MET:HE3	1.91	0.52
13:1M:294:MET:HA	13:1M:297:VAL:HG12	1.92	0.52
14:1N:310:ASN:HD22	15:1O:275:ILE:HD11	1.74	0.52
15:1O:26:THR:OG1	15:1O:28:ASP:OD1	2.24	0.52
17:1Q:37:ILE:HD11	17:1Q:105:VAL:HA	1.91	0.52
20:1U:47:GLN:HG3	20:1U:51:ILE:HG12	1.92	0.52
28:1c:32:ILE:HD12	28:1c:33:LYS:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:158:ILE:HG21	40:1o:30:PHE:CE2	2.45	0.52
2:1B:128:TYR:CD1	3:1C:194:PHE:HB2	2.45	0.51
2:1B:128:TYR:OH	3:1C:192:GLN:HG3	2.10	0.51
3:1C:175:ARG:NH2	3:1C:186:GLU:OE2	2.36	0.51
7:1G:385:ARG:HD2	7:1G:416:THR:HG23	1.90	0.51
8:1H:27:VAL:O	8:1H:31:MET:HG3	2.09	0.51
20:1U:45:LEU:C	20:1U:47:GLN:H	2.17	0.51
22:1W:115:PRO:HG2	22:1W:121:LYS:HE3	1.91	0.51
36:1k:22:LYS:HB2	36:1k:24:GLU:OE1	2.10	0.51
39:1n:68:GLU:OE1	39:1n:68:GLU:N	2.43	0.51
39:1n:120:LYS:HA	39:1n:123:GLN:OE1	2.10	0.51
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.35	0.51
7:1G:107:ILE:HD12	7:1G:215:PHE:HE2	1.75	0.51
7:1G:427:LYS:O	7:1G:430:GLN:HG2	2.11	0.51
8:1H:9:LEU:O	8:1H:13:ILE:HG12	2.11	0.51
12:1L:407:TRP:CE2	37:1l:115:MET:HB3	2.45	0.51
16:1P:157:ARG:HH21	16:1P:165:ILE:HG12	1.75	0.51
29:1d:100:ASP:OD1	33:1h:117:ARG:NH1	2.43	0.51
33:1h:55:ILE:HD13	33:1h:57:GLU:OE2	2.11	0.51
39:1n:134:ARG:O	39:1n:137:LYS:HG3	2.11	0.51
40:1o:6:ARG:HB2	40:1o:15:GLU:HG3	1.92	0.51
42:1q:55:PHE:HB3	43:1r:1:ALA:C	2.36	0.51
7:1G:440:SER:HA	7:1G:443:LEU:HD12	1.93	0.51
8:1H:79:LEU:HD22	8:1H:222:MET:HG3	1.91	0.51
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.92	0.51
11:1K:5:TYR:HA	11:1K:8:ILE:HD11	1.91	0.51
12:1L:68:TRP:HB3	12:1L:69:MET:CE	2.40	0.51
13:1M:216:LEU:HG	13:1M:220:HIS:CE1	2.46	0.51
13:1M:358:TRP:HA	13:1M:361:MET:SD	2.50	0.51
13:1M:398:MET:O	13:1M:402:ILE:HG12	2.10	0.51
14:1N:68:MET:HA	14:1N:68:MET:HE3	1.92	0.51
14:1N:308:THR:O	14:1N:311:MET:HB3	2.10	0.51
15:1O:94:TYR:CG	15:1O:148:CYS:HB3	2.46	0.51
20:1U:62:ILE:HG23	39:1n:20:LYS:HZ1	1.76	0.51
22:1W:23:ARG:HA	22:1W:23:ARG:NH1	2.25	0.51
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.29	0.51
36:1k:22:LYS:N	36:1k:22:LYS:HD2	2.24	0.51
37:1l:58:ARG:O	37:1l:70:ARG:NH1	2.43	0.51
1:1A:15:SER:HA	1:1A:18:VAL:HG22	1.92	0.51
1:1A:41:PHE:CD2	4:1D:53:PRO:HD3	2.45	0.51
2:1B:152:THR:OG1	2:1B:154:GLU:OE1	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:169:ARG:HG2	2:1B:169:ARG:O	2.11	0.51
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.74	0.51
8:1H:233:MET:HE3	8:1H:234:MET:N	2.24	0.51
9:1I:83:CYS:SG	9:1I:109:TYR:OH	2.69	0.51
10:1J:52:LEU:O	10:1J:56:VAL:HG12	2.11	0.51
12:1L:590:SER:O	12:1L:594:THR:OG1	2.19	0.51
13:1M:210:TYR:HA	13:1M:213:HIS:CD2	2.45	0.51
15:1O:43:ALA:HB2	15:1O:123:VAL:HG11	1.91	0.51
15:1O:207:LYS:HA	15:1O:211:LEU:HD23	1.92	0.51
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.11	0.51
29:1d:44:ILE:O	29:1d:48:ILE:HG12	2.10	0.51
34:1i:10:ARG:HD3	39:1n:155:PRO:HA	1.91	0.51
34:1i:56:TRP:CE2	34:1i:57:LYS:HG2	2.46	0.51
34:1i:74:VAL:O	34:1i:78:VAL:HG23	2.10	0.51
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.90	0.51
1:1A:44:MET:HE1	8:1H:126:LYS:NZ	2.24	0.51
4:1D:223:ASP:OD1	43:1r:17:ARG:NH2	2.42	0.51
8:1H:281:ARG:HE	8:1H:284:GLN:CD	2.11	0.51
12:1L:203:MET:HA	41:1p:120:TYR:HE2	1.74	0.51
12:1L:435:PRO:HB2	36:1k:51:ARG:HD2	1.92	0.51
15:1O:227:GLU:OE2	15:1O:234:VAL:HG13	2.10	0.51
20:1U:35:HIS:O	20:1U:39:ASP:HB2	2.10	0.51
22:1W:29:LYS:O	22:1W:33:ARG:NE	2.30	0.51
39:1n:131:SER:HB2	39:1n:162:LEU:HB2	1.91	0.51
39:1n:139:LEU:O	39:1n:143:THR:OG1	2.21	0.51
39:1n:175:GLU:O	39:1n:176:ARG:NH1	2.43	0.51
4:1D:40:LYS:HZ1	11:1K:85:TYR:HD1	1.59	0.51
6:1F:150:GLN:HE22	44:1s:51:PHE:HD2	1.57	0.51
8:1H:135:ALA:O	8:1H:139:THR:HG22	2.10	0.51
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.76	0.51
12:1L:322:PRO:HG2	12:1L:323:HIS:HD1	1.76	0.51
13:1M:25:ILE:O	13:1M:29:VAL:HG23	2.10	0.51
15:1O:145:ARG:NH2	15:1O:281:GLU:OE1	2.42	0.51
24:1Y:47:SER:N	24:1Y:50:GLU:OE1	2.40	0.51
24:1Y:72:THR:HA	24:1Y:75:ILE:HG12	1.92	0.51
28:1c:39:VAL:O	28:1c:43:LYS:HG3	2.11	0.51
32:1g:59:ARG:O	32:1g:63:PHE:HB2	2.10	0.51
33:1h:16:PHE:H	39:1n:107:HIS:CE1	2.28	0.51
5:1E:145:LEU:HD13	5:1E:160:TYR:CZ	2.46	0.51
10:1J:18:VAL:HA	11:1K:14:ILE:HD13	1.93	0.51
11:1K:26:LEU:N	11:1K:88:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:88:MET:HB3	12:1L:326:PHE:CZ	2.46	0.51
13:1M:119:TYR:CE2	13:1M:161:LEU:HB2	2.45	0.51
13:1M:268:GLY:O	13:1M:272:THR:HG22	2.10	0.51
15:1O:90:ASP:HA	32:1g:24:ILE:HD13	1.93	0.51
16:1P:137:ALA:HA	16:1P:146:LEU:HB3	1.92	0.51
16:1P:176:ASP:OD1	16:1P:179:LEU:N	2.44	0.51
26:1a:66:LEU:HD12	26:1a:66:LEU:H	1.74	0.51
2:1B:96:MET:O	2:1B:96:MET:HE3	2.10	0.51
3:1C:65:ARG:HA	3:1C:72:PHE:O	2.11	0.51
7:1G:588:THR:HG21	17:1Q:64:ARG:H	1.75	0.51
8:1H:79:LEU:O	8:1H:83:LEU:HD12	2.11	0.51
10:1J:110:GLU:O	10:1J:112:GLU:HG2	2.11	0.51
13:1M:2:LEU:HD22	13:1M:6:ILE:HD11	1.93	0.51
14:1N:206:LEU:O	14:1N:210:THR:HG22	2.10	0.51
14:1N:207:ILE:HG21	14:1N:262:PRO:HG2	1.93	0.51
20:1T:83:LYS:HG3	20:1T:84:LYS:N	2.26	0.51
21:1V:25:ILE:HG13	21:1V:26:LEU:HD22	1.93	0.51
22:1W:114:ARG:HA	22:1W:114:ARG:HH11	1.76	0.51
23:1X:93:LEU:HB2	23:1X:95:LEU:HG	1.92	0.51
32:1g:90:ARG:HA	41:1p:100:GLU:HG3	1.93	0.51
34:1i:46:TRP:HZ3	34:1i:60:ILE:HG22	1.75	0.51
34:1i:106:GLY:H	34:1i:116:ILE:HG23	1.75	0.51
37:1l:77:ILE:HD11	38:1m:67:TRP:CG	2.46	0.51
2:1B:152:THR:O	2:1B:155:ALA:N	2.44	0.51
2:1B:175:ILE:HG21	16:1P:51:CYS:HA	1.93	0.51
4:1D:161:ILE:HG22	8:1H:278:PRO:HB3	1.92	0.51
6:1F:104:THR:HA	6:1F:106:LYS:HZ2	1.75	0.51
12:1L:325:ALA:O	12:1L:329:ILE:HG22	2.11	0.51
12:1L:367:PRO:O	12:1L:371:THR:HG23	2.11	0.51
13:1M:193:ILE:HD12	13:1M:194:PHE:H	1.74	0.51
15:1O:91:GLY:C	15:1O:95:ARG:HE	2.19	0.51
20:1U:24:LYS:HG3	36:1k:41:ARG:CZ	2.41	0.51
20:1U:52:MET:HG3	39:1n:24:ARG:HH21	1.76	0.51
23:1X:84:TYR:CE2	23:1X:99:CYS:HB3	2.46	0.51
24:1Y:65:ILE:HG23	24:1Y:96:GLY:HA3	1.93	0.51
37:1l:7:ASP:O	37:1l:26:LYS:NZ	2.33	0.51
39:1n:163:PRO:HG2	39:1n:166:TRP:HB3	1.92	0.51
1:1A:30:TYR:CE1	1:1A:32:GLU:HG2	2.46	0.51
4:1D:220:PHE:CD2	43:1r:22:LYS:HE3	2.46	0.51
7:1G:60:GLU:HG2	7:1G:61:LYS:HE2	1.93	0.51
8:1H:92:PRO:HG3	8:1H:255:TYR:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:43:MET:HG3	14:1N:75:ILE:HG21	1.93	0.51
12:1L:596:MET:SD	12:1L:596:MET:N	2.84	0.51
14:1N:230:LEU:O	14:1N:233:THR:OG1	2.26	0.51
14:1N:316:GLN:OE1	14:1N:316:GLN:N	2.44	0.51
15:1O:246:GLY:O	15:1O:249:PRO:HD2	2.10	0.51
21:1V:88:SER:HB3	21:1V:92:LYS:HZ1	1.74	0.51
22:1W:51:GLN:HA	22:1W:51:GLN:OE1	2.10	0.51
25:1Z:98:MET:HG3	25:1Z:104:TRP:CD2	2.46	0.51
34:1i:99:ARG:NH1	41:1p:117:GLY:HA2	2.26	0.51
36:1k:44:TRP:CH2	36:1k:48:GLU:HB2	2.46	0.51
47:1D:501:U10:H412	8:1H:55:LEU:HD12	1.93	0.50
7:1G:535:GLN:OE1	7:1G:535:GLN:N	2.37	0.50
10:1J:121:GLY:HA2	11:1K:3:LEU:HD11	1.94	0.50
12:1L:312:LEU:HD23	12:1L:328:HIS:NE2	2.25	0.50
12:1L:424:THR:HA	12:1L:427:ILE:HD12	1.92	0.50
12:1L:489:THR:O	12:1L:493:VAL:HG22	2.11	0.50
13:1M:29:VAL:HG13	32:1g:64:PHE:HE2	1.77	0.50
13:1M:50:LEU:N	13:1M:58:SER:O	2.44	0.50
13:1M:168:GLN:HE22	33:1h:104:ARG:NH1	2.09	0.50
14:1N:282:MET:SD	14:1N:282:MET:N	2.72	0.50
15:1O:233:LYS:HE3	21:1V:91:ARG:HD3	1.92	0.50
20:1T:79:TYR:CD1	20:1T:80:ILE:HD12	2.45	0.50
31:1f:49:ARG:HE	31:1f:52:GLU:CD	2.19	0.50
35:1j:50:HIS:HB3	35:1j:51:PHE:CD2	2.46	0.50
37:1l:127:PRO:HD3	40:1o:3:HIS:CE1	2.45	0.50
38:1m:40:SER:O	38:1m:44:ARG:HG2	2.11	0.50
41:1p:5:ASP:OD2	41:1p:8:VAL:HG22	2.11	0.50
4:1D:87:THR:HA	4:1D:90:LEU:HB2	1.93	0.50
5:1E:48:LEU:HD11	5:1E:87:TYR:HE1	1.77	0.50
5:1E:183:LYS:HD3	44:1s:44:HIS:ND1	2.26	0.50
10:1J:40:GLY:O	10:1J:44:VAL:HG12	2.11	0.50
11:1K:48:ILE:HD13	11:1K:56:ALA:HB1	1.92	0.50
12:1L:15:LEU:HD12	12:1L:15:LEU:O	2.11	0.50
12:1L:362:LEU:HB2	12:1L:431:PHE:CD1	2.47	0.50
12:1L:402:SER:O	12:1L:404:THR:HG23	2.11	0.50
13:1M:76:MET:H	13:1M:76:MET:CE	2.25	0.50
16:1P:101:THR:HG22	16:1P:103:ASN:H	1.76	0.50
16:1P:220:ASP:OD1	16:1P:223:ALA:N	2.45	0.50
16:1P:328:THR:HB	22:1W:48:HIS:CE1	2.44	0.50
20:1T:52:MET:HB3	22:1W:41:ARG:HH12	1.75	0.50
33:1h:76:ALA:HA	33:1h:80:TYR:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:71:LYS:HG3	36:1k:72:TRP:CE3	2.46	0.50
6:1F:42:TRP:CZ2	6:1F:119:VAL:HG23	2.46	0.50
7:1G:70:ALA:O	7:1G:71:MET:HE2	2.11	0.50
12:1L:362:LEU:HB3	12:1L:366:MET:HB2	1.92	0.50
13:1M:187:SER:OG	13:1M:188:ASN:N	2.45	0.50
13:1M:410:MET:HE3	13:1M:411:LEU:N	2.26	0.50
18:1R:5:SER:N	18:1R:9:GLU:O	2.35	0.50
20:1T:48:VAL:HG12	20:1T:52:MET:HE1	1.94	0.50
22:1W:99:GLN:CD	22:1W:100:ARG:H	2.19	0.50
29:1d:113:LEU:HD13	32:1g:121:PRO:HG2	1.92	0.50
34:1i:82:HIS:CE1	34:1i:86:LYS:HG2	2.46	0.50
38:1m:44:ARG:HH21	39:1n:139:LEU:HD22	1.76	0.50
40:1o:59:ALA:O	40:1o:63:ILE:HD12	2.11	0.50
40:1o:68:CYS:O	40:1o:72:SER:OG	2.30	0.50
43:1r:63:MET:HE2	43:1r:63:MET:HA	1.92	0.50
2:1B:35:ASP:HA	2:1B:38:ASN:HD21	1.77	0.50
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.46	0.50
5:1E:22:ASP:O	5:1E:57:GLN:NE2	2.44	0.50
5:1E:46:ALA:O	5:1E:50:VAL:HG12	2.12	0.50
5:1E:155:GLN:HB2	5:1E:160:TYR:CD1	2.46	0.50
6:1F:121:GLY:HA3	6:1F:228:VAL:O	2.11	0.50
6:1F:165:ASN:OD1	6:1F:170:GLY:N	2.42	0.50
6:1F:261:HIS:H	6:1F:336:VAL:HG22	1.75	0.50
7:1G:383:ASN:ND2	7:1G:665:GLN:O	2.45	0.50
8:1H:224:PHE:HD1	8:1H:224:PHE:O	1.94	0.50
9:1I:64:GLU:OE1	9:1I:136:ASN:ND2	2.45	0.50
10:1J:86:ASN:HD21	10:1J:88:THR:HB	1.76	0.50
12:1L:88:MET:HB3	12:1L:326:PHE:HZ	1.75	0.50
13:1M:355:MET:HA	13:1M:355:MET:HE3	1.92	0.50
17:1Q:38:PHE:CE1	17:1Q:58:GLU:HG3	2.47	0.50
23:1X:122:GLY:N	25:1Z:66:GLU:OE1	2.40	0.50
39:1n:24:ARG:N	39:1n:25:HIS:HB2	2.17	0.50
40:1o:105:ARG:O	40:1o:109:GLN:HG2	2.11	0.50
3:1C:193:GLU:OE2	7:1G:223:ARG:NH2	2.45	0.50
4:1D:23:LYS:HA	4:1D:23:LYS:HE2	1.92	0.50
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.93	0.50
7:1G:276:ARG:HH21	7:1G:277:GLN:HG3	1.77	0.50
12:1L:176:ARG:NH1	13:1M:404:ALA:HB3	2.26	0.50
12:1L:237:MET:HB2	12:1L:244:SER:HB2	1.94	0.50
12:1L:484:LEU:HD22	35:1j:53:TYR:HB3	1.92	0.50
15:1O:161:CYS:SG	15:1O:162:GLU:N	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.93	0.50
21:1V:88:SER:HB3	21:1V:92:LYS:NZ	2.27	0.50
28:1c:27:LEU:HD12	29:1d:70:PHE:CD1	2.38	0.50
4:1D:218:PHE:HD2	4:1D:308:LEU:HD21	1.76	0.50
12:1L:246:LEU:HD12	12:1L:247:LEU:HD12	1.94	0.50
12:1L:331:MET:C	12:1L:331:MET:HE2	2.37	0.50
12:1L:492:ILE:HD13	51:1L:701:MYR:H131	1.94	0.50
12:1L:557:TRP:O	12:1L:561:ILE:HG12	2.11	0.50
13:1M:282:LEU:HD13	13:1M:286:ILE:HD11	1.94	0.50
13:1M:356:ALA:HA	13:1M:359:TRP:HD1	1.76	0.50
14:1N:162:ILE:HA	14:1N:185:ALA:HA	1.91	0.50
15:1O:42:ILE:HG12	15:1O:235:VAL:HG12	1.94	0.50
20:1U:48:VAL:O	20:1U:51:ILE:HB	2.11	0.50
26:1a:1:MET:HE2	26:1a:1:MET:H3	1.77	0.50
39:1n:97:LYS:HE3	39:1n:173:PRO:HB2	1.94	0.50
47:1D:501:U10:H303	8:1H:202:GLU:OE2	2.11	0.50
7:1G:115:ASP:O	7:1G:119:GLN:HG2	2.12	0.50
8:1H:137:ALA:O	8:1H:141:SER:OG	2.28	0.50
11:1K:90:VAL:HG22	12:1L:585:LYS:NZ	2.27	0.50
13:1M:11:LEU:HG	13:1M:14:MET:HE2	1.93	0.50
14:1N:87:THR:OG1	14:1N:88:LYS:N	2.44	0.50
14:1N:103:ALA:HB2	14:1N:157:MET:HE1	1.93	0.50
14:1N:164:ILE:H	14:1N:164:ILE:HD12	1.76	0.50
16:1P:8:HIS:N	16:1P:16:VAL:O	2.39	0.50
20:1T:15:VAL:HG23	20:1T:58:PHE:HZ	1.76	0.50
23:1X:36:ASP:OD2	27:1b:68:HIS:NE2	2.44	0.50
27:1b:39:ASN:N	27:1b:39:ASN:OD1	2.45	0.50
32:1g:48:ASP:OD1	32:1g:53:VAL:HG23	2.12	0.50
34:1i:99:ARG:HD3	34:1i:100:LYS:O	2.11	0.50
35:1j:10:ARG:NH2	35:1j:14:PHE:O	2.45	0.50
41:1p:91:TRP:NE1	41:1p:154:CYS:SG	2.84	0.50
4:1D:4:TRP:O	13:1M:142:ARG:NH2	2.42	0.50
6:1F:24:ASN:OD1	6:1F:28:ARG:N	2.44	0.50
6:1F:374:LYS:NZ	7:1G:133:GLY:O	2.29	0.50
12:1L:176:ARG:CZ	13:1M:404:ALA:H	2.24	0.50
12:1L:425:ARG:HG3	12:1L:428:PHE:HE1	1.76	0.50
14:1N:315:TRP:CD1	14:1N:315:TRP:N	2.79	0.50
15:1O:3:TYR:CD2	15:1O:261:MET:HE2	2.47	0.50
15:1O:141:GLN:HG3	15:1O:198:TYR:HD2	1.76	0.50
19:1S:19:ARG:HG2	19:1S:53:LEU:HB2	1.94	0.50
20:1U:14:ARG:NH1	20:1U:14:ARG:HA	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:65:PHE:O	25:1Z:68:ARG:N	2.45	0.50
27:1b:27:LEU:HB3	27:1b:31:LEU:CD2	2.42	0.50
28:1c:32:ILE:HD12	28:1c:33:LYS:H	1.77	0.50
33:1h:59:TYR:HE2	41:1p:63:TYR:HE2	1.60	0.50
34:1i:71:VAL:HA	34:1i:75:LEU:HD23	1.93	0.50
39:1n:64:ARG:O	39:1n:68:GLU:HB2	2.12	0.50
40:1o:27:ASP:HA	40:1o:30:PHE:HB2	1.93	0.50
40:1o:95:VAL:HA	40:1o:98:MET:HE3	1.94	0.50
41:1p:12:PRO:HD2	41:1p:115:ARG:HE	1.76	0.50
4:1D:83:LEU:O	4:1D:83:LEU:HD13	2.12	0.50
4:1D:206:GLY:N	25:1Z:9:ASP:OD1	2.41	0.50
5:1E:119:ALA:HB1	5:1E:169:ILE:HD11	1.93	0.50
7:1G:237:ASN:ND2	7:1G:581:GLN:OE1	2.45	0.50
7:1G:500:VAL:O	7:1G:504:ASP:N	2.44	0.50
11:1K:12:PHE:CD2	14:1N:72:MET:HE3	2.45	0.50
12:1L:552:LEU:HD13	37:1l:42:MET:HE1	1.92	0.50
13:1M:72:LEU:O	13:1M:73:LEU:C	2.55	0.50
16:1P:30:LEU:O	16:1P:34:VAL:HG12	2.12	0.50
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD21	1.92	0.50
16:1P:186:ARG:NH1	16:1P:186:ARG:O	2.44	0.50
20:1T:66:ASP:O	20:1T:70:LEU:HD13	2.12	0.50
21:1V:67:LEU:HA	21:1V:70:GLN:NE2	2.27	0.50
33:1h:87:TYR:O	33:1h:90:THR:HG22	2.12	0.50
35:1j:55:ASP:OD2	35:1j:58:GLN:NE2	2.45	0.50
36:1k:41:ARG:NH2	36:1k:46:ARG:HH12	2.09	0.50
38:1m:27:GLU:N	38:1m:27:GLU:OE2	2.41	0.50
38:1m:36:LEU:HD23	38:1m:36:LEU:H	1.77	0.50
40:1o:24:PHE:CE1	40:1o:104:GLU:HB2	2.46	0.50
3:1C:51:PHE:HE1	3:1C:108:LYS:HD3	1.76	0.49
3:1C:59:PRO:O	3:1C:62:THR:OG1	2.24	0.49
3:1C:179:GLU:OE2	16:1P:37:HIS:NE2	2.45	0.49
7:1G:337:ARG:HE	7:1G:609:MET:HB2	1.76	0.49
8:1H:70:MET:HE2	10:1J:28:TYR:CE1	2.47	0.49
10:1J:5:ILE:HD11	25:1Z:142:TRP:HZ2	1.77	0.49
12:1L:198:LEU:HA	12:1L:201:ILE:HD12	1.94	0.49
12:1L:338:MET:HE1	12:1L:375:ILE:HG13	1.94	0.49
15:1O:190:HIS:HA	15:1O:193:LYS:NZ	2.27	0.49
34:1i:24:ASP:HB2	39:1n:120:LYS:HD3	1.94	0.49
37:1l:54:SER:N	37:1l:91:THR:OG1	2.43	0.49
38:1m:84:LYS:O	38:1m:88:LEU:HD22	2.12	0.49
43:1r:43:GLY:H	43:1r:46:HIS:CD2	2.30	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:190:ARG:HA	5:1E:194:GLU:HG2	1.94	0.49
6:1F:68:ARG:HB2	6:1F:227:THR:OG1	2.12	0.49
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.47	0.49
12:1L:593:ILE:HD12	12:1L:594:THR:N	2.26	0.49
13:1M:36:LEU:HG	32:1g:69:VAL:HG22	1.94	0.49
13:1M:159:PRO:HG3	14:1N:284:MET:HE1	1.94	0.49
17:1Q:20:THR:HG23	17:1Q:30:ILE:HG12	1.94	0.49
21:1V:30:ILE:HD11	21:1V:51:THR:HG21	1.94	0.49
25:1Z:43:LEU:HB3	25:1Z:47:TYR:HE2	1.76	0.49
28:1c:25:VAL:O	28:1c:29:ILE:HG13	2.12	0.49
37:1l:125:TYR:O	40:1o:3:HIS:NE2	2.41	0.49
38:1m:49:GLN:O	38:1m:55:ARG:NE	2.33	0.49
1:1A:93:PHE:HE1	10:1J:155:ILE:HG12	1.76	0.49
3:1C:93:VAL:HG21	4:1D:377:TYR:CE2	2.47	0.49
3:1C:135:TRP:HE1	22:1W:88:MET:HE1	1.76	0.49
4:1D:120:LEU:HA	4:1D:123:GLU:OE1	2.12	0.49
4:1D:256:SER:OG	4:1D:257:GLY:N	2.45	0.49
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	1.93	0.49
5:1E:201:SER:OG	6:1F:20:ARG:NH1	2.45	0.49
6:1F:349:ARG:NH1	6:1F:352:GLU:OE1	2.45	0.49
7:1G:12:PHE:HA	7:1G:17:SER:HA	1.94	0.49
7:1G:102:PRO:HB2	7:1G:104:ASP:OD2	2.12	0.49
7:1G:215:PHE:HB2	9:1I:104:ARG:NH2	2.27	0.49
7:1G:455:SER:HB2	7:1G:494:HIS:HA	1.94	0.49
12:1L:589:LEU:O	12:1L:593:ILE:HG13	2.12	0.49
14:1N:26:TRP:HB3	14:1N:74:ILE:CD1	2.41	0.49
22:1W:52:LEU:CB	22:1W:54:ILE:HG22	2.32	0.49
25:1Z:72:MET:O	25:1Z:72:MET:HE3	2.12	0.49
25:1Z:104:TRP:HZ3	25:1Z:106:VAL:HA	1.77	0.49
29:1d:38:GLY:HA2	29:1d:68:PHE:HD2	1.77	0.49
36:1k:27:PRO:HD2	36:1k:52:TYR:HB3	1.93	0.49
1:1A:92:LEU:HD13	8:1H:302:MET:HG2	1.94	0.49
2:1B:57:VAL:HB	4:1D:189:MET:HE1	1.94	0.49
2:1B:60:MET:HE3	4:1D:167:PHE:CZ	2.47	0.49
2:1B:108:PRO:HB2	8:1H:58:LYS:HZ2	1.76	0.49
2:1B:149:CYS:SG	4:1D:105:ARG:NH2	2.85	0.49
4:1D:117:ALA:HB2	4:1D:367:ILE:HG12	1.93	0.49
7:1G:160:ILE:HG12	7:1G:173:GLY:HA2	1.93	0.49
13:1M:295:ALA:O	13:1M:299:VAL:HG22	2.12	0.49
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	1.94	0.49
20:1U:52:MET:HE1	39:1n:23:LEU:HG	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:43:TYR:OH	21:1V:86:GLU:OE2	2.29	0.49
22:1W:17:VAL:HG21	22:1W:77:ARG:NH1	2.27	0.49
22:1W:91:GLU:OE1	22:1W:91:GLU:N	2.45	0.49
24:1Y:85:ASP:H	24:1Y:125:LYS:NZ	2.09	0.49
27:1b:30:ILE:HD12	27:1b:31:LEU:N	2.26	0.49
32:1g:63:PHE:O	32:1g:65:GLY:N	2.46	0.49
33:1h:21:PHE:O	33:1h:24:LEU:HG	2.13	0.49
40:1o:92:LEU:HA	40:1o:95:VAL:HG12	1.95	0.49
41:1p:51:ILE:HA	41:1p:54:GLN:HE21	1.77	0.49
43:1r:26:ARG:HH21	43:1r:30:ILE:HG22	1.77	0.49
2:1B:123:GLY:H	2:1B:134:ARG:C	2.20	0.49
12:1L:97:THR:HG22	12:1L:246:LEU:HD21	1.95	0.49
12:1L:226:GLN:O	12:1L:230:HIS:N	2.45	0.49
13:1M:278:ARG:CZ	37:1l:82:ASP:HB3	2.43	0.49
15:1O:60:ASP:O	15:1O:66:GLY:HA2	2.12	0.49
30:1e:85:LEU:O	30:1e:89:GLY:N	2.45	0.49
35:1j:26:GLU:OE2	36:1k:68:LYS:NZ	2.41	0.49
40:1o:61:TYR:CD2	40:1o:89:CYS:HB2	2.48	0.49
41:1p:12:PRO:HG3	41:1p:116:GLU:OE2	2.13	0.49
2:1B:54:CYS:HB3	4:1D:108:TYR:HB2	1.95	0.49
4:1D:34:ASN:OD1	15:1O:158:VAL:HA	2.13	0.49
6:1F:276:LEU:O	6:1F:280:ILE:HG12	2.13	0.49
7:1G:408:LEU:HD21	7:1G:421:HIS:HD2	1.77	0.49
13:1M:10:MET:SD	31:1f:16:VAL:HA	2.53	0.49
14:1N:62:THR:HG21	14:1N:114:TRP:HB3	1.94	0.49
16:1P:248:VAL:HG13	16:1P:322:ARG:HH21	1.78	0.49
20:1T:22:TYR:HD1	20:1T:25:ILE:HG23	1.77	0.49
20:1T:36:PHE:HB2	20:1T:71:MET:HG2	1.94	0.49
23:1X:69:PHE:HA	23:1X:72:GLN:OE1	2.12	0.49
25:1Z:100:ASP:OD1	30:1e:81:GLN:NE2	2.46	0.49
30:1e:27:LYS:HZ1	33:1h:136:SER:HB2	1.77	0.49
31:1f:3:VAL:HA	31:1f:6:ILE:HD12	1.93	0.49
34:1i:7:GLU:OE2	34:1i:7:GLU:N	2.34	0.49
34:1i:78:VAL:HA	34:1i:81:ILE:CG2	2.42	0.49
37:1l:136:ASN:HD22	37:1l:153:VAL:HG23	1.77	0.49
38:1m:41:ARG:HD3	38:1m:44:ARG:HB2	1.95	0.49
41:1p:73:ILE:HG13	41:1p:151:ALA:HB1	1.93	0.49
3:1C:66:ASP:CB	21:1V:89:LEU:HB2	2.43	0.49
3:1C:78:LEU:HB3	3:1C:130:TYR:HB3	1.95	0.49
4:1D:62:LEU:HD11	4:1D:64:LEU:HD21	1.95	0.49
4:1D:325:VAL:HG22	4:1D:327:ASP:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:360:PRO:HG3	4:1D:382:GLY:HA3	1.94	0.49
6:1F:288:ILE:O	6:1F:293:ASN:ND2	2.41	0.49
8:1H:28:LEU:O	8:1H:32:GLN:HG2	2.12	0.49
8:1H:212:ASN:OD1	8:1H:212:ASN:N	2.43	0.49
9:1I:8:ARG:NH1	43:1r:112:LEU:O	2.46	0.49
10:1J:173:ARG:NH2	15:1O:254:ARG:HG2	2.27	0.49
12:1L:323:HIS:CG	12:1L:475:MET:HG3	2.48	0.49
12:1L:495:ILE:HD12	12:1L:496:MET:N	2.28	0.49
13:1M:31:SER:CB	13:1M:73:LEU:HD12	2.41	0.49
16:1P:328:THR:HA	22:1W:51:GLN:HE22	1.78	0.49
19:1S:63:LYS:HZ2	19:1S:65:TRP:CG	2.30	0.49
20:1U:11:ILE:HD12	20:1U:12:LYS:N	2.27	0.49
21:1V:16:CYS:N	21:1V:77:GLU:OE1	2.45	0.49
23:1X:3:ILE:HG23	25:1Z:105:LYS:NZ	2.28	0.49
23:1X:143:SER:OG	30:1e:38:GLU:OE1	2.28	0.49
25:1Z:87:LEU:HD21	25:1Z:119:PRO:HG3	1.95	0.49
25:1Z:133:ILE:HG13	25:1Z:134:LEU:N	2.26	0.49
33:1h:102:GLU:OE2	33:1h:103:LEU:N	2.46	0.49
33:1h:115:ARG:NH1	33:1h:123:TYR:OH	2.46	0.49
39:1n:30:CYS:O	39:1n:32:HIS:N	2.43	0.49
39:1n:60:THR:HB	39:1n:64:ARG:HH12	1.77	0.49
40:1o:38:MET:HE3	40:1o:38:MET:O	2.13	0.49
3:1C:211:GLN:CD	21:1V:114:PRO:HG2	2.38	0.49
4:1D:169:TRP:NE1	8:1H:32:GLN:HA	2.20	0.49
5:1E:30:ARG:HD2	5:1E:53:LEU:HD21	1.95	0.49
6:1F:66:ARG:HH12	6:1F:319:PHE:HB2	1.78	0.49
6:1F:189:GLU:HB2	6:1F:222:VAL:HG21	1.95	0.49
7:1G:84:GLU:HA	7:1G:87:LYS:HD3	1.94	0.49
8:1H:33:LEU:HD22	9:1I:46:ALA:H	1.77	0.49
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.78	0.49
12:1L:41:SER:O	12:1L:45:THR:HG23	2.12	0.49
12:1L:123:LEU:HA	12:1L:126:ILE:HD12	1.95	0.49
12:1L:231:PRO:HA	12:1L:234:PRO:HG2	1.95	0.49
12:1L:298:ILE:N	12:1L:354:GLN:O	2.36	0.49
14:1N:202:ILE:HG22	14:1N:346:LEU:HD13	1.94	0.49
20:1T:65:ILE:HD12	20:1T:66:ASP:H	1.78	0.49
21:1V:55:LEU:HA	21:1V:58:VAL:HG12	1.94	0.49
29:1d:114:GLU:OE1	29:1d:115:GLU:N	2.46	0.49
32:1g:51:PRO:O	32:1g:55:LEU:HG	2.13	0.49
35:1j:29:SER:HA	35:1j:32:MET:SD	2.52	0.49
38:1m:41:ARG:HH21	39:1n:148:PRO:HG3	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:94:TYR:HD1	40:1o:98:MET:HE2	1.78	0.49
4:1D:109:VAL:CG1	4:1D:152:MET:HG2	2.43	0.49
5:1E:89:MET:HE3	6:1F:181:ALA:O	2.12	0.49
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.45	0.49
8:1H:199:ASP:CG	8:1H:200:LEU:H	2.21	0.49
8:1H:225:MET:N	8:1H:225:MET:HE2	2.28	0.49
9:1I:103:SER:OG	9:1I:105:ARG:NE	2.45	0.49
12:1L:331:MET:HA	12:1L:334:PHE:CD2	2.43	0.49
12:1L:466:PHE:HD1	12:1L:469:SER:HB2	1.77	0.49
12:1L:577:VAL:HG13	14:1N:164:ILE:HG23	1.95	0.49
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.13	0.49
14:1N:196:TYR:HD1	14:1N:273:ASN:ND2	2.11	0.49
15:1O:144:ILE:HG23	15:1O:148:CYS:HB2	1.94	0.49
17:1Q:37:ILE:CD1	17:1Q:105:VAL:HA	2.42	0.49
23:1X:79:GLU:CD	23:1X:80:PRO:HD3	2.36	0.49
35:1j:7:ILE:HG23	35:1j:15:PRO:HB2	1.94	0.49
38:1m:18:ASP:HB2	38:1m:21:GLU:CG	2.39	0.49
39:1n:23:LEU:HA	39:1n:26:LEU:HB2	1.94	0.49
5:1E:56:ARG:NH1	44:1s:48:THR:O	2.46	0.49
5:1E:58:ASN:O	5:1E:58:ASN:ND2	2.44	0.49
6:1F:194:GLU:OE1	6:1F:199:LYS:HD3	2.12	0.49
6:1F:263:ASN:ND2	6:1F:285:GLY:O	2.46	0.49
7:1G:232:ASP:OD2	7:1G:388:ALA:HA	2.12	0.49
7:1G:644:GLN:H	7:1G:644:GLN:CD	2.21	0.49
10:1J:130:THR:HG22	25:1Z:121:MET:HB3	1.94	0.49
12:1L:56:HIS:NE2	41:1p:27:ASN:OD1	2.46	0.49
51:1L:701:MYR:H22	40:1o:3:HIS:CE1	2.48	0.49
13:1M:326:LEU:HD22	13:1M:362:ALA:HB1	1.95	0.49
32:1g:26:LEU:CD1	32:1g:28:GLU:HB2	2.43	0.49
6:1F:99:GLU:OE2	6:1F:107:ASP:N	2.44	0.48
6:1F:140:GLY:HA2	6:1F:179:ARG:HE	1.78	0.48
6:1F:261:HIS:HD2	6:1F:337:MET:HA	1.78	0.48
7:1G:6:SER:HG	7:1G:7:ASN:H	1.57	0.48
7:1G:143:GLY:CA	7:1G:190:MET:HE1	2.42	0.48
7:1G:194:GLU:OE1	7:1G:385:ARG:NH1	2.45	0.48
12:1L:291:CYS:HA	12:1L:523:SER:O	2.13	0.48
12:1L:306:THR:O	12:1L:310:LEU:HG	2.13	0.48
12:1L:407:TRP:O	12:1L:411:MET:HB2	2.13	0.48
13:1M:425:ASN:HD21	38:1m:58:VAL:HG23	1.77	0.48
14:1N:198:THR:HA	14:1N:201:THR:HG22	1.93	0.48
14:1N:249:LEU:HD13	14:1N:254:LEU:HD12	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:57:HIS:NE2	15:1O:69:LEU:O	2.46	0.48
15:1O:65:ASP:N	15:1O:65:ASP:OD1	2.45	0.48
16:1P:144:ARG:O	16:1P:148:SER:OG	2.27	0.48
19:1S:36:ILE:HA	19:1S:40:TYR:HB2	1.94	0.48
28:1c:35:HIS:O	28:1c:39:VAL:HG12	2.13	0.48
1:1A:68:GLU:OE1	1:1A:98:LEU:HD22	2.12	0.48
1:1A:87:MET:HE3	1:1A:88:LEU:N	2.28	0.48
3:1C:50:ILE:HG22	3:1C:52:ILE:HG22	1.95	0.48
7:1G:258:ILE:HD11	7:1G:579:ARG:NE	2.28	0.48
12:1L:199:GLN:HE22	41:1p:110:LYS:HB3	1.78	0.48
12:1L:490:ALA:O	12:1L:494:THR:HG23	2.13	0.48
12:1L:570:GLN:OE1	14:1N:167:TRP:NE1	2.41	0.48
14:1N:8:THR:O	14:1N:12:THR:HG22	2.13	0.48
14:1N:89:MET:HE2	14:1N:89:MET:HA	1.94	0.48
14:1N:217:MET:HE1	14:1N:324:LYS:O	2.13	0.48
16:1P:203:GLN:HG2	16:1P:231:VAL:HB	1.95	0.48
17:1Q:27:GLU:OE2	17:1Q:27:GLU:N	2.25	0.48
20:1T:74:GLN:CD	20:1T:74:GLN:N	2.67	0.48
23:1X:119:PRO:HA	27:1b:70:GLN:HE22	1.78	0.48
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.47	0.48
30:1e:57:ILE:HA	30:1e:60:ASP:OD1	2.13	0.48
34:1i:76:ILE:HA	34:1i:79:TRP:CD1	2.48	0.48
37:1l:4:VAL:HG13	37:1l:8:MET:HE1	1.95	0.48
37:1l:54:SER:CB	37:1l:91:THR:H	2.26	0.48
40:1o:51:MET:O	40:1o:55:ARG:HG3	2.13	0.48
41:1p:138:PHE:HE1	41:1p:142:TYR:HB2	1.78	0.48
1:1A:25:PRO:HB2	8:1H:60:PRO:HD3	1.95	0.48
2:1B:145:TYR:N	9:1I:141:THR:O	2.42	0.48
4:1D:79:HIS:NE2	22:1W:97:TRP:CD1	2.81	0.48
4:1D:133:ARG:O	4:1D:137:ILE:HG13	2.13	0.48
5:1E:100:ILE:HG13	5:1E:138:THR:O	2.13	0.48
6:1F:118:LEU:HD23	6:1F:225:VAL:HG13	1.95	0.48
7:1G:48:VAL:HG23	17:1Q:118:TYR:HD1	1.78	0.48
7:1G:199:ILE:HG23	7:1G:202:ILE:HD11	1.95	0.48
7:1G:324:ASP:OD2	7:1G:324:ASP:N	2.38	0.48
8:1H:207:LEU:O	8:1H:209:SER:N	2.46	0.48
12:1L:166:THR:O	12:1L:170:GLN:HG2	2.12	0.48
12:1L:381:THR:HG21	12:1L:420:ALA:HB2	1.95	0.48
13:1M:263:MET:HG2	38:1m:101:TYR:HB2	1.95	0.48
14:1N:1:FME:C	15:1O:254:ARG:HD2	2.43	0.48
14:1N:7:THR:O	14:1N:11:MET:HG3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:42:GLU:OE2	19:1S:42:GLU:N	2.46	0.48
21:1V:48:GLU:O	21:1V:52:ASN:ND2	2.46	0.48
25:1Z:93:GLU:OE1	30:1e:91:TYR:OH	2.17	0.48
34:1i:4:THR:N	34:1i:7:GLU:OE1	2.46	0.48
34:1i:104:PHE:CE2	40:1o:63:ILE:HG22	2.49	0.48
42:1q:32:ASP:OD1	42:1q:34:ARG:N	2.44	0.48
3:1C:58:ILE:HD11	3:1C:118:GLU:HB3	1.95	0.48
4:1D:47:LEU:HD12	4:1D:49:LEU:HD21	1.96	0.48
4:1D:259:MET:HA	4:1D:259:MET:HE3	1.96	0.48
7:1G:303:VAL:HG22	7:1G:544:ILE:HD13	1.96	0.48
12:1L:38:THR:HB	12:1L:42:TYR:OH	2.13	0.48
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.36	0.48
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.48	0.48
14:1N:261:MET:HE2	14:1N:337:LEU:HA	1.95	0.48
23:1X:147:PRO:HB3	30:1e:54:GLU:OE1	2.13	0.48
30:1e:46:ILE:HG22	30:1e:50:ARG:HG2	1.94	0.48
32:1g:47:TYR:OH	32:1g:61:VAL:HG11	2.14	0.48
36:1k:21:TRP:C	36:1k:22:LYS:HD2	2.39	0.48
36:1k:46:ARG:N	36:1k:46:ARG:HD3	2.27	0.48
3:1C:45:PHE:CE1	4:1D:363:THR:HG22	2.48	0.48
4:1D:215:SER:HB2	25:1Z:19:ILE:HG21	1.95	0.48
4:1D:287:ILE:O	9:1I:5:VAL:HG12	2.13	0.48
6:1F:19:ASP:HA	6:1F:241:TRP:HZ2	1.78	0.48
7:1G:104:ASP:HB3	7:1G:107:ILE:HG22	1.94	0.48
7:1G:546:GLN:HG2	7:1G:547:GLY:H	1.78	0.48
10:1J:13:PHE:HE2	11:1K:8:ILE:HG22	1.78	0.48
12:1L:13:ILE:O	12:1L:17:ILE:HG12	2.13	0.48
12:1L:247:LEU:HA	12:1L:251:THR:OG1	2.14	0.48
12:1L:359:MET:O	12:1L:436:ARG:N	2.47	0.48
13:1M:41:LEU:O	13:1M:41:LEU:HD13	2.13	0.48
13:1M:176:PHE:HB3	13:1M:245:ARG:HH21	1.77	0.48
13:1M:368:ALA:HA	13:1M:374:ASN:HB3	1.95	0.48
15:1O:65:ASP:CG	15:1O:67:LYS:HG2	2.38	0.48
16:1P:33:TYR:O	16:1P:37:HIS:ND1	2.46	0.48
22:1W:47:VAL:HA	22:1W:52:LEU:HB2	1.96	0.48
32:1g:58:MET:HE2	32:1g:62:PHE:CE2	2.48	0.48
33:1h:115:ARG:HD2	33:1h:123:TYR:CZ	2.48	0.48
37:1l:72:ASN:HD21	38:1m:43:LYS:HE2	1.78	0.48
40:1o:62:LEU:HG	40:1o:86:TRP:CE2	2.48	0.48
2:1B:81:ARG:HH11	8:1H:61:LEU:HD22	1.78	0.48
2:1B:88:VAL:HG21	2:1B:136:CYS:SG	2.53	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:40:VAL:HG12	3:1C:50:ILE:HG23	1.95	0.48
4:1D:46:ASN:OD1	4:1D:74:ARG:HG3	2.14	0.48
5:1E:86:PHE:HZ	6:1F:359:CYS:HB2	1.79	0.48
6:1F:212:ASP:OD2	6:1F:212:ASP:N	2.40	0.48
7:1G:283:MET:HB2	7:1G:560:ILE:HB	1.96	0.48
10:1J:70:TYR:O	10:1J:74:MET:N	2.34	0.48
13:1M:299:VAL:O	13:1M:303:ILE:HG12	2.14	0.48
14:1N:7:THR:HA	14:1N:10:ILE:HG12	1.95	0.48
14:1N:210:THR:HA	14:1N:329:MET:HE1	1.95	0.48
15:1O:260:ARG:HA	15:1O:263:VAL:HG22	1.95	0.48
25:1Z:104:TRP:CZ3	25:1Z:106:VAL:HA	2.48	0.48
26:1a:28:LYS:HE3	26:1a:28:LYS:HB2	1.62	0.48
29:1d:109:TYR:HA	29:1d:112:ILE:HG12	1.96	0.48
33:1h:21:PHE:C	33:1h:21:PHE:CD2	2.89	0.48
33:1h:48:GLY:O	41:1p:60:TYR:OH	2.31	0.48
33:1h:140:THR:OG1	33:1h:143:ASN:ND2	2.46	0.48
34:1i:7:GLU:HA	34:1i:10:ARG:HB2	1.95	0.48
39:1n:105:ASP:N	39:1n:105:ASP:OD1	2.46	0.48
7:1G:140:LYS:NZ	7:1G:182:GLN:HB3	2.29	0.48
12:1L:36:VAL:HG23	12:1L:101:MET:CE	2.44	0.48
12:1L:203:MET:HA	41:1p:120:TYR:CE2	2.47	0.48
13:1M:19:LYS:HD2	13:1M:22:MET:CE	2.44	0.48
13:1M:443:PRO:HA	13:1M:446:LEU:HB3	1.95	0.48
15:1O:292:VAL:HG12	15:1O:295:LYS:HE3	1.95	0.48
16:1P:3:HIS:ND1	42:1q:132:LYS:HE3	2.28	0.48
16:1P:315:ILE:HD11	16:1P:319:ARG:NH2	2.26	0.48
19:1S:23:CYS:SG	19:1S:24:GLN:N	2.87	0.48
19:1S:82:SER:O	19:1S:86:VAL:HG12	2.13	0.48
24:1Y:53:ALA:O	24:1Y:57:ARG:HG2	2.13	0.48
30:1e:89:GLY:C	30:1e:90:LYS:HD2	2.39	0.48
34:1i:3:TYR:O	34:1i:8:LYS:NZ	2.28	0.48
37:1l:51:PRO:O	37:1l:53:ARG:HD3	2.14	0.48
37:1l:149:GLU:OE1	37:1l:149:GLU:N	2.47	0.48
1:1A:42:ASP:OD1	1:1A:42:ASP:N	2.40	0.48
2:1B:166:LYS:HA	2:1B:169:ARG:NH2	2.28	0.48
4:1D:103:PHE:CE1	4:1D:391:ILE:HD11	2.48	0.48
8:1H:93:TYR:OH	26:1a:35:GLU:OE1	2.31	0.48
9:1I:93:THR:C	9:1I:94:ILE:HD12	2.39	0.48
13:1M:313:THR:O	13:1M:317:ILE:HD12	2.14	0.48
13:1M:329:LEU:HB3	13:1M:359:TRP:CZ2	2.48	0.48
14:1N:137:ALA:O	14:1N:141:VAL:HG23	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:337:LEU:O	14:1N:340:THR:OG1	2.31	0.48
16:1P:80:SER:O	16:1P:84:VAL:HG23	2.14	0.48
17:1Q:37:ILE:HG22	17:1Q:57:MET:HB3	1.96	0.48
18:1R:82:GLY:O	18:1R:91:PHE:N	2.39	0.48
20:1T:72:CYS:HB3	20:1T:75:GLU:OE1	2.13	0.48
21:1V:33:VAL:O	21:1V:36:GLN:HB3	2.14	0.48
21:1V:39:LYS:HA	21:1V:44:ARG:HD3	1.95	0.48
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.46	0.48
34:1i:69:PHE:O	34:1i:73:HIS:HB2	2.14	0.48
34:1i:123:PRO:HD3	40:1o:39:VAL:HG21	1.96	0.48
1:1A:2:ASN:O	1:1A:6:THR:HG23	2.14	0.48
1:1A:21:ALA:CB	8:1H:218:GLY:HA3	2.41	0.48
2:1B:101:ARG:HH12	2:1B:104:TYR:HD2	1.62	0.48
4:1D:230:THR:O	4:1D:294:TYR:OH	2.22	0.48
47:1D:501:U10:H48	8:1H:52:ALA:HB2	1.94	0.48
5:1E:88:THR:O	5:1E:89:MET:HG2	2.13	0.48
6:1F:137:TYR:CG	6:1F:192:LEU:HD21	2.49	0.48
6:1F:280:ILE:HG13	6:1F:291:TRP:HZ3	1.79	0.48
6:1F:389:ILE:HG23	6:1F:419:ILE:HD12	1.94	0.48
7:1G:195:LEU:HD12	7:1G:198:ASN:HD21	1.79	0.48
7:1G:690:ALA:HB2	7:1G:698:VAL:HG11	1.94	0.48
8:1H:138:GLN:NE2	8:1H:198:PHE:O	2.47	0.48
9:1I:122:CYS:CB	45:1I:201:SF4:S1	3.01	0.48
11:1K:62:ILE:HG21	14:1N:27:LEU:HD21	1.96	0.48
12:1L:137:LEU:HD12	12:1L:196:TRP:HA	1.94	0.48
14:1N:118:VAL:O	14:1N:122:ILE:HG13	2.12	0.48
15:1O:101:TYR:CE1	15:1O:128:ILE:HG23	2.46	0.48
18:1R:22:ASP:O	18:1R:25:ARG:HG3	2.14	0.48
20:1T:70:LEU:HB3	20:1T:76:ILE:HD13	1.96	0.48
22:1W:47:VAL:HG22	22:1W:54:ILE:CG2	2.44	0.48
25:1Z:105:LYS:HD2	25:1Z:105:LYS:C	2.39	0.48
29:1d:119:VAL:HB	41:1p:146:GLY:HA2	1.96	0.48
41:1p:14:ARG:NE	41:1p:15:ARG:H	2.12	0.48
41:1p:102:VAL:HG12	41:1p:134:VAL:CG2	2.44	0.48
2:1B:112:TYR:HB2	2:1B:163:LEU:HD11	1.96	0.48
5:1E:100:ILE:HA	5:1E:156:ILE:HG22	1.96	0.48
7:1G:437:HIS:ND1	7:1G:438:PRO:HD2	2.28	0.48
8:1H:152:SER:HB3	8:1H:301:CYS:HA	1.95	0.48
10:1J:64:MET:N	10:1J:64:MET:HE3	2.29	0.48
10:1J:157:THR:O	10:1J:161:LEU:HD22	2.14	0.48
12:1L:384:PRO:HG3	12:1L:491:LEU:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:235:LEU:HA	13:1M:238:LEU:HG	1.96	0.48
14:1N:187:MET:O	14:1N:191:THR:OG1	2.29	0.48
14:1N:234:TRP:NE1	14:1N:305:PHE:O	2.41	0.48
15:1O:3:TYR:O	15:1O:264:GLN:NE2	2.23	0.48
16:1P:317:VAL:HG23	16:1P:318:LEU:HD22	1.94	0.48
17:1Q:59:PHE:CE2	17:1Q:79:LEU:HD23	2.49	0.48
21:1V:26:LEU:O	21:1V:30:ILE:HG23	2.14	0.48
22:1W:34:GLU:HA	22:1W:37:ARG:HB2	1.94	0.48
53:1a:101:CDL:H542	53:1a:101:CDL:H741	1.96	0.48
29:1d:78:ARG:HH22	46:1d:201:PC1:H252	1.79	0.48
32:1g:68:ILE:HD12	32:1g:69:VAL:N	2.28	0.48
37:1l:114:PHE:O	37:1l:118:VAL:HG13	2.13	0.48
40:1o:113:ARG:HH21	40:1o:117:ARG:HG2	1.79	0.48
2:1B:58:GLU:OE1	2:1B:153:ALA:N	2.42	0.47
2:1B:90:GLY:HA2	45:1B:201:SF4:S2	2.54	0.47
8:1H:26:LYS:HD2	8:1H:36:GLY:HA3	1.96	0.47
8:1H:312:ALA:HB3	25:1Z:55:ARG:HH12	1.79	0.47
9:1I:151:LYS:HE2	18:1R:13:HIS:HE2	1.78	0.47
14:1N:268:GLN:NE2	14:1N:272:LYS:HD2	2.29	0.47
15:1O:29:GLY:HA2	15:1O:171:TYR:CZ	2.49	0.47
15:1O:164:LEU:HB2	15:1O:165:PRO:HD3	1.96	0.47
19:1S:24:GLN:HB3	19:1S:25:ARG:HD2	1.96	0.47
20:1U:36:PHE:HA	20:1U:40:LEU:HD23	1.96	0.47
22:1W:80:ASP:HA	22:1W:83:VAL:HG12	1.96	0.47
25:1Z:55:ARG:CZ	27:1b:83:LEU:HD22	2.44	0.47
25:1Z:121:MET:HE3	25:1Z:137:THR:HG22	1.95	0.47
37:1l:78:HIS:NE2	37:1l:80:ASP:HB2	2.29	0.47
39:1n:89:SER:HA	39:1n:92:ARG:HB2	1.96	0.47
39:1n:104:ASP:OD1	39:1n:121:ARG:NH2	2.47	0.47
43:1r:42:VAL:HB	43:1r:46:HIS:CD2	2.49	0.47
1:1A:16:LEU:O	1:1A:20:ILE:HG13	2.14	0.47
1:1A:43:PRO:HB3	8:1H:126:LYS:CG	2.44	0.47
2:1B:58:GLU:HA	2:1B:58:GLU:OE2	2.14	0.47
4:1D:413:ASP:CG	8:1H:281:ARG:HH11	2.20	0.47
12:1L:137:LEU:HA	12:1L:140:LEU:HB2	1.95	0.47
12:1L:359:MET:HG3	12:1L:430:ALA:HA	1.96	0.47
12:1L:435:PRO:HD2	36:1k:51:ARG:O	2.14	0.47
12:1L:521:LYS:HA	12:1L:524:ASN:ND2	2.29	0.47
12:1L:585:LYS:O	12:1L:589:LEU:HD12	2.14	0.47
13:1M:190:TRP:CE3	24:1Y:126:MET:HE1	2.49	0.47
16:1P:145:TYR:CD2	16:1P:286:ARG:HD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:45:LEU:O	20:1U:48:VAL:HG12	2.13	0.47
25:1Z:6:VAL:HA	43:1r:39:LYS:HG3	1.96	0.47
26:1a:3:PHE:O	26:1a:6:LEU:HB2	2.14	0.47
34:1i:11:LEU:O	34:1i:14:LEU:HG	2.14	0.47
37:1l:102:CYS:O	37:1l:105:LEU:HD12	2.13	0.47
40:1o:89:CYS:HA	40:1o:92:LEU:HG	1.94	0.47
42:1q:44:TYR:HE2	42:1q:83:PRO:HB3	1.79	0.47
2:1B:70:ASP:OD1	8:1H:25:ARG:HD2	2.14	0.47
6:1F:24:ASN:ND2	6:1F:29:HIS:O	2.47	0.47
6:1F:367:GLU:OE2	7:1G:100:ASN:ND2	2.40	0.47
12:1L:174:TYR:CD2	12:1L:232:TRP:HB3	2.49	0.47
12:1L:425:ARG:HA	12:1L:428:PHE:CD1	2.49	0.47
13:1M:64:PRO:O	13:1M:68:LEU:HB2	2.14	0.47
15:1O:4:GLY:HA2	15:1O:261:MET:HE1	1.96	0.47
15:1O:189:PRO:HA	15:1O:192:MET:HG2	1.96	0.47
20:1T:57:GLU:OE2	20:1T:58:PHE:HD1	1.97	0.47
20:1U:18:VAL:HG21	20:1U:58:PHE:CZ	2.48	0.47
23:1X:29:HIS:NE2	25:1Z:63:GLU:OE2	2.47	0.47
24:1Y:119:LEU:HD12	24:1Y:120:THR:HG23	1.96	0.47
46:1d:201:PC1:H392	46:1d:201:PC1:H3C1	1.74	0.47
32:1g:67:SER:O	32:1g:70:LEU:N	2.41	0.47
33:1h:64:TRP:CE3	33:1h:77:ARG:HA	2.50	0.47
34:1i:77:PRO:O	34:1i:80:ILE:HD12	2.13	0.47
40:1o:93:ASP:HA	40:1o:96:LYS:HB3	1.96	0.47
41:1p:109:LEU:CD2	41:1p:127:GLU:HB3	2.44	0.47
5:1E:184:PRO:HD2	44:1s:44:HIS:ND1	2.30	0.47
7:1G:231:MET:HE2	7:1G:231:MET:H	1.78	0.47
8:1H:1:FME:HA	8:1H:4:ILE:HD12	1.96	0.47
12:1L:535:ARG:HA	37:1l:89:VAL:HG23	1.95	0.47
13:1M:30:HIS:O	13:1M:34:ILE:HG13	2.14	0.47
14:1N:270:MET:HB3	14:1N:279:PRO:HG3	1.96	0.47
15:1O:27:VAL:HG21	15:1O:39:ALA:HB2	1.96	0.47
17:1Q:28:GLU:O	17:1Q:32:THR:OG1	2.22	0.47
25:1Z:23:ARG:HE	43:1r:112:LEU:HD11	1.80	0.47
27:1b:62:MET:SD	27:1b:62:MET:N	2.87	0.47
38:1m:106:THR:O	38:1m:110:LYS:HG2	2.13	0.47
38:1m:114:LEU:HD22	38:1m:119:LYS:HG2	1.96	0.47
41:1p:156:ALA:O	41:1p:160:GLN:HG2	2.15	0.47
2:1B:72:PHE:HA	8:1H:39:VAL:HG11	1.97	0.47
2:1B:116:MET:HA	2:1B:146:VAL:HB	1.96	0.47
3:1C:20:LYS:N	3:1C:20:LYS:HE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:54:GLN:CD	4:1D:56:PRO:HD3	2.39	0.47
4:1D:143:GLU:OE1	4:1D:307:SER:HB3	2.15	0.47
4:1D:149:ASN:OD1	4:1D:371:LYS:HE3	2.14	0.47
4:1D:150:HIS:CB	4:1D:304:MET:HE2	2.43	0.47
5:1E:26:GLU:O	5:1E:30:ARG:HG3	2.14	0.47
5:1E:49:PRO:O	5:1E:53:LEU:N	2.38	0.47
6:1F:138:ILE:HG12	6:1F:149:LEU:HD21	1.95	0.47
7:1G:306:MET:SD	7:1G:542:PHE:CG	3.08	0.47
7:1G:561:LEU:HD13	7:1G:599:ILE:HD11	1.96	0.47
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.95	0.47
7:1G:623:LEU:HD23	7:1G:623:LEU:C	2.39	0.47
10:1J:132:ASP:N	10:1J:132:ASP:OD1	2.47	0.47
11:1K:83:ASN:OD1	11:1K:83:ASN:N	2.46	0.47
12:1L:298:ILE:HG22	12:1L:354:GLN:HB3	1.96	0.47
12:1L:562:LEU:HB2	12:1L:563:PRO:HD3	1.96	0.47
12:1L:604:TYR:CD2	14:1N:153:LEU:HG	2.49	0.47
13:1M:356:ALA:HA	13:1M:359:TRP:CD1	2.50	0.47
13:1M:409:TYR:O	13:1M:412:ILE:HG13	2.14	0.47
21:1V:115:ILE:HD12	21:1V:115:ILE:HA	1.79	0.47
24:1Y:100:LEU:O	24:1Y:104:THR:HG22	2.14	0.47
30:1e:88:GLU:OE1	30:1e:90:LYS:HD3	2.13	0.47
32:1g:26:LEU:HD12	32:1g:28:GLU:HB2	1.97	0.47
34:1i:99:ARG:NH2	41:1p:114:GLN:HA	2.29	0.47
39:1n:29:TRP:HA	39:1n:75:HIS:NE2	2.30	0.47
41:1p:98:ASP:O	41:1p:101:ILE:HG13	2.15	0.47
4:1D:9:GLU:HA	4:1D:12:GLU:HB2	1.96	0.47
7:1G:153:CYS:SG	7:1G:154:ILE:N	2.87	0.47
7:1G:534:ARG:NH1	42:1q:144:TYR:OH	2.48	0.47
12:1L:190:LEU:HD21	12:1L:196:TRP:CD2	2.49	0.47
13:1M:278:ARG:HH21	38:1m:67:TRP:HZ2	1.62	0.47
13:1M:293:HIS:HA	13:1M:296:LEU:HD12	1.96	0.47
13:1M:433:GLU:O	13:1M:437:MET:SD	2.73	0.47
14:1N:18:MET:HA	14:1N:21:MET:HE3	1.96	0.47
14:1N:309:ASN:HD22	15:1O:95:ARG:HG2	1.79	0.47
15:1O:53:GLU:OE1	15:1O:126:ARG:NH1	2.47	0.47
15:1O:80:GLU:HB3	15:1O:190:HIS:ND1	2.30	0.47
24:1Y:90:PHE:C	24:1Y:90:PHE:CD2	2.92	0.47
27:1b:24:ILE:HA	27:1b:27:LEU:HD23	1.95	0.47
37:1l:44:TYR:HA	37:1l:79:TRP:CZ3	2.49	0.47
44:1s:43:HIS:HA	44:1s:46:TYR:CE2	2.49	0.47
4:1D:184:VAL:HB	4:1D:193:TYR:HE2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:347:HIS:NE2	7:1G:126:ASP:HA	2.29	0.47
5:1E:155:GLN:HB2	5:1E:160:TYR:HD1	1.80	0.47
6:1F:112:ARG:HH22	44:1s:43:HIS:CE1	2.33	0.47
6:1F:337:MET:HE2	6:1F:337:MET:N	2.30	0.47
7:1G:466:ILE:HG12	7:1G:656:LEU:HD21	1.96	0.47
7:1G:517:ASN:OD1	7:1G:517:ASN:N	2.48	0.47
8:1H:43:TYR:CZ	53:1a:101:CDL:H141	2.50	0.47
11:1K:40:LEU:HD23	11:1K:40:LEU:HA	1.54	0.47
12:1L:139:GLN:HA	12:1L:142:ILE:HD12	1.96	0.47
12:1L:177:ILE:HA	12:1L:180:ILE:HD12	1.95	0.47
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.23	0.47
12:1L:391:SER:O	12:1L:394:LEU:N	2.48	0.47
12:1L:499:MET:SD	12:1L:500:LEU:N	2.88	0.47
12:1L:593:ILE:O	12:1L:597:ILE:HD12	2.14	0.47
13:1M:401:MET:O	13:1M:405:LEU:HD12	2.15	0.47
13:1M:433:GLU:O	13:1M:436:LEU:N	2.48	0.47
13:1M:442:LEU:HD12	32:1g:70:LEU:HD11	1.97	0.47
14:1N:192:ALA:HB1	14:1N:270:MET:HE1	1.96	0.47
15:1O:51:PHE:HE2	15:1O:111:ALA:HA	1.80	0.47
15:1O:209:THR:O	15:1O:213:GLU:HB3	2.15	0.47
17:1Q:11:ILE:HD11	22:1W:19:PRO:HD3	1.97	0.47
20:1T:8:LEU:H	20:1T:88:GLU:HG2	1.80	0.47
20:1U:52:MET:CE	39:1n:23:LEU:HG	2.45	0.47
21:1V:53:GLU:O	21:1V:57:MET:HG2	2.15	0.47
22:1W:54:ILE:HD11	22:1W:58:GLN:O	2.15	0.47
22:1W:54:ILE:HD12	22:1W:58:GLN:CD	2.38	0.47
31:1f:41:SER:HB3	33:1h:87:TYR:HE1	1.80	0.47
32:1g:83:TYR:HD1	32:1g:84:ARG:HG3	1.79	0.47
37:1l:16:THR:O	37:1l:20:ARG:HG2	2.15	0.47
39:1n:122:GLU:O	39:1n:125:LYS:HG2	2.15	0.47
43:1r:59:ARG:HH21	43:1r:60:ARG:NH2	2.12	0.47
5:1E:162:GLU:HB2	5:1E:186:PRO:HG3	1.97	0.47
7:1G:358:LEU:HD22	7:1G:645:ALA:HB2	1.97	0.47
7:1G:448:LYS:HG3	7:1G:487:TRP:CD2	2.50	0.47
7:1G:477:ILE:C	7:1G:477:ILE:HD12	2.40	0.47
9:1I:10:PRO:HB2	9:1I:20:ARG:HH21	1.80	0.47
9:1I:136:ASN:HB2	9:1I:161:TRP:CE2	2.50	0.47
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.49	0.47
10:1J:33:LEU:HD12	10:1J:33:LEU:O	2.15	0.47
11:1K:96:LEU:HB3	14:1N:117:GLU:CD	2.40	0.47
12:1L:82:MET:HE3	12:1L:82:MET:N	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:115:ASN:O	12:1L:119:LYS:HD2	2.14	0.47
12:1L:323:HIS:CD2	12:1L:476:THR:HA	2.50	0.47
12:1L:345:SER:O	12:1L:349:SER:OG	2.32	0.47
13:1M:257:MET:O	13:1M:260:PRO:HD2	2.14	0.47
16:1P:23:VAL:HB	16:1P:26:ALA:HB2	1.97	0.47
19:1S:24:GLN:C	19:1S:25:ARG:HD2	2.39	0.47
20:1U:73:PRO:O	20:1U:77:VAL:HG22	2.15	0.47
32:1g:103:ASN:OD1	32:1g:103:ASN:N	2.43	0.47
35:1j:27:PHE:C	35:1j:27:PHE:CD2	2.93	0.47
38:1m:6:LYS:NZ	38:1m:7:PRO:O	2.39	0.47
40:1o:6:ARG:NH2	40:1o:15:GLU:OE2	2.47	0.47
42:1q:6:VAL:HB	42:1q:9:ARG:HH21	1.79	0.47
1:1A:51:PHE:CE2	8:1H:130:ILE:HD13	2.50	0.47
3:1C:14:ARG:NH2	3:1C:44:CYS:SG	2.88	0.47
4:1D:202:ASP:OD1	4:1D:203:LEU:N	2.48	0.47
4:1D:217:ASN:O	4:1D:221:ARG:NH2	2.34	0.47
7:1G:190:MET:HA	7:1G:190:MET:HE3	1.96	0.47
8:1H:25:ARG:NH1	8:1H:25:ARG:HB2	2.29	0.47
9:1I:26:LEU:HD12	25:1Z:35:MET:HG3	1.96	0.47
10:1J:15:ILE:HG21	10:1J:97:LEU:HD13	1.97	0.47
10:1J:152:TRP:CD2	30:1e:13:LEU:HD11	2.50	0.47
14:1N:8:THR:HA	14:1N:11:MET:CE	2.45	0.47
14:1N:220:ILE:HD13	14:1N:323:MET:SD	2.55	0.47
15:1O:22:SER:HB3	15:1O:115:LEU:HD11	1.96	0.47
15:1O:94:TYR:CE2	15:1O:282:ILE:HD11	2.49	0.47
16:1P:176:ASP:H	16:1P:180:ASN:ND2	2.12	0.47
19:1S:63:LYS:HZ1	19:1S:75:ASN:HA	1.80	0.47
20:1U:24:LYS:HG3	36:1k:41:ARG:NH1	2.29	0.47
22:1W:42:GLU:HG2	22:1W:94:ILE:HD11	1.97	0.47
33:1h:55:ILE:HD12	33:1h:55:ILE:O	2.14	0.47
35:1j:32:MET:HE1	36:1k:68:LYS:HB3	1.96	0.47
37:1l:56:GLN:HG2	37:1l:86:ARG:HD3	1.97	0.47
40:1o:14:LYS:O	40:1o:109:GLN:NE2	2.43	0.47
42:1q:11:LEU:O	42:1q:14:VAL:HG12	2.13	0.47
1:1A:42:ASP:OD1	2:1B:102:LYS:NZ	2.48	0.47
1:1A:62:PHE:CD2	8:1H:140:ILE:HD13	2.50	0.47
3:1C:42:VAL:HB	3:1C:48:LEU:HD12	1.96	0.47
4:1D:339:LYS:HB3	18:1R:69:PRO:HA	1.97	0.47
6:1F:121:GLY:HA2	6:1F:232:PRO:HD3	1.97	0.47
6:1F:206:LYS:HG2	6:1F:210:PRO:HD3	1.98	0.47
7:1G:12:PHE:HB2	7:1G:78:ASN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:673:MET:SD	7:1G:679:ARG:HA	2.54	0.47
8:1H:179:TRP:NE1	25:1Z:43:LEU:HG	2.29	0.47
10:1J:157:THR:HG21	11:1K:62:ILE:HD13	1.97	0.47
12:1L:258:PHE:O	12:1L:262:ARG:HG2	2.14	0.47
12:1L:474:PRO:HG3	40:1o:65:LEU:HD22	1.97	0.47
13:1M:25:ILE:H	13:1M:25:ILE:HD12	1.80	0.47
13:1M:88:THR:HB	13:1M:91:ARG:HD3	1.97	0.47
13:1M:106:LEU:HD11	13:1M:238:LEU:HD23	1.97	0.47
16:1P:274:PRO:HD2	16:1P:275:PHE:N	2.28	0.47
20:1T:73:PRO:O	20:1T:77:VAL:HG22	2.15	0.47
25:1Z:22:LYS:HD2	43:1r:109:GLN:OE1	2.14	0.47
25:1Z:127:LEU:HB2	30:1e:97:HIS:NE2	2.30	0.47
32:1g:85:MET:HE3	32:1g:85:MET:H	1.80	0.47
32:1g:96:LEU:O	32:1g:100:ARG:HG2	2.15	0.47
37:1l:105:LEU:HD12	37:1l:106:SER:N	2.30	0.47
39:1n:46:ARG:NH1	39:1n:46:ARG:O	2.47	0.47
39:1n:81:PHE:HB2	39:1n:84:SER:OG	2.14	0.47
1:1A:54:LYS:HZ3	4:1D:71:GLU:HG2	1.80	0.46
7:1G:236:SER:HB3	7:1G:259:ASN:HD22	1.79	0.46
8:1H:19:PHE:O	8:1H:23:VAL:HG13	2.14	0.46
8:1H:272:TRP:HZ2	9:1I:38:LEU:HB2	1.78	0.46
9:1I:52:PHE:CZ	42:1q:30:ALA:HA	2.51	0.46
10:1J:31:LEU:O	10:1J:35:VAL:HG13	2.15	0.46
11:1K:66:PHE:CZ	14:1N:31:ILE:HG23	2.49	0.46
12:1L:79:SER:N	12:1L:139:GLN:OE1	2.48	0.46
12:1L:416:THR:HG21	12:1L:493:VAL:HG23	1.95	0.46
12:1L:546:GLN:HB3	12:1L:547:LYS:HD2	1.97	0.46
13:1M:300:ALA:HB2	13:1M:381:ILE:HG12	1.97	0.46
15:1O:266:LYS:O	15:1O:270:LEU:HD22	2.15	0.46
21:1V:30:ILE:HD11	21:1V:51:THR:CG2	2.46	0.46
21:1V:46:TYR:O	21:1V:50:ILE:HG12	2.14	0.46
21:1V:64:VAL:O	21:1V:68:GLU:HG2	2.15	0.46
29:1d:111:GLU:HA	32:1g:119:GLN:HE21	1.79	0.46
32:1g:57:ASN:HA	32:1g:60:VAL:HG22	1.96	0.46
36:1k:61:SER:O	36:1k:65:ALA:N	2.40	0.46
39:1n:26:LEU:HA	39:1n:29:TRP:HD1	1.79	0.46
41:1p:80:ASP:O	41:1p:84:MET:HB2	2.15	0.46
3:1C:51:PHE:HB3	21:1V:111:TRP:CZ2	2.49	0.46
4:1D:169:TRP:HB2	4:1D:170:MET:HE2	1.98	0.46
4:1D:371:LYS:HZ3	4:1D:422:ASP:HB2	1.79	0.46
4:1D:423:ILE:HD11	4:1D:428:VAL:CG1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:27:ASN:O	5:1E:31:ILE:HG12	2.15	0.46
6:1F:95:VAL:HB	6:1F:136:ILE:HD13	1.97	0.46
11:1K:22:TYR:HB3	12:1L:585:LYS:HG3	1.96	0.46
12:1L:278:LEU:HD21	12:1L:319:ILE:HG23	1.97	0.46
13:1M:244:MET:HA	13:1M:244:MET:HE2	1.98	0.46
13:1M:266:MET:O	13:1M:269:MET:HG3	2.16	0.46
15:1O:80:GLU:HB3	15:1O:190:HIS:CG	2.51	0.46
16:1P:107:GLU:OE2	16:1P:112:LYS:NZ	2.45	0.46
16:1P:198:LYS:HA	16:1P:237:LEU:HD11	1.96	0.46
24:1Y:119:LEU:O	24:1Y:123:LEU:HG	2.15	0.46
26:1a:7:PRO:HG3	53:1a:101:CDL:H152	1.96	0.46
34:1i:87:TYR:HB3	41:1p:48:ARG:NH2	2.30	0.46
37:1l:46:ASP:OD1	37:1l:46:ASP:N	2.39	0.46
39:1n:111:LYS:HA	39:1n:118:PHE:CD2	2.51	0.46
40:1o:80:LYS:HZ1	40:1o:83:GLN:CD	2.20	0.46
4:1D:6:PRO:HB3	4:1D:10:TRP:HD1	1.80	0.46
4:1D:132:PRO:O	4:1D:136:TRP:HD1	1.98	0.46
7:1G:635:ASP:N	7:1G:635:ASP:OD1	2.48	0.46
9:1I:112:ASP:OD1	9:1I:114:THR:HG22	2.16	0.46
11:1K:10:MET:O	11:1K:10:MET:HE3	2.14	0.46
13:1M:278:ARG:NH2	37:1l:80:ASP:HA	2.30	0.46
13:1M:282:LEU:HD21	13:1M:410:MET:CG	2.46	0.46
13:1M:328:CYS:O	13:1M:332:THR:HG23	2.15	0.46
13:1M:430:PHE:HB2	13:1M:433:GLU:OE1	2.15	0.46
53:1N:401:CDL:H731	53:1N:401:CDL:OB7	2.14	0.46
16:1P:202:LYS:NZ	16:1P:287:VAL:O	2.42	0.46
24:1Y:119:LEU:HD12	24:1Y:120:THR:N	2.30	0.46
25:1Z:105:LYS:HD2	25:1Z:106:VAL:N	2.30	0.46
30:1e:85:LEU:HA	30:1e:88:GLU:HG3	1.97	0.46
33:1h:27:PHE:CE1	33:1h:28:TYR:HE2	2.33	0.46
34:1i:99:ARG:NH2	41:1p:117:GLY:HA2	2.29	0.46
40:1o:72:SER:HG	40:1o:79:CYS:HG	1.52	0.46
2:1B:50:PHE:CZ	2:1B:100:LEU:HD23	2.51	0.46
2:1B:91:THR:HG22	2:1B:119:CYS:SG	2.55	0.46
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.97	0.46
6:1F:242:PHE:CZ	6:1F:252:GLY:HA3	2.50	0.46
8:1H:167:THR:HG23	23:1X:97:ARG:HH22	1.80	0.46
9:1I:76:ARG:NH2	18:1R:66:LEU:O	2.48	0.46
12:1L:316:THR:O	12:1L:319:ILE:HD12	2.15	0.46
12:1L:511:LEU:HD21	39:1n:38:TYR:CD2	2.51	0.46
13:1M:34:ILE:HD12	13:1M:35:SER:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:47:GLU:OE2	41:1p:92:ARG:HB3	2.16	0.46
13:1M:193:ILE:HG22	13:1M:253:LEU:HD11	1.97	0.46
14:1N:5:ILE:O	14:1N:8:THR:HG22	2.15	0.46
15:1O:30:ASN:ND2	15:1O:202:ILE:HD11	2.30	0.46
16:1P:91:VAL:HG23	16:1P:126:VAL:HG21	1.97	0.46
16:1P:108:ASP:HB3	16:1P:112:LYS:HZ3	1.81	0.46
17:1Q:37:ILE:HG21	17:1Q:92:ALA:HB1	1.97	0.46
18:1R:58:SER:HB2	18:1R:72:TYR:CE1	2.50	0.46
20:1T:35:HIS:O	20:1T:40:LEU:N	2.37	0.46
20:1T:74:GLN:NE2	20:1T:74:GLN:HA	2.29	0.46
23:1X:100:ARG:O	23:1X:103:GLN:HB3	2.15	0.46
28:1c:13:ASP:OD1	28:1c:16:LYS:HD3	2.16	0.46
32:1g:48:ASP:OD2	32:1g:50:ASP:N	2.49	0.46
36:1k:48:GLU:HG2	36:1k:51:ARG:CB	2.43	0.46
40:1o:7:ARG:HB2	40:1o:15:GLU:HB3	1.98	0.46
40:1o:117:ARG:O	40:1o:121:MET:HB3	2.15	0.46
44:1s:52:LEU:HA	44:1s:55:ASN:HB3	1.96	0.46
2:1B:33:LEU:HD11	46:1B:202:PC1:H3A1	1.98	0.46
2:1B:86:MET:HG3	2:1B:107:MET:SD	2.55	0.46
3:1C:189:GLU:OE2	16:1P:15:SER:N	2.49	0.46
4:1D:19:MET:H	4:1D:19:MET:HE3	1.80	0.46
4:1D:168:PHE:HZ	47:1D:501:U10:H153	1.79	0.46
5:1E:7:PHE:HA	5:1E:92:ARG:HH12	1.80	0.46
8:1H:53:LEU:O	8:1H:57:THR:HG23	2.15	0.46
8:1H:79:LEU:HD22	8:1H:222:MET:CG	2.46	0.46
8:1H:179:TRP:CZ3	9:1I:26:LEU:HD21	2.51	0.46
12:1L:34:ASN:O	12:1L:38:THR:OG1	2.34	0.46
12:1L:203:MET:CE	41:1p:109:LEU:HB3	2.45	0.46
12:1L:575:ILE:O	12:1L:579:ASN:HB2	2.16	0.46
13:1M:19:LYS:O	13:1M:23:ILE:HG23	2.16	0.46
13:1M:29:VAL:HG13	32:1g:64:PHE:CE2	2.50	0.46
14:1N:35:MET:HE3	14:1N:35:MET:HB2	1.72	0.46
16:1P:45:VAL:HG23	16:1P:47:VAL:H	1.80	0.46
25:1Z:54:ASN:O	25:1Z:58:ARG:HG2	2.15	0.46
33:1h:18:ASP:O	33:1h:22:LEU:HG	2.16	0.46
35:1j:16:GLN:NE2	35:1j:18:THR:HG22	2.31	0.46
39:1n:17:ARG:HB2	39:1n:21:ARG:HH21	1.81	0.46
39:1n:162:LEU:HD13	39:1n:163:PRO:HD2	1.96	0.46
41:1p:98:ASP:O	41:1p:102:VAL:HG13	2.14	0.46
41:1p:138:PHE:CE1	41:1p:142:TYR:HB2	2.51	0.46
6:1F:165:ASN:ND2	6:1F:168:GLY:HA2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:241:SER:OG	7:1G:249:ARG:HG3	2.15	0.46
7:1G:296:TRP:O	7:1G:300:LEU:HD22	2.16	0.46
7:1G:404:LEU:HD22	7:1G:406:VAL:HG23	1.96	0.46
8:1H:38:ASN:HA	8:1H:44:GLY:N	2.31	0.46
9:1I:64:GLU:OE2	9:1I:149:TYR:OH	2.27	0.46
12:1L:314:MET:O	12:1L:317:ILE:HG13	2.16	0.46
12:1L:488:MET:HE3	12:1L:488:MET:HB2	1.77	0.46
12:1L:602:PHE:C	12:1L:602:PHE:CD2	2.94	0.46
13:1M:182:TRP:CG	41:1p:79:LYS:HZ3	2.34	0.46
13:1M:373:ILE:HG23	13:1M:448:THR:HA	1.97	0.46
14:1N:115:VAL:HG13	14:1N:116:PRO:HD3	1.96	0.46
16:1P:29:PHE:HB3	16:1P:30:LEU:H	1.58	0.46
17:1Q:59:PHE:N	17:1Q:59:PHE:CD1	2.84	0.46
31:1f:13:HIS:O	31:1f:13:HIS:ND1	2.49	0.46
32:1g:51:PRO:O	32:1g:54:ASP:HB2	2.15	0.46
34:1i:4:THR:OG1	34:1i:7:GLU:OE2	2.28	0.46
34:1i:104:PHE:HB3	34:1i:107:ASP:CG	2.40	0.46
40:1o:67:LYS:HG3	40:1o:70:ARG:HH12	1.80	0.46
40:1o:104:GLU:HA	40:1o:107:LEU:HB2	1.97	0.46
40:1o:106:ARG:HA	40:1o:109:GLN:HG2	1.98	0.46
41:1p:2:ASP:OD1	41:1p:3:SER:N	2.49	0.46
41:1p:159:LYS:HD2	41:1p:159:LYS:HA	1.76	0.46
3:1C:209:TYR:CD1	4:1D:360:PRO:HD2	2.51	0.46
5:1E:33:ALA:O	5:1E:37:ASN:ND2	2.48	0.46
6:1F:22:PHE:CE2	6:1F:255:LEU:HB2	2.50	0.46
7:1G:35:MET:HE1	7:1G:37:ILE:CD1	2.45	0.46
8:1H:29:GLY:O	8:1H:34:ARG:N	2.40	0.46
9:1I:155:LEU:HD23	9:1I:155:LEU:HA	1.80	0.46
12:1L:101:MET:HE3	12:1L:101:MET:HB3	1.56	0.46
12:1L:291:CYS:O	12:1L:295:GLN:HG2	2.16	0.46
12:1L:423:SER:O	12:1L:427:ILE:HG13	2.15	0.46
12:1L:463:PHE:O	12:1L:467:ILE:HG12	2.16	0.46
13:1M:412:ILE:HA	13:1M:416:ARG:HD3	1.97	0.46
14:1N:170:LEU:HD23	14:1N:292:PHE:CD2	2.51	0.46
53:1N:401:CDL:OA4	15:1O:258:ARG:NH1	2.36	0.46
15:1O:197:ALA:O	15:1O:201:ASP:HB2	2.16	0.46
16:1P:174:ARG:HA	16:1P:174:ARG:NE	2.30	0.46
18:1R:89:LEU:HB2	18:1R:91:PHE:HE1	1.80	0.46
22:1W:90:LEU:O	22:1W:94:ILE:HD13	2.16	0.46
28:1c:40:LEU:O	28:1c:44:ARG:HG2	2.15	0.46
29:1d:86:ARG:O	29:1d:90:MET:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:59:HIS:HD2	47:1D:501:U10:H3M3	1.80	0.46
7:1G:354:ALA:HB3	7:1G:361:ASN:ND2	2.31	0.46
11:1K:55:LEU:HD21	30:1e:24:GLN:HA	1.98	0.46
12:1L:55:MET:HA	12:1L:55:MET:HE3	1.97	0.46
13:1M:151:PHE:HD1	14:1N:287:LEU:HD12	1.81	0.46
13:1M:302:MET:O	13:1M:304:GLN:NE2	2.48	0.46
13:1M:355:MET:SD	13:1M:434:ASN:ND2	2.89	0.46
14:1N:190:MET:HE3	14:1N:190:MET:HB2	1.84	0.46
15:1O:56:ILE:O	15:1O:99:TRP:NE1	2.38	0.46
16:1P:115:HIS:HB2	16:1P:155:GLU:HG2	1.97	0.46
20:1U:11:ILE:HD13	20:1U:77:VAL:HG12	1.98	0.46
20:1U:18:VAL:C	20:1U:20:LYS:H	2.24	0.46
21:1V:44:ARG:HG3	21:1V:45:LYS:N	2.30	0.46
25:1Z:36:PHE:O	25:1Z:40:ILE:HD13	2.15	0.46
25:1Z:83:VAL:HG23	25:1Z:124:LEU:HD21	1.98	0.46
26:1a:1:MET:SD	53:1a:101:CDL:HA21	2.56	0.46
26:1a:41:PHE:N	26:1a:44:GLN:OE1	2.49	0.46
27:1b:27:LEU:HB3	27:1b:31:LEU:HD21	1.98	0.46
27:1b:68:HIS:ND1	27:1b:70:GLN:HB2	2.31	0.46
35:1j:11:TYR:CE2	35:1j:12:ARG:HG3	2.51	0.46
2:1B:157:LEU:HD23	9:1I:50:TYR:CD2	2.51	0.46
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.96	0.46
12:1L:100:ILE:O	12:1L:104:SER:OG	2.28	0.46
12:1L:396:ILE:O	12:1L:400:ASN:ND2	2.34	0.46
12:1L:593:ILE:HD12	12:1L:594:THR:H	1.81	0.46
13:1M:135:ARG:NH2	14:1N:304:MET:HE1	2.31	0.46
13:1M:391:ILE:H	13:1M:391:ILE:HD12	1.80	0.46
14:1N:59:TYR:O	14:1N:59:TYR:HD1	1.99	0.46
16:1P:264:ARG:HE	16:1P:264:ARG:HB3	1.64	0.46
19:1S:12:LYS:HD2	19:1S:14:GLY:H	1.80	0.46
23:1X:144:ARG:NE	30:1e:58:GLU:OE2	2.28	0.46
30:1e:32:CYS:SG	30:1e:66:LEU:HD23	2.56	0.46
32:1g:85:MET:HB3	32:1g:88:TRP:HB3	1.96	0.46
33:1h:48:GLY:HA3	41:1p:55:HIS:CE1	2.51	0.46
34:1i:99:ARG:HH21	41:1p:114:GLN:C	2.21	0.46
42:1q:14:VAL:HG23	42:1q:23:TYR:CD2	2.51	0.46
42:1q:39:VAL:HG11	42:1q:50:GLU:HB3	1.97	0.46
3:1C:15:ASN:HB3	3:1C:46:ASN:ND2	2.31	0.46
3:1C:175:ARG:HD2	3:1C:176:TYR:O	2.16	0.46
6:1F:376:MET:HE3	6:1F:377:ALA:N	2.31	0.46
7:1G:628:PRO:HD2	19:1S:55:ARG:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:63:GLY:H	9:1I:133:GLU:HB3	1.80	0.46
12:1L:123:LEU:O	12:1L:127:THR:HG22	2.16	0.46
13:1M:364:LEU:HB3	13:1M:369:LEU:HD21	1.97	0.46
14:1N:272:LYS:NZ	33:1h:108:LEU:HD21	2.28	0.46
33:1h:42:LEU:HA	33:1h:45:VAL:HG22	1.98	0.46
37:1l:140:LEU:HA	37:1l:144:GLY:HA3	1.97	0.46
39:1n:27:GLU:HB3	39:1n:36:TYR:CD1	2.50	0.46
42:1q:2:GLU:HB3	43:1r:4:THR:HG23	1.98	0.46
42:1q:65:THR:HG21	42:1q:68:MET:HB2	1.98	0.46
3:1C:74:SER:OG	3:1C:97:LEU:O	2.33	0.45
4:1D:406:SER:HB3	4:1D:417:ILE:HD13	1.98	0.45
6:1F:277:LYS:HZ3	6:1F:291:TRP:CG	2.34	0.45
7:1G:258:ILE:HD11	7:1G:579:ARG:HE	1.80	0.45
7:1G:333:ASP:HB3	7:1G:611:LEU:HD11	1.98	0.45
8:1H:161:THR:O	8:1H:164:THR:HG22	2.16	0.45
9:1I:109:TYR:OH	45:1I:202:SF4:S1	2.74	0.45
10:1J:67:VAL:O	10:1J:71:THR:OG1	2.34	0.45
12:1L:296:ASN:HA	12:1L:356:ILE:HG13	1.98	0.45
13:1M:35:SER:O	13:1M:39:LEU:HD12	2.16	0.45
13:1M:318:ALA:O	13:1M:322:THR:HG23	2.16	0.45
19:1S:19:ARG:HB2	19:1S:65:TRP:HB2	1.97	0.45
20:1U:10:ALA:O	20:1U:14:ARG:HG2	2.15	0.45
32:1g:45:HIS:HB3	32:1g:58:MET:HE3	1.97	0.45
32:1g:118:ILE:HD11	41:1p:159:LYS:HD3	1.97	0.45
34:1i:10:ARG:HA	34:1i:13:GLN:OE1	2.16	0.45
35:1j:38:TRP:O	35:1j:42:HIS:HB2	2.15	0.45
36:1k:35:LEU:HB3	39:1n:41:CYS:SG	2.56	0.45
37:1l:47:TYR:OH	37:1l:77:ILE:O	2.23	0.45
43:1r:44:PRO:O	43:1r:47:LYS:NZ	2.50	0.45
6:1F:8:LYS:HE3	6:1F:8:LYS:HB3	1.70	0.45
7:1G:35:MET:HE3	7:1G:35:MET:C	2.41	0.45
7:1G:217:ALA:HB2	7:1G:243:ARG:HH11	1.82	0.45
7:1G:240:VAL:HG22	7:1G:250:ILE:HD12	1.98	0.45
7:1G:316:ALA:HB1	7:1G:514:ILE:HD11	1.98	0.45
8:1H:260:VAL:HG12	26:1a:16:LEU:HB3	1.98	0.45
9:1I:10:PRO:HB2	9:1I:20:ARG:NH2	2.31	0.45
12:1L:128:MET:O	12:1L:132:VAL:HG23	2.16	0.45
12:1L:132:VAL:HA	12:1L:258:PHE:CE2	2.51	0.45
12:1L:136:ASN:OD1	12:1L:139:GLN:N	2.37	0.45
18:1R:9:GLU:OE2	18:1R:25:ARG:HD2	2.16	0.45
28:1c:26:PHE:O	28:1c:29:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:86:LYS:HE2	34:1i:87:TYR:CE1	2.52	0.45
37:1l:10:PRO:HA	37:1l:26:LYS:HD3	1.98	0.45
37:1l:50:LEU:HD12	37:1l:50:LEU:HA	1.84	0.45
39:1n:29:TRP:HE1	39:1n:74:GLN:HA	1.81	0.45
4:1D:29:LYS:HE2	4:1D:29:LYS:N	2.31	0.45
47:1D:501:U10:H122	47:1D:501:U10:H101	1.63	0.45
6:1F:205:LEU:HD21	7:1G:50:GLY:HA3	1.99	0.45
10:1J:153:LEU:HD13	11:1K:62:ILE:HG13	1.97	0.45
12:1L:44:PHE:CE1	12:1L:95:PHE:HB2	2.52	0.45
12:1L:61:MET:HB3	12:1L:82:MET:SD	2.57	0.45
12:1L:399:VAL:HG23	12:1L:404:THR:HG21	1.98	0.45
12:1L:409:LEU:O	12:1L:413:LEU:HD23	2.16	0.45
13:1M:68:LEU:HD23	13:1M:72:LEU:CD1	2.37	0.45
13:1M:382:ILE:HD12	13:1M:396:MET:SD	2.55	0.45
14:1N:245:MET:HE3	14:1N:245:MET:C	2.42	0.45
24:1Y:10:ASP:OD1	24:1Y:11:ILE:N	2.49	0.45
30:1e:56:LYS:HD3	30:1e:56:LYS:O	2.16	0.45
31:1f:37:PHE:HB3	31:1f:40:LYS:HB2	1.98	0.45
37:1l:129:GLY:H	40:1o:97:ARG:HB3	1.81	0.45
39:1n:107:HIS:O	39:1n:111:LYS:N	2.35	0.45
42:1q:9:ARG:HE	42:1q:9:ARG:HB3	1.51	0.45
42:1q:48:TYR:CD1	42:1q:62:VAL:HG22	2.51	0.45
4:1D:92:GLU:OE1	4:1D:92:GLU:N	2.48	0.45
4:1D:148:LEU:HD21	4:1D:177:MET:HB2	1.98	0.45
4:1D:169:TRP:CE2	9:1I:40:TYR:CD2	3.04	0.45
5:1E:78:MET:HB2	5:1E:78:MET:HE3	1.70	0.45
5:1E:146:GLY:HA3	6:1F:142:PHE:HZ	1.81	0.45
6:1F:104:THR:HG22	6:1F:106:LYS:NZ	2.32	0.45
7:1G:91:GLU:OE1	7:1G:125:SER:N	2.49	0.45
8:1H:265:ALA:O	8:1H:269:THR:HG23	2.16	0.45
10:1J:7:PHE:C	10:1J:7:PHE:CD2	2.94	0.45
12:1L:10:THR:HG21	34:1i:78:VAL:HG22	1.99	0.45
12:1L:249:SER:HA	12:1L:306:THR:HG21	1.98	0.45
12:1L:254:VAL:HG12	12:1L:310:LEU:HD22	1.98	0.45
12:1L:483:PRO:O	12:1L:487:LYS:N	2.50	0.45
12:1L:486:MET:HA	12:1L:489:THR:OG1	2.17	0.45
13:1M:95:TYR:HD2	13:1M:136:TRP:CD2	2.34	0.45
15:1O:30:ASN:HA	15:1O:202:ILE:HD11	1.97	0.45
15:1O:132:PHE:HB3	15:1O:156:LYS:HE3	1.97	0.45
15:1O:275:ILE:HG21	15:1O:282:ILE:HG21	1.98	0.45
20:1T:71:MET:HE1	20:1T:72:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1a:30:THR:OG1	26:1a:31:ASN:OD1	2.21	0.45
37:1l:125:TYR:CD1	40:1o:18:PRO:HB3	2.52	0.45
37:1l:141:GLU:OE1	37:1l:141:GLU:N	2.49	0.45
38:1m:107:ASP:O	38:1m:111:LYS:HG2	2.15	0.45
40:1o:96:LYS:HA	40:1o:99:LYS:HE3	1.98	0.45
42:1q:90:LEU:HD12	42:1q:90:LEU:HA	1.78	0.45
5:1E:169:ILE:O	5:1E:172:ILE:HG13	2.17	0.45
7:1G:343:LEU:HB3	7:1G:507:TYR:CD2	2.51	0.45
8:1H:31:MET:HE2	9:1I:37:THR:HB	1.99	0.45
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.23	0.45
12:1L:12:LEU:HA	12:1L:129:MET:CE	2.47	0.45
12:1L:28:LYS:HG2	12:1L:31:LEU:H	1.81	0.45
12:1L:310:LEU:HA	12:1L:313:MET:SD	2.56	0.45
12:1L:409:LEU:O	12:1L:412:THR:HG22	2.17	0.45
13:1M:222:GLU:HA	13:1M:340:ARG:HH12	1.82	0.45
13:1M:282:LEU:HD21	13:1M:410:MET:HG2	1.99	0.45
13:1M:373:ILE:HG23	13:1M:448:THR:HG23	1.99	0.45
19:1S:29:SER:O	19:1S:33:ARG:HG3	2.17	0.45
21:1V:75:GLN:O	21:1V:79:VAL:HG23	2.17	0.45
28:1c:33:LYS:O	28:1c:37:GLU:HG3	2.16	0.45
31:1f:15:LEU:HD12	31:1f:16:VAL:N	2.31	0.45
32:1g:64:PHE:HA	32:1g:67:SER:HB2	1.99	0.45
34:1i:21:TRP:HE3	34:1i:22:LEU:HD22	1.80	0.45
36:1k:33:GLU:O	36:1k:36:ALA:HB3	2.16	0.45
37:1l:69:LEU:HA	37:1l:69:LEU:HD13	1.67	0.45
38:1m:48:LEU:HD23	39:1n:132:TRP:CH2	2.52	0.45
41:1p:6:LYS:HZ2	41:1p:11:GLU:HB3	1.81	0.45
1:1A:106:TRP:CZ2	8:1H:291:LYS:HD3	2.52	0.45
2:1B:147:PRO:HG3	9:1I:147:LEU:HD11	1.98	0.45
2:1B:147:PRO:HB3	9:1I:147:LEU:HD21	1.98	0.45
4:1D:176:LYS:NZ	43:1r:26:ARG:HD2	2.31	0.45
6:1F:141:GLU:OE1	6:1F:141:GLU:N	2.50	0.45
8:1H:121:TRP:CH2	10:1J:27:ILE:HG12	2.52	0.45
10:1J:117:PHE:HD2	10:1J:119:PHE:HZ	1.63	0.45
11:1K:6:MET:HA	11:1K:6:MET:HE3	1.98	0.45
12:1L:36:VAL:HA	12:1L:39:THR:OG1	2.17	0.45
12:1L:100:ILE:HD11	12:1L:245:ALA:HB3	1.98	0.45
12:1L:148:GLY:O	12:1L:151:SER:OG	2.33	0.45
12:1L:176:ARG:HH22	13:1M:404:ALA:H	1.65	0.45
12:1L:383:MET:SD	12:1L:384:PRO:HD2	2.57	0.45
12:1L:396:ILE:HA	12:1L:399:VAL:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:288:GLN:O	15:1O:292:VAL:HG22	2.17	0.45
16:1P:177:ARG:O	16:1P:181:TYR:HB2	2.17	0.45
17:1Q:54:LYS:HA	17:1Q:54:LYS:HD3	1.85	0.45
19:1S:63:LYS:NZ	19:1S:75:ASN:HA	2.31	0.45
26:1a:59:ARG:HD2	26:1a:59:ARG:HA	1.65	0.45
29:1d:70:PHE:C	29:1d:70:PHE:CD2	2.93	0.45
36:1k:41:ARG:HH22	36:1k:43:PRO:HA	1.82	0.45
39:1n:51:LYS:HA	39:1n:51:LYS:HD2	1.71	0.45
40:1o:41:THR:HB	40:1o:44:GLU:HG3	1.99	0.45
1:1A:38:GLU:OE1	8:1H:126:LYS:NZ	2.50	0.45
2:1B:104:TYR:CE1	2:1B:111:ARG:HD2	2.51	0.45
2:1B:147:PRO:HD3	9:1I:140:SER:HA	1.98	0.45
3:1C:131:GLU:HG3	3:1C:142:PHE:CD2	2.51	0.45
3:1C:150:ARG:NH2	22:1W:92:GLU:OE2	2.49	0.45
4:1D:226:GLU:HG2	4:1D:301:VAL:HG11	1.99	0.45
7:1G:324:ASP:OD2	7:1G:327:ALA:HB3	2.16	0.45
7:1G:432:ILE:HG22	7:1G:473:ILE:HG12	1.98	0.45
7:1G:575:ASN:ND2	7:1G:579:ARG:HB3	2.31	0.45
10:1J:20:PHE:CD2	10:1J:33:LEU:HB2	2.52	0.45
11:1K:20:LEU:O	12:1L:588:PHE:HB3	2.17	0.45
12:1L:32:TYR:CE2	12:1L:119:LYS:HE3	2.51	0.45
13:1M:305:THR:HG22	13:1M:307:TRP:HE3	1.82	0.45
15:1O:138:MET:HB2	15:1O:138:MET:HE3	1.66	0.45
16:1P:145:TYR:OH	56:1P:501:NDP:O2D	2.28	0.45
16:1P:322:ARG:HB2	16:1P:327:LEU:HD23	1.98	0.45
16:1P:332:GLU:H	16:1P:332:GLU:HG3	1.60	0.45
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.50	0.45
24:1Y:80:ARG:HB3	24:1Y:82:LYS:HG2	1.99	0.45
24:1Y:115:ALA:O	24:1Y:119:LEU:HG	2.17	0.45
39:1n:74:GLN:NE2	39:1n:75:HIS:O	2.49	0.45
42:1q:1:MET:HE2	42:1q:1:MET:O	2.17	0.45
1:1A:51:PHE:HE2	8:1H:130:ILE:HD13	1.81	0.45
2:1B:77:ARG:NH1	2:1B:77:ARG:O	2.50	0.45
3:1C:21:GLN:HE21	43:1r:97:ALA:HA	1.79	0.45
4:1D:294:TYR:CE2	4:1D:298:LEU:HD11	2.52	0.45
4:1D:346:ILE:HD12	7:1G:98:LEU:HD11	1.98	0.45
6:1F:248:GLU:O	6:1F:250:ASN:N	2.50	0.45
8:1H:25:ARG:HB2	8:1H:25:ARG:HH11	1.82	0.45
10:1J:146:LEU:HD12	10:1J:150:GLY:HA3	1.99	0.45
11:1K:73:LEU:HD11	14:1N:60:PHE:CD1	2.51	0.45
11:1K:90:VAL:HG22	12:1L:585:LYS:HZ2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:9:LEU:HD12	34:1i:81:ILE:HD12	1.99	0.45
12:1L:65:ASN:HB2	34:1i:84:TYR:OH	2.16	0.45
12:1L:524:ASN:HD21	39:1n:76:PRO:HG2	1.82	0.45
13:1M:450:ASN:ND2	32:1g:78:ALA:HA	2.30	0.45
14:1N:163:LEU:HD11	14:1N:167:TRP:CH2	2.51	0.45
15:1O:30:ASN:CG	15:1O:179:ILE:HD13	2.41	0.45
15:1O:171:TYR:HE2	15:1O:206:TYR:CG	2.35	0.45
16:1P:248:VAL:O	16:1P:322:ARG:NE	2.50	0.45
20:1U:43:ASP:OD1	20:1U:43:ASP:N	2.47	0.45
35:1j:7:ILE:O	35:1j:7:ILE:HG22	2.16	0.45
36:1k:13:MET:SD	36:1k:15:LEU:HB3	2.57	0.45
37:1l:36:PRO:HA	37:1l:48:PRO:HA	1.99	0.45
41:1p:130:GLN:HA	41:1p:133:GLN:HE21	1.82	0.45
2:1B:33:LEU:O	2:1B:37:VAL:HG23	2.17	0.45
3:1C:173:GLU:CD	3:1C:188:VAL:HA	2.41	0.45
3:1C:175:ARG:HD3	16:1P:13:ARG:NH1	2.31	0.45
5:1E:127:LYS:HA	5:1E:127:LYS:HD2	1.62	0.45
6:1F:77:LEU:H	6:1F:77:LEU:HD23	1.82	0.45
7:1G:650:LYS:HZ2	7:1G:650:LYS:HB3	1.81	0.45
10:1J:127:ILE:CG2	11:1K:50:ASN:HD21	2.30	0.45
12:1L:466:PHE:CD1	12:1L:469:SER:HB2	2.52	0.45
13:1M:373:ILE:HD12	13:1M:374:ASN:N	2.32	0.45
13:1M:427:LYS:HE2	32:1g:39:GLU:OE2	2.17	0.45
14:1N:265:MET:O	14:1N:268:GLN:HG3	2.16	0.45
15:1O:17:LYS:HE2	15:1O:17:LYS:HB2	1.86	0.45
15:1O:65:ASP:HB3	28:1c:2:PHE:CD1	2.52	0.45
15:1O:114:HIS:O	15:1O:118:THR:OG1	2.33	0.45
18:1R:93:GLN:O	18:1R:95:HIS:N	2.50	0.45
20:1T:71:MET:CE	20:1T:72:CYS:HB2	2.47	0.45
31:1f:56:TRP:CD2	33:1h:85:LYS:HG2	2.52	0.45
34:1i:86:LYS:HE2	34:1i:87:TYR:CZ	2.52	0.45
39:1n:44:ARG:NH1	39:1n:48:ASP:OD1	2.50	0.45
40:1o:36:ARG:HB2	40:1o:57:TYR:CE2	2.52	0.45
2:1B:86:MET:HE3	2:1B:86:MET:HB3	1.73	0.45
2:1B:166:LYS:HA	2:1B:169:ARG:HH22	1.81	0.45
4:1D:301:VAL:HA	4:1D:304:MET:HG3	1.98	0.45
5:1E:128:VAL:HA	5:1E:139:LEU:HD22	1.99	0.45
6:1F:206:LYS:HB3	6:1F:209:PHE:CD1	2.51	0.45
7:1G:104:ASP:OD2	7:1G:104:ASP:N	2.49	0.45
7:1G:372:GLU:OE2	7:1G:394:ARG:NE	2.48	0.45
10:1J:125:TRP:CZ3	25:1Z:122:GLY:HA2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:355:ASP:OD1	12:1L:355:ASP:N	2.49	0.45
12:1L:432:LEU:HB2	12:1L:509:TYR:OH	2.17	0.45
12:1L:561:ILE:O	12:1L:565:THR:HB	2.17	0.45
13:1M:108:MET:CB	13:1M:121:LEU:HD13	2.40	0.45
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD11	2.00	0.45
17:1Q:123:SER:OG	17:1Q:126:LYS:N	2.49	0.45
20:1T:58:PHE:CD2	20:1T:80:ILE:HG12	2.52	0.45
21:1V:93:MET:HB3	21:1V:96:TRP:CE3	2.48	0.45
23:1X:56:LEU:O	23:1X:60:LYS:HG2	2.17	0.45
25:1Z:119:PRO:HB2	25:1Z:124:LEU:HD13	1.97	0.45
26:1a:31:ASN:OD1	26:1a:31:ASN:N	2.50	0.45
28:1c:43:LYS:NZ	28:1c:43:LYS:HB2	2.31	0.45
32:1g:56:TRP:HA	32:1g:59:ARG:HG2	1.99	0.45
36:1k:41:ARG:HH11	36:1k:41:ARG:HG3	1.81	0.45
1:1A:4:MET:HA	1:1A:7:LEU:HD13	1.99	0.44
3:1C:189:GLU:HG2	16:1P:14:SER:OG	2.17	0.44
4:1D:83:LEU:O	4:1D:85:ARG:HD3	2.17	0.44
4:1D:242:ILE:HD12	4:1D:242:ILE:O	2.17	0.44
5:1E:56:ARG:NH2	6:1F:179:ARG:HH12	2.14	0.44
5:1E:196:ALA:H	6:1F:264:HIS:HB3	1.83	0.44
6:1F:111:ILE:HD11	6:1F:149:LEU:HB3	1.98	0.44
7:1G:97:LEU:HA	7:1G:97:LEU:HD23	1.71	0.44
7:1G:313:ASN:OD1	7:1G:517:ASN:ND2	2.50	0.44
8:1H:227:GLU:O	8:1H:231:ILE:HG12	2.17	0.44
10:1J:111:GLU:CD	30:1e:80:ARG:HH12	2.25	0.44
12:1L:297:ASP:O	12:1L:301:ILE:HD12	2.18	0.44
13:1M:37:ILE:O	13:1M:40:SER:OG	2.29	0.44
13:1M:147:LEU:HG	13:1M:151:PHE:HE2	1.83	0.44
14:1N:277:ILE:O	14:1N:280:THR:OG1	2.34	0.44
15:1O:292:VAL:HA	15:1O:295:LYS:HG3	1.98	0.44
24:1Y:4:LEU:HD23	24:1Y:4:LEU:H	1.82	0.44
24:1Y:19:ARG:HA	24:1Y:19:ARG:HD2	1.82	0.44
24:1Y:30:ALA:O	24:1Y:33:LEU:HG	2.17	0.44
34:1i:85:LEU:HD12	34:1i:89:VAL:HG11	1.99	0.44
38:1m:24:ILE:H	38:1m:24:ILE:HG13	1.51	0.44
39:1n:176:ARG:HA	39:1n:176:ARG:HD3	1.75	0.44
40:1o:66:LEU:O	40:1o:70:ARG:N	2.46	0.44
40:1o:95:VAL:HA	40:1o:98:MET:CE	2.46	0.44
2:1B:70:ASP:HA	2:1B:74:VAL:O	2.17	0.44
2:1B:76:PHE:CD1	2:1B:76:PHE:C	2.94	0.44
2:1B:150:PRO:HG3	4:1D:189:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:68:LEU:HA	4:1D:74:ARG:HG2	1.99	0.44
4:1D:265:ILE:H	4:1D:265:ILE:HD12	1.81	0.44
5:1E:183:LYS:HB3	44:1s:44:HIS:HE1	1.82	0.44
6:1F:226:GLU:O	6:1F:230:VAL:HG22	2.18	0.44
7:1G:105:CYS:O	7:1G:218:ARG:NH2	2.51	0.44
8:1H:314:ILE:HD12	8:1H:314:ILE:O	2.17	0.44
9:1I:112:ASP:OD2	9:1I:115:LYS:HE3	2.18	0.44
10:1J:117:PHE:HB2	10:1J:119:PHE:CE2	2.52	0.44
10:1J:164:GLY:HA2	14:1N:38:LEU:HD11	1.98	0.44
11:1K:44:SER:HB3	14:1N:75:ILE:HD11	1.98	0.44
12:1L:60:GLU:O	34:1i:99:ARG:HB3	2.17	0.44
12:1L:244:SER:HA	12:1L:248:HIS:ND1	2.33	0.44
12:1L:271:LYS:HE2	12:1L:271:LYS:HB2	1.72	0.44
14:1N:134:GLN:O	14:1N:135:LYS:HD3	2.17	0.44
20:1T:20:LYS:NZ	20:1T:27:PRO:HB3	2.32	0.44
22:1W:20:ILE:HG22	22:1W:21:PHE:N	2.33	0.44
24:1Y:27:ILE:O	24:1Y:31:THR:HG22	2.16	0.44
24:1Y:46:ALA:N	24:1Y:50:GLU:OE1	2.49	0.44
26:1a:21:MET:HB2	26:1a:25:HIS:CD2	2.51	0.44
27:1b:15:GLU:HB3	27:1b:18:LEU:HD23	2.00	0.44
27:1b:23:ALA:O	27:1b:27:LEU:HD22	2.17	0.44
34:1i:90:THR:O	41:1p:4:TRP:HH2	2.01	0.44
39:1n:108:PRO:HA	39:1n:111:LYS:HB2	1.99	0.44
41:1p:100:GLU:O	41:1p:104:ILE:HG13	2.17	0.44
41:1p:109:LEU:HD12	41:1p:131:PHE:CD2	2.51	0.44
41:1p:141:ARG:HG3	41:1p:142:TYR:CD2	2.53	0.44
43:1r:5:ARG:HD3	43:1r:6:VAL:N	2.32	0.44
1:1A:39:CYS:SG	8:1H:127:TYR:OH	2.60	0.44
1:1A:72:LEU:HA	10:1J:147:TYR:OH	2.17	0.44
3:1C:28:TYR:OH	3:1C:67:HIS:NE2	2.36	0.44
3:1C:182:ARG:NH2	22:1W:104:MET:HB3	2.33	0.44
7:1G:317:ALA:HB1	7:1G:331:LEU:HD21	2.00	0.44
7:1G:460:ARG:HE	7:1G:460:ARG:HB3	1.73	0.44
12:1L:161:ARG:HD2	12:1L:161:ARG:HA	1.79	0.44
12:1L:285:THR:HA	12:1L:308:SER:HB3	2.00	0.44
12:1L:394:LEU:HA	12:1L:397:GLU:OE2	2.16	0.44
12:1L:436:ARG:HA	36:1k:51:ARG:CZ	2.47	0.44
14:1N:264:TRP:HZ3	14:1N:337:LEU:HD21	1.82	0.44
14:1N:323:MET:HE2	14:1N:323:MET:HB3	1.78	0.44
15:1O:116:LEU:HD23	15:1O:260:ARG:HB2	1.99	0.44
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:14:ARG:HG2	20:1T:58:PHE:CE1	2.52	0.44
20:1U:71:MET:HG3	20:1U:72:CYS:SG	2.58	0.44
22:1W:25:MET:O	22:1W:29:LYS:HB2	2.17	0.44
23:1X:39:ASN:HB3	25:1Z:73:PRO:HG2	1.98	0.44
23:1X:69:PHE:O	23:1X:73:ILE:HG22	2.18	0.44
35:1j:59:TRP:N	35:1j:59:TRP:CD1	2.86	0.44
1:1A:68:GLU:O	1:1A:72:LEU:HG	2.18	0.44
2:1B:33:LEU:HD21	46:1B:202:PC1:H3A1	2.00	0.44
2:1B:34:ASP:O	2:1B:38:ASN:ND2	2.50	0.44
3:1C:108:LYS:HE3	3:1C:108:LYS:HB3	1.81	0.44
3:1C:113:GLU:H	3:1C:113:GLU:CD	2.26	0.44
4:1D:339:LYS:NZ	9:1I:129:ASP:OD2	2.50	0.44
5:1E:111:ARG:HB2	5:1E:152:PRO:HD3	1.98	0.44
7:1G:147:LYS:HG3	7:1G:211:LYS:HG2	2.00	0.44
7:1G:243:ARG:HG2	7:1G:248:MET:CE	2.42	0.44
8:1H:307:LEU:HD23	8:1H:310:MET:SD	2.57	0.44
12:1L:20:MET:C	12:1L:20:MET:HE2	2.43	0.44
12:1L:428:PHE:HB2	36:1k:62:PHE:CZ	2.52	0.44
12:1L:524:ASN:O	39:1n:77:GLN:NE2	2.49	0.44
12:1L:546:GLN:HE21	37:1l:79:TRP:CD1	2.35	0.44
13:1M:325:MET:HB2	13:1M:440:HIS:CD2	2.52	0.44
15:1O:31:ILE:HG23	54:1O:401:GTP:H3'	1.99	0.44
15:1O:209:THR:C	15:1O:212:PRO:HD2	2.43	0.44
15:1O:268:GLU:HA	15:1O:271:ASN:HB2	1.99	0.44
16:1P:24:PHE:N	16:1P:92:ILE:O	2.49	0.44
20:1U:19:LEU:H	20:1U:21:LEU:HG	1.82	0.44
20:1U:87:TYR:HE1	34:1i:18:ARG:HG2	1.81	0.44
21:1V:28:THR:HA	21:1V:31:LEU:HD12	2.00	0.44
21:1V:75:GLN:N	21:1V:78:GLU:OE2	2.50	0.44
40:1o:67:LYS:HG3	40:1o:70:ARG:NH1	2.32	0.44
4:1D:149:ASN:HD21	4:1D:371:LYS:CE	2.31	0.44
4:1D:243:GLY:O	4:1D:405:MET:HE1	2.17	0.44
6:1F:251:SER:OG	6:1F:252:GLY:N	2.51	0.44
7:1G:75:LYS:HB2	7:1G:75:LYS:HE2	1.63	0.44
9:1I:13:ASP:C	9:1I:13:ASP:OD1	2.60	0.44
10:1J:115:ILE:HG13	10:1J:116:ILE:HG12	2.00	0.44
11:1K:66:PHE:O	11:1K:69:CYS:HB2	2.17	0.44
12:1L:297:ASP:OD2	12:1L:354:GLN:NE2	2.43	0.44
13:1M:41:LEU:HD21	13:1M:52:PHE:HZ	1.83	0.44
13:1M:91:ARG:HD2	52:1M:501:3PE:C32	2.48	0.44
13:1M:336:ARG:HD2	13:1M:426:ILE:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:379:LEU:CA	13:1M:382:ILE:HG12	2.45	0.44
19:1S:26:SER:O	19:1S:33:ARG:NH2	2.45	0.44
20:1U:45:LEU:N	58:1n:201:EHZ:O9	2.50	0.44
23:1X:165:ARG:NH1	29:1d:87:ASP:OD2	2.33	0.44
24:1Y:23:ALA:O	24:1Y:27:ILE:HD13	2.16	0.44
28:1c:29:ILE:HD12	28:1c:30:TYR:N	2.32	0.44
33:1h:127:THR:OG1	33:1h:128:ILE:N	2.51	0.44
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.52	0.44
12:1L:312:LEU:HG	12:1L:395:ILE:HG21	2.00	0.44
12:1L:335:PHE:HE2	12:1L:380:LEU:HB3	1.83	0.44
12:1L:500:LEU:O	12:1L:504:LEU:HD13	2.18	0.44
13:1M:114:GLU:OE2	13:1M:116:ILE:HG22	2.17	0.44
15:1O:101:TYR:OH	15:1O:156:LYS:HA	2.17	0.44
17:1Q:38:PHE:HE1	17:1Q:58:GLU:HG3	1.83	0.44
17:1Q:40:PRO:HG2	17:1Q:56:LYS:HD3	2.00	0.44
21:1V:4:LEU:HD23	21:1V:4:LEU:H	1.83	0.44
23:1X:5:GLU:OE2	23:1X:53:ARG:NE	2.49	0.44
34:1i:119:MET:HE1	40:1o:60:HIS:O	2.18	0.44
36:1k:23:ILE:HG12	36:1k:29:GLU:HG2	2.00	0.44
38:1m:46:TYR:HA	38:1m:49:GLN:NE2	2.33	0.44
2:1B:143:ASP:OD1	2:1B:166:LYS:NZ	2.28	0.44
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.52	0.44
5:1E:56:ARG:HD3	5:1E:56:ARG:HA	1.74	0.44
6:1F:140:GLY:O	6:1F:179:ARG:NH2	2.47	0.44
6:1F:300:GLY:O	6:1F:330:GLY:HA3	2.18	0.44
6:1F:385:ARG:HG3	6:1F:386:PRO:HD2	2.00	0.44
7:1G:54:MET:HE1	7:1G:94:MET:HE2	1.99	0.44
7:1G:113:GLU:CD	7:1G:219:PRO:HB2	2.43	0.44
8:1H:31:MET:HG2	9:1I:41:LEU:HD12	1.99	0.44
12:1L:134:ALA:HB3	12:1L:140:LEU:HD23	1.99	0.44
13:1M:382:ILE:HG23	13:1M:396:MET:SD	2.57	0.44
14:1N:75:ILE:HD13	14:1N:75:ILE:HA	1.82	0.44
15:1O:258:ARG:HD2	15:1O:258:ARG:HA	1.73	0.44
19:1S:17:GLU:HB3	19:1S:51:PRO:HG2	1.99	0.44
20:1T:24:LYS:HE3	20:1T:42:LEU:HG	2.00	0.44
20:1T:81:ALA:HA	20:1T:86:VAL:CG2	2.48	0.44
20:1U:20:LYS:HG3	20:1U:30:LEU:HD21	2.00	0.44
28:1c:15:LEU:HD23	28:1c:15:LEU:H	1.82	0.44
38:1m:116:GLN:OE1	38:1m:116:GLN:N	2.51	0.44
1:1A:75:LEU:HB2	8:1H:151:LEU:HD11	1.99	0.44
4:1D:152:MET:HA	4:1D:152:MET:HE2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:110:LEU:HD21	6:1F:337:MET:HG3	1.99	0.44
5:1E:134:ASP:OD2	5:1E:136:LEU:HB2	2.17	0.44
6:1F:232:PRO:O	6:1F:236:ARG:HG3	2.18	0.44
6:1F:250:ASN:ND2	6:1F:250:ASN:H	2.15	0.44
6:1F:425:GLU:O	6:1F:428:GLU:HG3	2.18	0.44
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.58	0.44
8:1H:26:LYS:NZ	26:1a:4:GLU:HB3	2.33	0.44
10:1J:15:ILE:HD12	10:1J:16:GLY:N	2.33	0.44
10:1J:125:TRP:HZ3	25:1Z:122:GLY:HA2	1.83	0.44
10:1J:173:ARG:HH22	15:1O:254:ARG:CG	2.28	0.44
12:1L:142:ILE:HG12	13:1M:370:PRO:HB2	1.99	0.44
12:1L:233:LEU:HD22	12:1L:236:ALA:HB3	1.99	0.44
12:1L:371:THR:HG22	36:1k:68:LYS:HG2	1.99	0.44
13:1M:267:TRP:O	13:1M:271:MET:HG2	2.18	0.44
13:1M:319:HIS:O	13:1M:323:SER:OG	2.35	0.44
14:1N:1:FME:HG3	14:1N:46:LYS:NZ	2.33	0.44
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.53	0.44
22:1W:58:GLN:HA	22:1W:61:ASP:OD2	2.18	0.44
23:1X:92:GLY:N	26:1a:35:GLU:OE2	2.44	0.44
25:1Z:69:ILE:HG23	27:1b:52:TYR:CD2	2.52	0.44
28:1c:29:ILE:O	28:1c:32:ILE:HD12	2.18	0.44
40:1o:95:VAL:HA	40:1o:98:MET:HG2	1.99	0.44
1:1A:40:GLY:HA3	4:1D:53:PRO:HD2	1.99	0.44
1:1A:106:TRP:HH2	27:1b:18:LEU:HD21	1.83	0.44
3:1C:168:LEU:HD21	4:1D:90:LEU:HD23	1.99	0.44
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.17	0.44
5:1E:206:PRO:HB2	6:1F:39:ARG:HG3	1.99	0.44
6:1F:57:LEU:HA	6:1F:60:VAL:HG12	2.00	0.44
7:1G:43:HIS:HB3	7:1G:46:LEU:HB2	1.99	0.44
7:1G:171:ASP:OD2	7:1G:171:ASP:C	2.61	0.44
7:1G:483:VAL:HG23	7:1G:487:TRP:HD1	1.83	0.44
8:1H:9:LEU:HD22	26:1a:19:PRO:HB3	2.00	0.44
8:1H:272:TRP:CE2	9:1I:34:LEU:HD23	2.53	0.44
10:1J:63:GLY:O	10:1J:66:VAL:HG23	2.18	0.44
12:1L:203:MET:SD	12:1L:203:MET:C	3.01	0.44
12:1L:463:PHE:C	12:1L:467:ILE:HG12	2.43	0.44
13:1M:127:VAL:HG22	14:1N:249:LEU:HD12	2.00	0.44
13:1M:206:LYS:HA	13:1M:215:TRP:CZ2	2.53	0.44
16:1P:320:ARG:HE	16:1P:321:HIS:CD2	2.36	0.44
19:1S:38:LYS:HE2	19:1S:38:LYS:HB2	1.74	0.44
21:1V:30:ILE:HG22	21:1V:87:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:80:ARG:O	24:1Y:81:GLU:HG3	2.18	0.44
27:1b:77:LEU:HA	27:1b:79:TRP:NE1	2.33	0.44
30:1e:88:GLU:OE2	30:1e:90:LYS:NZ	2.45	0.44
32:1g:50:ASP:OD1	32:1g:53:VAL:HG22	2.18	0.44
34:1i:75:LEU:HD12	34:1i:79:TRP:CZ2	2.53	0.44
2:1B:35:ASP:HA	2:1B:38:ASN:ND2	2.32	0.43
2:1B:117:GLY:HA2	2:1B:148:GLY:O	2.18	0.43
3:1C:182:ARG:NH2	3:1C:184:VAL:HG12	2.33	0.43
5:1E:161:TYR:OH	5:1E:182:PRO:HG2	2.17	0.43
6:1F:27:GLY:HA3	44:1s:38:TYR:HE1	1.83	0.43
6:1F:262:VAL:HB	6:1F:284:ALA:HB1	2.00	0.43
9:1I:17:VAL:CG2	27:1b:13:ALA:HB2	2.47	0.43
12:1L:176:ARG:NH1	13:1M:404:ALA:H	2.15	0.43
12:1L:220:ALA:HB2	12:1L:260:LEU:HD23	1.99	0.43
12:1L:533:MET:O	12:1L:537:PRO:HD2	2.18	0.43
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.82	0.43
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	1.99	0.43
16:1P:154:LYS:HG3	16:1P:155:GLU:N	2.31	0.43
17:1Q:35:VAL:O	17:1Q:103:PHE:HA	2.18	0.43
41:1p:35:ILE:O	41:1p:38:LEU:HG	2.18	0.43
2:1B:27:GLU:OE1	2:1B:31:ALA:HB2	2.18	0.43
2:1B:47:PRO:HB3	2:1B:87:ILE:CD1	2.48	0.43
2:1B:61:HIS:NE2	4:1D:174:ARG:HB3	2.33	0.43
4:1D:51:PHE:CE1	8:1H:206:GLU:HA	2.51	0.43
5:1E:10:ARG:HH21	18:1R:77:LYS:HE2	1.82	0.43
5:1E:93:LYS:HE2	5:1E:93:LYS:HB2	1.78	0.43
8:1H:281:ARG:HH21	8:1H:284:GLN:NE2	2.16	0.43
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.17	0.43
12:1L:558:LEU:HD22	13:1M:211:GLY:HA2	2.00	0.43
13:1M:329:LEU:HD21	13:1M:437:MET:HG2	2.00	0.43
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.99	0.43
14:1N:343:LEU:HD23	14:1N:344:SER:H	1.83	0.43
15:1O:128:ILE:HG21	15:1O:160:ALA:HB2	2.01	0.43
15:1O:308:TYR:CE1	15:1O:320:LYS:HB3	2.52	0.43
22:1W:102:HIS:O	22:1W:105:ARG:HB2	2.18	0.43
25:1Z:121:MET:C	25:1Z:121:MET:SD	3.01	0.43
29:1d:38:GLY:HA2	29:1d:68:PHE:CD2	2.53	0.43
33:1h:21:PHE:C	33:1h:21:PHE:HD2	2.26	0.43
37:1l:156:TYR:CD2	40:1o:33:ARG:HG2	2.53	0.43
2:1B:31:ALA:HA	2:1B:174:ARG:HD2	1.99	0.43
2:1B:41:ARG:NH1	8:1H:57:THR:OG1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:188:GLU:HG3	6:1F:405:CYS:HB2	2.00	0.43
7:1G:276:ARG:O	7:1G:278:ARG:HG2	2.17	0.43
7:1G:426:PRO:O	7:1G:429:LEU:HB2	2.19	0.43
9:1I:164:GLU:OE2	42:1q:87:HIS:HB3	2.18	0.43
12:1L:19:ILE:HG13	12:1L:123:LEU:HD13	1.99	0.43
12:1L:585:LYS:HE2	12:1L:585:LYS:HB2	1.65	0.43
13:1M:151:PHE:HZ	14:1N:291:TYR:HA	1.83	0.43
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	2.01	0.43
13:1M:342:MET:HE2	13:1M:413:THR:CG2	2.46	0.43
14:1N:45:MET:HE3	14:1N:45:MET:HB3	1.76	0.43
14:1N:303:THR:C	14:1N:304:MET:HE2	2.42	0.43
15:1O:96:LEU:HD22	15:1O:100:LEU:HD13	2.00	0.43
15:1O:234:VAL:O	15:1O:238:ILE:HD13	2.19	0.43
16:1P:230:PHE:HA	16:1P:300:LEU:HG	2.00	0.43
16:1P:234:ASN:OD1	16:1P:234:ASN:C	2.61	0.43
18:1R:11:VAL:HG23	18:1R:17:ALA:HB2	1.99	0.43
20:1T:47:GLN:O	20:1T:50:ILE:HD12	2.18	0.43
20:1U:8:LEU:O	20:1U:12:LYS:CB	2.66	0.43
22:1W:95:ASN:HB2	22:1W:97:TRP:CE3	2.53	0.43
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.51	0.43
29:1d:104:LYS:H	29:1d:104:LYS:HG3	1.63	0.43
30:1e:49:ILE:HD12	30:1e:49:ILE:C	2.43	0.43
32:1g:77:VAL:O	32:1g:80:LEU:HG	2.18	0.43
39:1n:158:LYS:HE2	39:1n:158:LYS:HB2	1.80	0.43
44:1s:60:LYS:HB3	44:1s:60:LYS:HE3	1.72	0.43
2:1B:130:TYR:OH	3:1C:137:MET:HE1	2.18	0.43
3:1C:157:PHE:HE2	3:1C:161:PRO:HG3	1.83	0.43
4:1D:151:ILE:HD11	4:1D:218:PHE:HZ	1.83	0.43
4:1D:161:ILE:CG2	8:1H:278:PRO:HB3	2.49	0.43
4:1D:205:LEU:C	43:1r:35:GLN:HE21	2.26	0.43
6:1F:15:LEU:HB3	6:1F:20:ARG:NH2	2.34	0.43
6:1F:30:ASP:OD1	6:1F:32:ARG:NE	2.50	0.43
8:1H:90:PRO:HG3	8:1H:162:LEU:HD23	1.99	0.43
9:1I:74:GLU:OE2	9:1I:105:ARG:NE	2.51	0.43
12:1L:100:ILE:HG13	12:1L:341:MET:HE1	2.00	0.43
12:1L:250:SER:HG	12:1L:332:HIS:CE1	2.37	0.43
12:1L:295:GLN:OE1	39:1n:77:GLN:NE2	2.50	0.43
12:1L:378:LEU:HD12	12:1L:383:MET:CE	2.49	0.43
12:1L:486:MET:HE2	12:1L:486:MET:C	2.44	0.43
13:1M:408:LEU:O	13:1M:412:ILE:HG23	2.18	0.43
16:1P:302:ASP:OD1	16:1P:302:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:27:PRO:HA	20:1U:30:LEU:HB3	2.00	0.43
20:1U:45:LEU:HD21	39:1n:47:PHE:HE2	1.83	0.43
22:1W:62:LYS:HE2	22:1W:62:LYS:HB2	1.77	0.43
22:1W:113:PRO:O	22:1W:114:ARG:NH1	2.51	0.43
27:1b:38:THR:O	27:1b:42:ILE:HG13	2.18	0.43
32:1g:45:HIS:HD2	32:1g:54:ASP:HB3	1.83	0.43
32:1g:79:TYR:HH	33:1h:69:HIS:CD2	2.34	0.43
32:1g:88:TRP:NE1	41:1p:65:ARG:HB3	2.34	0.43
38:1m:4:LYS:HE2	38:1m:4:LYS:HA	2.01	0.43
38:1m:35:ARG:CZ	38:1m:39:ARG:HB2	2.48	0.43
41:1p:109:LEU:HD12	41:1p:131:PHE:HD2	1.83	0.43
41:1p:131:PHE:HA	41:1p:134:VAL:CG1	2.48	0.43
2:1B:168:LYS:HE3	42:1q:76:ASP:OD2	2.19	0.43
3:1C:134:ILE:HB	3:1C:142:PHE:HE2	1.82	0.43
4:1D:5:GLN:HG2	15:1O:287:HIS:NE2	2.32	0.43
4:1D:182:GLU:OE1	9:1I:58:SER:N	2.52	0.43
6:1F:106:LYS:HE3	6:1F:257:ASN:ND2	2.32	0.43
6:1F:194:GLU:HB3	6:1F:200:GLN:O	2.19	0.43
6:1F:322:LEU:HB3	6:1F:327:THR:HG23	2.00	0.43
7:1G:515:ARG:HG2	7:1G:532:ILE:HD11	1.99	0.43
10:1J:173:ARG:HH12	15:1O:254:ARG:NE	2.17	0.43
11:1K:96:LEU:HD23	11:1K:96:LEU:HA	1.88	0.43
12:1L:98:TRP:O	12:1L:102:GLU:HG3	2.18	0.43
12:1L:136:ASN:HA	12:1L:197:ASP:HA	2.00	0.43
13:1M:321:LEU:O	13:1M:440:HIS:NE2	2.51	0.43
13:1M:404:ALA:HB1	13:1M:408:LEU:HD23	2.00	0.43
13:1M:423:ILE:HB	13:1M:426:ILE:HD11	2.00	0.43
14:1N:315:TRP:H	14:1N:315:TRP:HD1	1.62	0.43
14:1N:321:LYS:HG3	14:1N:323:MET:CG	2.46	0.43
15:1O:135:LEU:HA	15:1O:138:MET:HB3	2.01	0.43
15:1O:271:ASN:C	15:1O:271:ASN:OD1	2.60	0.43
17:1Q:11:ILE:HG12	22:1W:23:ARG:NH1	2.33	0.43
22:1W:75:ASP:O	22:1W:79:VAL:HG23	2.18	0.43
29:1d:46:ASN:HB2	29:1d:53:VAL:HA	2.00	0.43
34:1i:13:GLN:HA	34:1i:16:GLU:OE1	2.18	0.43
35:1j:27:PHE:C	35:1j:27:PHE:HD2	2.26	0.43
37:1l:23:ALA:HA	37:1l:26:LYS:HB3	2.01	0.43
41:1p:132:THR:O	41:1p:136:LYS:HG2	2.18	0.43
1:1A:53:MET:HB3	1:1A:53:MET:HE3	1.74	0.43
1:1A:108:GLN:O	1:1A:110:GLY:N	2.51	0.43
4:1D:391:ILE:HD13	4:1D:391:ILE:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:35:GLY:O	6:1F:39:ARG:NE	2.38	0.43
7:1G:266:LYS:NZ	7:1G:674:THR:HB	2.34	0.43
8:1H:6:ILE:HG22	8:1H:10:ILE:CD1	2.47	0.43
9:1I:95:GLU:HG3	9:1I:108:ARG:HB3	1.99	0.43
9:1I:174:LEU:HD12	9:1I:174:LEU:HA	1.83	0.43
12:1L:60:GLU:HB3	12:1L:83:ASP:HB3	2.00	0.43
12:1L:159:HIS:HE1	39:1n:95:CYS:HB3	1.83	0.43
13:1M:59:ASP:H	13:1M:62:SER:HG	1.63	0.43
13:1M:280:THR:HG21	38:1m:68:THR:HA	1.99	0.43
14:1N:103:ALA:HA	14:1N:106:LEU:HD12	2.00	0.43
15:1O:105:LEU:HA	15:1O:128:ILE:HD11	2.01	0.43
15:1O:194:ILE:HD12	15:1O:194:ILE:O	2.19	0.43
15:1O:200:GLN:HE22	15:1O:204:ASN:HD21	1.67	0.43
17:1Q:26:PRO:HG2	17:1Q:29:HIS:HB2	2.00	0.43
20:1U:36:PHE:HA	20:1U:40:LEU:HB2	2.01	0.43
22:1W:28:ALA:O	22:1W:32:VAL:HG12	2.19	0.43
28:1c:41:GLU:OE2	28:1c:45:ARG:HD2	2.18	0.43
29:1d:25:LYS:HD3	29:1d:25:LYS:HA	1.76	0.43
30:1e:21:SER:O	30:1e:21:SER:OG	2.36	0.43
40:1o:114:ARG:HG2	40:1o:118:GLU:OE1	2.19	0.43
2:1B:133:VAL:HG23	2:1B:135:GLY:H	1.83	0.43
4:1D:228:MET:HE3	4:1D:228:MET:HB2	1.83	0.43
4:1D:236:ARG:O	4:1D:240:VAL:N	2.30	0.43
6:1F:28:ARG:HA	44:1s:39:ARG:HH21	1.84	0.43
7:1G:104:ASP:HB2	45:1G:801:SF4:S2	2.59	0.43
8:1H:39:VAL:HA	42:1q:31:ASN:OD1	2.19	0.43
11:1K:12:PHE:HE2	14:1N:72:MET:CB	2.32	0.43
12:1L:392:LYS:NZ	12:1L:416:THR:HG23	2.33	0.43
13:1M:252:PRO:HG3	29:1d:117:HIS:CE1	2.54	0.43
13:1M:453:MET:HG3	32:1g:77:VAL:HG23	2.00	0.43
14:1N:95:MET:HE1	14:1N:145:ILE:HD12	1.99	0.43
16:1P:196:LEU:HD23	16:1P:196:LEU:HA	1.77	0.43
16:1P:276:GLU:OE1	16:1P:276:GLU:N	2.52	0.43
22:1W:98:LYS:HG3	22:1W:102:HIS:HB2	2.00	0.43
23:1X:162:HIS:NE2	33:1h:99:GLU:HB3	2.34	0.43
29:1d:-1:MET:HE2	29:1d:86:ARG:HD3	2.00	0.43
33:1h:7:ARG:HH22	34:1i:32:PRO:HG3	1.83	0.43
36:1k:28:LEU:HD22	36:1k:52:TYR:CE2	2.53	0.43
36:1k:44:TRP:O	36:1k:44:TRP:CG	2.72	0.43
38:1m:2:PHE:HB2	39:1n:72:TYR:CE2	2.54	0.43
41:1p:36:PHE:O	41:1p:40:VAL:HB	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:50:PHE:CD2	41:1p:50:PHE:C	2.96	0.43
41:1p:73:ILE:HG12	41:1p:87:ALA:HB1	2.00	0.43
2:1B:72:PHE:CD2	2:1B:72:PHE:N	2.85	0.43
6:1F:115:PRO:O	6:1F:119:VAL:HG13	2.19	0.43
8:1H:236:ALA:HB1	8:1H:259:PHE:CZ	2.53	0.43
10:1J:100:GLU:HA	10:1J:103:MET:SD	2.59	0.43
10:1J:150:GLY:O	10:1J:154:VAL:HG12	2.18	0.43
12:1L:113:PHE:HB3	12:1L:116:ARG:HD2	2.01	0.43
12:1L:280:LEU:O	12:1L:284:THR:HG22	2.18	0.43
12:1L:338:MET:HE3	12:1L:461:SER:CB	2.49	0.43
13:1M:5:ILE:HD11	13:1M:108:MET:SD	2.59	0.43
13:1M:238:LEU:HD12	13:1M:239:GLY:N	2.33	0.43
14:1N:25:HIS:NE2	30:1e:17:MET:SD	2.92	0.43
14:1N:219:LEU:O	14:1N:223:SER:N	2.50	0.43
15:1O:94:TYR:CD1	15:1O:148:CYS:HB3	2.54	0.43
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	2.01	0.43
16:1P:182:PHE:HB2	16:1P:245:ILE:HD11	2.01	0.43
20:1U:50:ILE:HD12	20:1U:50:ILE:C	2.44	0.43
21:1V:81:LEU:HD13	21:1V:85:ASN:ND2	2.28	0.43
24:1Y:126:MET:O	24:1Y:130:GLU:HG2	2.18	0.43
25:1Z:94:GLU:HA	25:1Z:97:ILE:HB	2.01	0.43
33:1h:53:ALA:HB2	41:1p:61:TYR:CD1	2.53	0.43
35:1j:19:ARG:HA	35:1j:22:LEU:HB2	2.01	0.43
42:1q:9:ARG:O	42:1q:13:GLN:HG2	2.18	0.43
5:1E:72:ILE:HG22	5:1E:73:LEU:HD22	2.00	0.43
7:1G:279:LEU:HD13	7:1G:550:GLY:H	1.83	0.43
7:1G:549:HIS:CE1	7:1G:677:ILE:HG12	2.53	0.43
8:1H:184:MET:HE3	8:1H:184:MET:HB2	1.87	0.43
12:1L:499:MET:C	12:1L:499:MET:HE2	2.44	0.43
12:1L:517:SER:OG	12:1L:518:GLN:N	2.51	0.43
13:1M:209:LEU:HD23	13:1M:209:LEU:H	1.84	0.43
14:1N:245:MET:HE3	14:1N:246:VAL:N	2.34	0.43
15:1O:266:LYS:H	15:1O:266:LYS:HG2	1.66	0.43
16:1P:97:ARG:NH2	56:1P:501:NDP:H2B	2.33	0.43
16:1P:186:ARG:HD2	16:1P:251:ARG:NE	2.34	0.43
20:1T:72:CYS:O	20:1T:76:ILE:HG12	2.18	0.43
20:1U:11:ILE:HA	20:1U:14:ARG:CG	2.49	0.43
22:1W:76:PRO:O	22:1W:79:VAL:N	2.52	0.43
29:1d:9:VAL:HA	29:1d:10:PRO:HD3	1.92	0.43
29:1d:120:ARG:NH2	41:1p:144:ASP:OD2	2.52	0.43
31:1f:15:LEU:O	31:1f:18:VAL:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:21:PHE:CE2	33:1h:25:MET:HE2	2.52	0.43
37:1l:117:TRP:O	37:1l:120:GLU:HG3	2.19	0.43
38:1m:110:LYS:O	38:1m:114:LEU:HG	2.18	0.43
39:1n:26:LEU:HA	39:1n:29:TRP:CD1	2.54	0.43
39:1n:97:LYS:HE3	39:1n:97:LYS:HB2	1.87	0.43
40:1o:47:ASP:O	40:1o:49:GLN:NE2	2.49	0.43
42:1q:71:ARG:HD3	42:1q:115:PHE:CZ	2.54	0.43
1:1A:1:FME:HE1	10:1J:2:THR:HG21	2.01	0.43
3:1C:137:MET:HB3	3:1C:162:PHE:CD2	2.54	0.43
4:1D:136:TRP:HZ3	4:1D:314:CYS:HA	1.84	0.43
6:1F:205:LEU:H	6:1F:205:LEU:HD12	1.83	0.43
6:1F:224:ASN:O	6:1F:228:VAL:HG22	2.19	0.43
8:1H:91:MET:O	8:1H:92:PRO:C	2.61	0.43
12:1L:531:SER:HG	12:1L:535:ARG:HH22	1.59	0.43
14:1N:213:LEU:HB2	14:1N:329:MET:HE2	2.00	0.43
53:1N:401:CDL:H152	53:1N:401:CDL:HA61	2.00	0.43
16:1P:105:ASP:OD2	16:1P:107:GLU:HG3	2.19	0.43
16:1P:108:ASP:OD1	16:1P:108:ASP:N	2.33	0.43
25:1Z:50:MET:O	25:1Z:50:MET:HE3	2.18	0.43
28:1c:26:PHE:HA	28:1c:29:ILE:HD11	2.00	0.43
29:1d:106:LYS:HB2	41:1p:77:GLU:CD	2.44	0.43
30:1e:93:PRO:HA	30:1e:94:PRO:HD3	1.91	0.43
34:1i:15:ARG:O	34:1i:19:ARG:HG3	2.18	0.43
34:1i:79:TRP:HA	34:1i:79:TRP:CE3	2.54	0.43
34:1i:99:ARG:HD3	34:1i:100:LYS:N	2.33	0.43
35:1j:45:ASP:HA	35:1j:48:LEU:HB3	2.01	0.43
1:1A:62:PHE:CD1	1:1A:62:PHE:C	2.94	0.42
3:1C:125:LYS:HD2	4:1D:253:TYR:CE1	2.54	0.42
4:1D:223:ASP:OD2	4:1D:223:ASP:C	2.62	0.42
4:1D:413:ASP:OD2	8:1H:281:ARG:NH1	2.48	0.42
47:1D:501:U10:H471	47:1D:501:U10:H451	1.82	0.42
5:1E:161:TYR:CZ	5:1E:182:PRO:HG2	2.54	0.42
7:1G:198:ASN:HA	7:1G:268:ARG:NH2	2.33	0.42
7:1G:357:ASP:HA	19:1S:53:LEU:HD23	2.01	0.42
7:1G:365:ASN:N	7:1G:491:ASN:OD1	2.52	0.42
10:1J:86:ASN:O	10:1J:89:VAL:HG22	2.18	0.42
11:1K:17:ALA:O	11:1K:21:MET:HB3	2.18	0.42
12:1L:48:LEU:O	12:1L:52:LEU:HD22	2.19	0.42
12:1L:140:LEU:HD11	12:1L:198:LEU:HD11	2.00	0.42
13:1M:42:LEU:CD2	13:1M:67:VAL:HG11	2.49	0.42
16:1P:270:PHE:CD2	16:1P:279:THR:HG22	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:58:GLU:C	17:1Q:59:PHE:HD1	2.27	0.42
18:1R:74:ASN:OD1	18:1R:76:ASP:HB2	2.19	0.42
25:1Z:97:ILE:HG22	25:1Z:98:MET:HE3	2.01	0.42
30:1e:79:LYS:HD2	30:1e:79:LYS:C	2.44	0.42
31:1f:53:GLU:N	31:1f:53:GLU:OE1	2.51	0.42
32:1g:97:VAL:HG12	41:1p:8:VAL:HG12	2.01	0.42
35:1j:33:TRP:CZ2	36:1k:67:LEU:HA	2.52	0.42
37:1l:156:TYR:HB3	40:1o:33:ARG:NH1	2.34	0.42
2:1B:50:PHE:CE2	2:1B:100:LEU:HD23	2.53	0.42
4:1D:29:LYS:H	4:1D:29:LYS:CE	2.33	0.42
4:1D:302:GLU:HG2	9:1I:3:LYS:HD2	2.01	0.42
5:1E:186:PRO:HG2	5:1E:190:ARG:O	2.19	0.42
5:1E:199:LEU:HD12	5:1E:199:LEU:HA	1.80	0.42
6:1F:150:GLN:HG3	44:1s:54:LEU:HD21	2.01	0.42
6:1F:261:HIS:CD2	6:1F:337:MET:HA	2.54	0.42
6:1F:384:ALA:HB3	6:1F:430:MET:HE3	2.00	0.42
6:1F:388:GLU:OE1	6:1F:388:GLU:N	2.52	0.42
7:1G:11:VAL:HG11	7:1G:73:VAL:HG21	2.00	0.42
7:1G:255:HIS:CE1	7:1G:257:ASP:HB2	2.54	0.42
8:1H:20:LEU:HD23	8:1H:228:TYR:HB3	2.01	0.42
8:1H:91:MET:HE2	8:1H:91:MET:N	2.35	0.42
8:1H:138:GLN:OE1	8:1H:200:LEU:HD13	2.19	0.42
8:1H:272:TRP:NE1	9:1I:34:LEU:O	2.52	0.42
9:1I:146:GLU:OE2	42:1q:124:TYR:HD2	2.03	0.42
12:1L:104:SER:O	12:1L:108:MET:N	2.51	0.42
12:1L:292:ALA:HB2	12:1L:304:PHE:CD2	2.52	0.42
13:1M:104:LEU:HD23	13:1M:108:MET:HG3	2.01	0.42
13:1M:453:MET:HG3	32:1g:77:VAL:CG2	2.49	0.42
15:1O:145:ARG:NH2	15:1O:148:CYS:SG	2.81	0.42
19:1S:16:ARG:NH2	19:1S:69:ALA:HB2	2.34	0.42
21:1V:69:GLU:OE1	21:1V:69:GLU:C	2.63	0.42
23:1X:146:ARG:HE	30:1e:41:GLU:HG3	1.85	0.42
25:1Z:50:MET:O	25:1Z:54:ASN:HB2	2.19	0.42
26:1a:31:ASN:ND2	26:1a:36:LYS:HA	2.35	0.42
37:1l:13:TYR:HB3	37:1l:15:LYS:NZ	2.34	0.42
37:1l:75:GLU:OE2	38:1m:39:ARG:NH1	2.50	0.42
39:1n:102:CYS:O	39:1n:106:TRP:NE1	2.52	0.42
39:1n:133:GLU:HA	39:1n:136:VAL:HG22	2.00	0.42
40:1o:114:ARG:CG	40:1o:117:ARG:HH21	2.24	0.42
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	2.00	0.42
6:1F:206:LYS:HB2	6:1F:206:LYS:HE2	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:522:LEU:HD23	7:1G:537:LEU:HD11	2.00	0.42
8:1H:186:PHE:O	8:1H:189:THR:HB	2.19	0.42
10:1J:120:ASN:HD22	30:1e:72:MET:CG	2.32	0.42
11:1K:8:ILE:HD12	11:1K:9:ILE:H	1.83	0.42
12:1L:264:TYR:CD2	12:1L:322:PRO:HG3	2.55	0.42
12:1L:365:ALA:HA	35:1j:17:LEU:HD22	2.01	0.42
13:1M:290:SER:HB2	13:1M:319:HIS:NE2	2.34	0.42
14:1N:289:ASN:HB3	14:1N:293:TYR:CE1	2.54	0.42
16:1P:58:HIS:H	16:1P:58:HIS:CD2	2.38	0.42
19:1S:44:LYS:HE2	19:1S:44:LYS:HB2	1.60	0.42
19:1S:49:ASP:N	19:1S:49:ASP:OD1	2.52	0.42
20:1U:42:LEU:HD13	20:1U:46:ASP:HB2	2.01	0.42
22:1W:24:ASP:H	22:1W:27:GLU:CD	2.27	0.42
27:1b:25:GLY:O	27:1b:29:ILE:HD12	2.19	0.42
27:1b:30:ILE:HD12	27:1b:30:ILE:C	2.44	0.42
29:1d:15:PRO:HG2	29:1d:81:TYR:CZ	2.53	0.42
37:1l:136:ASN:ND2	37:1l:151:GLU:O	2.53	0.42
39:1n:12:GLN:H	39:1n:12:GLN:CD	2.27	0.42
39:1n:84:SER:O	39:1n:90:TYR:HB2	2.20	0.42
40:1o:88:TYR:CE1	40:1o:91:HIS:HD2	2.37	0.42
41:1p:135:SER:O	41:1p:139:GLN:HG3	2.19	0.42
2:1B:47:PRO:HD2	2:1B:76:PHE:H	1.82	0.42
2:1B:161:LEU:HB3	2:1B:165:ARG:HH12	1.84	0.42
7:1G:70:ALA:HB1	17:1Q:118:TYR:HB2	2.01	0.42
7:1G:145:LEU:HD21	7:1G:687:CYS:HB3	2.01	0.42
7:1G:560:ILE:HD13	7:1G:560:ILE:HA	1.85	0.42
7:1G:622:ARG:HH21	7:1G:626:VAL:HG22	1.84	0.42
8:1H:195:ARG:O	8:1H:198:PHE:N	2.53	0.42
10:1J:162:LEU:O	10:1J:165:VAL:HG12	2.20	0.42
12:1L:42:TYR:HH	34:1i:69:PHE:HD2	1.63	0.42
12:1L:550:SER:O	12:1L:552:LEU:N	2.52	0.42
12:1L:604:TYR:OH	14:1N:156:THR:HG21	2.19	0.42
13:1M:269:MET:O	13:1M:273:SER:OG	2.25	0.42
17:1Q:13:VAL:N	22:1W:15:THR:O	2.49	0.42
23:1X:167:PHE:O	33:1h:104:ARG:NH2	2.47	0.42
25:1Z:111:PHE:CD2	25:1Z:117:VAL:HG11	2.54	0.42
33:1h:39:GLY:O	33:1h:43:VAL:HG22	2.19	0.42
35:1j:12:ARG:HD3	36:1k:50:TRP:CD1	2.54	0.42
2:1B:42:ARG:NE	2:1B:168:LYS:HB2	2.33	0.42
6:1F:82:MET:HE1	6:1F:211:ALA:HB1	2.01	0.42
6:1F:208:PRO:HB2	6:1F:213:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:45:ARG:HD3	7:1G:262:TRP:CZ2	2.54	0.42
10:1J:105:TYR:CE2	10:1J:109:LYS:HD3	2.55	0.42
12:1L:123:LEU:HB2	12:1L:150:MET:CE	2.42	0.42
12:1L:127:THR:O	12:1L:130:ILE:HG13	2.20	0.42
12:1L:137:LEU:HB2	12:1L:196:TRP:HE3	1.84	0.42
12:1L:150:MET:O	12:1L:150:MET:HG3	2.19	0.42
12:1L:374:ILE:HG21	36:1k:66:LEU:HA	2.00	0.42
12:1L:560:THR:HA	12:1L:564:LYS:HB2	2.01	0.42
13:1M:116:ILE:HD12	13:1M:119:TYR:HB3	2.00	0.42
13:1M:127:VAL:HB	13:1M:128:PRO:HD3	2.02	0.42
13:1M:341:THR:HG21	38:1m:64:LEU:HD11	2.02	0.42
14:1N:154:MET:HE1	14:1N:191:THR:HB	2.01	0.42
15:1O:251:GLN:HB2	15:1O:255:THR:OG1	2.19	0.42
18:1R:44:ILE:HD12	18:1R:44:ILE:HA	1.88	0.42
24:1Y:139:LYS:HD3	33:1h:112:ARG:HG3	2.02	0.42
28:1c:29:ILE:HD12	28:1c:30:TYR:H	1.83	0.42
33:1h:130:LYS:O	33:1h:133:ILE:HG12	2.20	0.42
34:1i:8:LYS:O	34:1i:12:GLN:HG3	2.19	0.42
35:1j:16:GLN:NE2	35:1j:16:GLN:O	2.53	0.42
36:1k:48:GLU:OE1	36:1k:52:TYR:OH	2.22	0.42
43:1r:91:LYS:HE2	43:1r:91:LYS:HB3	1.72	0.42
1:1A:58:VAL:HA	1:1A:61:THR:HG22	2.02	0.42
2:1B:45:LEU:HG	2:1B:74:VAL:HG13	2.02	0.42
2:1B:47:PRO:HB3	2:1B:87:ILE:HD11	2.01	0.42
2:1B:96:MET:SD	4:1D:82:LEU:HD22	2.59	0.42
2:1B:145:TYR:CZ	9:1I:144:HIS:HB2	2.54	0.42
2:1B:171:LYS:N	16:1P:52:GLU:OE2	2.41	0.42
3:1C:88:ASN:OD1	3:1C:88:ASN:N	2.53	0.42
4:1D:115:GLU:O	4:1D:119:SER:OG	2.26	0.42
4:1D:282:GLU:OE1	4:1D:282:GLU:N	2.48	0.42
4:1D:346:ILE:HG23	7:1G:117:GLN:HG2	2.00	0.42
5:1E:36:LYS:NZ	44:1s:59:SER:HA	2.34	0.42
6:1F:56:ILE:HD13	6:1F:124:VAL:HG13	2.01	0.42
6:1F:104:THR:HG22	6:1F:106:LYS:HZ3	1.84	0.42
6:1F:189:GLU:CD	6:1F:190:THR:HG23	2.45	0.42
7:1G:272:ASP:OD1	7:1G:272:ASP:N	2.52	0.42
7:1G:512:GLU:OE2	7:1G:515:ARG:NH1	2.53	0.42
10:1J:56:VAL:O	10:1J:60:TYR:HB2	2.19	0.42
12:1L:2:ASN:HB3	12:1L:3:PRO:HD3	2.02	0.42
12:1L:140:LEU:HD23	12:1L:140:LEU:HA	1.86	0.42
12:1L:190:LEU:HD21	12:1L:196:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:389:PHE:HE2	35:1j:46:ALA:HB1	1.85	0.42
13:1M:86:LYS:HE2	13:1M:86:LYS:HB2	1.73	0.42
13:1M:278:ARG:C	38:1m:71:ARG:HH22	2.28	0.42
13:1M:349:GLN:OE1	13:1M:349:GLN:HA	2.19	0.42
15:1O:21:THR:O	15:1O:21:THR:OG1	2.32	0.42
15:1O:70:ASP:O	15:1O:74:SER:N	2.52	0.42
15:1O:92:ASN:O	15:1O:96:LEU:HB2	2.19	0.42
15:1O:200:GLN:O	15:1O:203:GLU:HB2	2.19	0.42
16:1P:211:SER:O	16:1P:215:ILE:HG12	2.19	0.42
21:1V:34:LEU:HD13	21:1V:48:GLU:HG2	2.00	0.42
23:1X:70:PHE:HA	23:1X:73:ILE:HG22	2.00	0.42
23:1X:89:ASP:OD2	26:1a:63:THR:HG21	2.20	0.42
23:1X:110:VAL:HB	23:1X:116:TRP:CE3	2.55	0.42
25:1Z:120:MET:SD	25:1Z:121:MET:N	2.92	0.42
26:1a:13:ALA:O	26:1a:17:PHE:N	2.53	0.42
29:1d:77:LYS:HB3	29:1d:77:LYS:HE3	1.87	0.42
34:1i:92:LYS:HB2	34:1i:92:LYS:HE3	1.74	0.42
41:1p:116:GLU:HG2	41:1p:123:ASN:HB2	2.02	0.42
41:1p:170:LYS:O	41:1p:174:ALA:N	2.53	0.42
1:1A:90:MET:HE1	10:1J:151:THR:HG23	2.01	0.42
4:1D:145:THR:HG23	4:1D:181:TYR:OH	2.19	0.42
4:1D:167:PHE:C	4:1D:167:PHE:CD2	2.98	0.42
4:1D:224:GLU:O	4:1D:227:GLU:HG3	2.20	0.42
5:1E:46:ALA:O	5:1E:49:PRO:HD2	2.19	0.42
7:1G:9:ILE:HD11	7:1G:75:LYS:HG3	2.02	0.42
7:1G:213:TYR:O	7:1G:213:TYR:CG	2.73	0.42
9:1I:160:LYS:HD2	9:1I:161:TRP:CD1	2.55	0.42
10:1J:120:ASN:HD22	30:1e:72:MET:HG2	1.84	0.42
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	2.01	0.42
13:1M:322:THR:O	13:1M:325:MET:HB3	2.19	0.42
14:1N:24:SER:OG	30:1e:14:ASP:OD1	2.36	0.42
14:1N:196:TYR:OH	24:1Y:136:ALA:O	2.21	0.42
15:1O:86:PRO:HB2	15:1O:143:PHE:CD1	2.55	0.42
16:1P:319:ARG:NH2	22:1W:51:GLN:OE1	2.52	0.42
23:1X:146:ARG:HH11	23:1X:147:PRO:HD3	1.85	0.42
32:1g:48:ASP:CG	32:1g:53:VAL:HG23	2.45	0.42
32:1g:99:TYR:C	32:1g:99:TYR:CD1	2.97	0.42
32:1g:106:PRO:HB2	32:1g:108:MET:HE1	2.01	0.42
33:1h:6:LYS:HE3	33:1h:8:LEU:HD13	2.02	0.42
36:1k:67:LEU:HB3	36:1k:70:PHE:CD1	2.55	0.42
37:1l:98:TRP:CE2	38:1m:10:LEU:HD13	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:128:VAL:C	40:1o:101:PHE:HB2	2.44	0.42
39:1n:80:ILE:HD12	39:1n:80:ILE:O	2.20	0.42
1:1A:2:ASN:OD1	1:1A:2:ASN:N	2.50	0.42
1:1A:64:LEU:HA	1:1A:64:LEU:HD23	1.76	0.42
2:1B:93:THR:OG1	2:1B:94:ASN:N	2.53	0.42
2:1B:169:ARG:HB3	2:1B:169:ARG:CZ	2.50	0.42
2:1B:171:LYS:HA	2:1B:174:ARG:NH2	2.35	0.42
3:1C:172:VAL:HG21	3:1C:185:ALA:HB1	2.02	0.42
4:1D:262:GLY:HA3	4:1D:296:ARG:HG2	2.02	0.42
4:1D:265:ILE:HD12	4:1D:265:ILE:N	2.34	0.42
6:1F:189:GLU:N	6:1F:189:GLU:OE2	2.53	0.42
6:1F:298:ILE:HD12	6:1F:302:SER:HA	2.02	0.42
7:1G:456:SER:HB3	7:1G:495:ARG:HD3	2.02	0.42
10:1J:10:SER:HB2	11:1K:7:ASN:HB2	2.01	0.42
12:1L:176:ARG:NH2	13:1M:403:THR:HB	2.35	0.42
12:1L:315:VAL:O	12:1L:319:ILE:HG13	2.19	0.42
12:1L:371:THR:O	12:1L:375:ILE:HG12	2.19	0.42
12:1L:545:SER:HA	12:1L:549:ALA:HB3	2.02	0.42
13:1M:167:ILE:HB	13:1M:174:LEU:HD21	2.02	0.42
15:1O:165:PRO:O	15:1O:165:PRO:HD2	2.19	0.42
15:1O:232:GLU:O	15:1O:236:GLU:HG2	2.20	0.42
16:1P:200:THR:O	16:1P:237:LEU:HD22	2.19	0.42
17:1Q:70:MET:SD	17:1Q:70:MET:N	2.93	0.42
19:1S:34:ASP:O	19:1S:37:GLU:HB3	2.20	0.42
21:1V:30:ILE:HG22	21:1V:87:LEU:HB2	2.01	0.42
21:1V:39:LYS:HE3	21:1V:39:LYS:HB3	1.77	0.42
22:1W:57:LYS:HD2	22:1W:61:ASP:OD2	2.19	0.42
27:1b:15:GLU:N	27:1b:15:GLU:OE1	2.53	0.42
32:1g:25:ARG:O	32:1g:26:LEU:HB2	2.20	0.42
34:1i:27:LEU:HB2	34:1i:31:GLU:HB2	2.00	0.42
35:1j:67:LEU:O	35:1j:68:PRO:C	2.63	0.42
41:1p:82:LEU:HD22	41:1p:82:LEU:H	1.84	0.42
41:1p:138:PHE:HA	41:1p:141:ARG:HG2	2.02	0.42
1:1A:36:PRO:HB2	1:1A:43:PRO:HD2	2.00	0.42
46:1B:202:PC1:H322	46:1B:202:PC1:H31	1.70	0.42
4:1D:175:GLU:O	4:1D:179:GLU:HG3	2.20	0.42
4:1D:225:LEU:HA	4:1D:228:MET:CE	2.50	0.42
4:1D:314:CYS:O	4:1D:318:MET:HG3	2.20	0.42
7:1G:134:LYS:HB2	18:1R:72:TYR:CD2	2.54	0.42
7:1G:334:LEU:HD23	7:1G:604:SER:HB2	2.02	0.42
7:1G:632:ARG:NH2	19:1S:57:CYS:SG	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:307:LEU:HD23	8:1H:307:LEU:HA	1.79	0.42
10:1J:20:PHE:HA	10:1J:29:GLY:HA2	2.02	0.42
11:1K:20:LEU:HD22	12:1L:592:LEU:HD23	2.01	0.42
11:1K:96:LEU:HB2	14:1N:54:GLU:CG	2.47	0.42
11:1K:96:LEU:HD13	14:1N:117:GLU:OE1	2.20	0.42
12:1L:203:MET:CE	41:1p:109:LEU:HD13	2.46	0.42
12:1L:559:GLU:O	12:1L:563:PRO:HD2	2.20	0.42
12:1L:563:PRO:HG3	13:1M:152:TYR:OH	2.20	0.42
13:1M:10:MET:SD	13:1M:10:MET:C	3.02	0.42
14:1N:299:SER:HA	14:1N:305:PHE:CE1	2.54	0.42
15:1O:25:ILE:HA	15:1O:168:VAL:O	2.19	0.42
15:1O:139:TYR:OH	15:1O:146:LYS:HB3	2.20	0.42
18:1R:1:GLY:N	18:1R:42:ASP:OD2	2.44	0.42
20:1T:51:ILE:HG23	20:1T:62:ILE:HG21	2.01	0.42
22:1W:58:GLN:HA	22:1W:61:ASP:CG	2.44	0.42
23:1X:52:PRO:HD2	23:1X:53:ARG:HH12	1.84	0.42
32:1g:84:ARG:HD3	41:1p:96:LYS:NZ	2.34	0.42
37:1l:115:MET:HA	37:1l:118:VAL:HG22	2.01	0.42
41:1p:105:ILE:HG13	41:1p:108:ARG:HH11	1.83	0.42
41:1p:109:LEU:HA	41:1p:109:LEU:HD23	1.64	0.42
43:1r:51:ASN:C	43:1r:56:ARG:HH12	2.28	0.42
1:1A:106:TRP:CH2	27:1b:18:LEU:HD21	2.55	0.42
2:1B:96:MET:HG2	4:1D:82:LEU:O	2.20	0.42
4:1D:341:SER:HB2	7:1G:128:SER:HB3	2.02	0.42
4:1D:347:HIS:O	4:1D:351:LEU:HB2	2.19	0.42
5:1E:202:LEU:HD12	5:1E:202:LEU:HA	1.92	0.42
7:1G:210:SER:OG	7:1G:213:TYR:HB3	2.20	0.42
7:1G:460:ARG:HB3	7:1G:461:SER:H	1.55	0.42
8:1H:200:LEU:HD11	8:1H:282:TYR:CD2	2.53	0.42
11:1K:37:MET:HE2	11:1K:37:MET:O	2.20	0.42
12:1L:319:ILE:HD12	12:1L:321:GLN:HB2	2.02	0.42
12:1L:356:ILE:HD13	12:1L:429:PHE:CE2	2.55	0.42
12:1L:406:ALA:O	12:1L:409:LEU:N	2.53	0.42
12:1L:566:THR:HA	12:1L:569:ILE:HD12	2.02	0.42
13:1M:31:SER:O	13:1M:34:ILE:HD12	2.20	0.42
13:1M:244:MET:HE1	13:1M:309:PHE:CE1	2.55	0.42
13:1M:263:MET:C	13:1M:263:MET:HE2	2.45	0.42
15:1O:188:ASN:HB3	15:1O:191:GLU:OE1	2.20	0.42
37:1l:60:PRO:HG3	37:1l:70:ARG:CZ	2.50	0.42
40:1o:40:ALA:CB	40:1o:59:ALA:HB3	2.49	0.42
42:1q:6:VAL:C	42:1q:9:ARG:HH21	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:1D:501:U10:H272	47:1D:501:U10:H23	1.82	0.41
12:1L:439:PRO:HA	36:1k:50:TRP:CZ2	2.55	0.41
15:1O:91:GLY:HA2	15:1O:281:GLU:HG2	2.01	0.41
16:1P:8:HIS:O	16:1P:16:VAL:N	2.53	0.41
17:1Q:63:GLU:OE1	22:1W:126:HIS:ND1	2.52	0.41
21:1V:43:TYR:CE1	21:1V:47:THR:HG21	2.55	0.41
28:1c:26:PHE:C	28:1c:26:PHE:CD2	2.97	0.41
32:1g:108:MET:HG2	41:1p:137:ALA:HB3	2.01	0.41
34:1i:3:TYR:CE2	34:1i:8:LYS:HB3	2.55	0.41
35:1j:67:LEU:HB2	40:1o:110:ARG:HE	1.85	0.41
37:1l:27:TYR:CZ	37:1l:47:TYR:HA	2.54	0.41
39:1n:27:GLU:O	39:1n:31:VAL:N	2.46	0.41
2:1B:30:VAL:HG13	2:1B:174:ARG:HD3	2.01	0.41
4:1D:95:THR:O	4:1D:99:ALA:N	2.53	0.41
4:1D:271:LYS:HG2	4:1D:283:PHE:CZ	2.56	0.41
7:1G:40:PHE:HB2	7:1G:52:CYS:HB3	2.02	0.41
7:1G:378:LEU:HB3	7:1G:451:VAL:HG12	2.03	0.41
8:1H:54:LYS:O	8:1H:58:LYS:N	2.52	0.41
8:1H:90:PRO:HG3	8:1H:162:LEU:CD2	2.50	0.41
10:1J:7:PHE:O	10:1J:10:SER:OG	2.38	0.41
10:1J:70:TYR:HB2	11:1K:27:MET:HE1	2.02	0.41
10:1J:139:GLU:HA	11:1K:57:ASN:ND2	2.35	0.41
11:1K:27:MET:SD	11:1K:78:LEU:HD13	2.60	0.41
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.20	0.41
11:1K:66:PHE:CE2	14:1N:31:ILE:HG12	2.55	0.41
12:1L:428:PHE:CE2	12:1L:505:ASN:HA	2.55	0.41
12:1L:452:ASN:O	12:1L:455:LYS:HG3	2.19	0.41
13:1M:24:TRP:HB3	13:1M:81:GLN:HE22	1.84	0.41
13:1M:36:LEU:HA	13:1M:39:LEU:HD12	2.01	0.41
13:1M:358:TRP:HE1	13:1M:434:ASN:HB3	1.84	0.41
14:1N:263:LYS:HE3	14:1N:263:LYS:HB3	1.74	0.41
15:1O:14:THR:HG21	15:1O:256:PHE:HB3	2.01	0.41
15:1O:15:THR:HA	15:1O:18:LEU:HD23	2.02	0.41
16:1P:59:LEU:O	16:1P:62:MET:HG2	2.20	0.41
20:1U:69:LYS:H	34:1i:1:SAC:HB2	1.86	0.41
20:1U:87:TYR:OH	34:1i:18:ARG:NE	2.45	0.41
28:1c:6:GLU:CD	28:1c:7:PRO:HD2	2.45	0.41
32:1g:64:PHE:CD1	32:1g:68:ILE:HD11	2.52	0.41
33:1h:30:LEU:HB3	33:1h:34:ILE:CD1	2.50	0.41
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.27	0.41
38:1m:62:PRO:O	38:1m:66:ARG:HG3	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:62:PRO:O	38:1m:65:ILE:HD12	2.20	0.41
39:1n:24:ARG:O	39:1n:24:ARG:HD3	2.20	0.41
41:1p:170:LYS:HD2	41:1p:171:GLU:N	2.35	0.41
42:1q:51:ASP:OD2	42:1q:54:GLN:HG2	2.19	0.41
1:1A:53:MET:SD	1:1A:55:PHE:N	2.93	0.41
3:1C:66:ASP:HB3	21:1V:89:LEU:HB2	2.03	0.41
3:1C:150:ARG:NH1	3:1C:154:GLY:O	2.31	0.41
4:1D:159:LEU:HD22	4:1D:159:LEU:HA	1.83	0.41
4:1D:191:ALA:HB1	4:1D:193:TYR:HB2	2.02	0.41
4:1D:204:PRO:HA	9:1I:175:TYR:CZ	2.55	0.41
4:1D:210:ASP:OD2	43:1r:26:ARG:NH2	2.53	0.41
4:1D:360:PRO:HA	4:1D:380:SER:O	2.20	0.41
47:1D:501:U10:H521	47:1D:501:U10:H501	1.88	0.41
47:1D:501:U10:H372	8:1H:224:PHE:CE2	2.56	0.41
5:1E:85:THR:HG23	7:1G:176:GLY:H	1.85	0.41
6:1F:262:VAL:HA	6:1F:287:VAL:HA	2.02	0.41
7:1G:8:LEU:HB3	7:1G:19:MET:HE2	2.02	0.41
8:1H:75:PRO:HG2	8:1H:219:PRO:HB3	2.03	0.41
8:1H:104:PHE:CD1	8:1H:108:MET:HE2	2.56	0.41
8:1H:128:ALA:HA	8:1H:210:GLY:O	2.20	0.41
10:1J:160:SER:CB	11:1K:66:PHE:HE1	2.33	0.41
11:1K:69:CYS:O	11:1K:72:ALA:HB3	2.19	0.41
12:1L:306:THR:HG22	12:1L:336:LYS:CG	2.51	0.41
12:1L:381:THR:HG22	12:1L:494:THR:HG22	2.01	0.41
13:1M:160:LEU:HD22	13:1M:164:LEU:HD13	2.03	0.41
14:1N:200:MET:HG3	14:1N:269:GLU:OE1	2.20	0.41
15:1O:173:ASP:N	15:1O:223:TYR:O	2.45	0.41
17:1Q:112:LYS:HB3	17:1Q:112:LYS:HE2	1.78	0.41
23:1X:70:PHE:HA	23:1X:70:PHE:HD1	1.78	0.41
31:1f:6:ILE:O	31:1f:10:HIS:N	2.44	0.41
33:1h:87:TYR:HA	33:1h:90:THR:HG22	2.02	0.41
33:1h:88:GLU:HA	33:1h:91:MET:SD	2.60	0.41
33:1h:114:MET:HE1	33:1h:122:TRP:H	1.86	0.41
34:1i:30:ARG:NH2	39:1n:116:ASP:HB3	2.35	0.41
36:1k:18:TYR:HD2	36:1k:19:LYS:HE2	1.85	0.41
37:1l:44:TYR:HD1	37:1l:79:TRP:CZ3	2.38	0.41
37:1l:126:GLN:HG2	37:1l:128:VAL:HG22	2.01	0.41
37:1l:130:PRO:O	37:1l:132:GLN:NE2	2.53	0.41
39:1n:109:SER:O	39:1n:113:MET:HB3	2.20	0.41
42:1q:78:ASP:H	42:1q:81:MET:HE3	1.85	0.41
1:1A:4:MET:H	1:1A:4:MET:HG2	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:150:ARG:HH21	22:1W:92:GLU:CD	2.28	0.41
4:1D:225:LEU:HA	4:1D:228:MET:HE3	2.03	0.41
4:1D:407:LYS:HA	4:1D:407:LYS:HD3	1.74	0.41
5:1E:38:TYR:N	5:1E:38:TYR:CD1	2.88	0.41
5:1E:162:GLU:O	5:1E:186:PRO:HA	2.19	0.41
6:1F:140:GLY:HA2	6:1F:179:ARG:NE	2.34	0.41
6:1F:277:LYS:O	6:1F:281:GLU:HG2	2.20	0.41
7:1G:130:PHE:CE1	7:1G:132:GLU:HB2	2.56	0.41
10:1J:109:LYS:HE2	10:1J:109:LYS:HB2	1.87	0.41
12:1L:90:ILE:O	12:1L:93:ALA:N	2.54	0.41
12:1L:203:MET:SD	12:1L:204:LEU:N	2.93	0.41
12:1L:335:PHE:CD1	12:1L:336:LYS:N	2.89	0.41
12:1L:386:LEU:HD12	12:1L:386:LEU:HA	1.92	0.41
12:1L:407:TRP:CZ2	37:1L:115:MET:HG2	2.55	0.41
12:1L:558:LEU:HD13	13:1M:211:GLY:HA2	2.01	0.41
12:1L:564:LYS:HA	12:1L:564:LYS:HD2	1.79	0.41
13:1M:30:HIS:HA	13:1M:33:LEU:HG	2.03	0.41
13:1M:457:PRO:HA	32:1g:84:ARG:HH12	1.85	0.41
14:1N:3:PRO:O	14:1N:7:THR:HG23	2.20	0.41
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	2.01	0.41
14:1N:258:SER:OG	14:1N:333:SER:O	2.31	0.41
15:1O:234:VAL:HG23	15:1O:235:VAL:HG13	2.02	0.41
16:1P:83:LYS:HE3	16:1P:83:LYS:HB3	1.63	0.41
20:1T:43:ASP:OD2	20:1T:43:ASP:C	2.63	0.41
22:1W:121:LYS:HD3	22:1W:121:LYS:HA	1.73	0.41
23:1X:84:TYR:HE2	23:1X:99:CYS:HB3	1.85	0.41
24:1Y:47:SER:OG	24:1Y:50:GLU:HG3	2.20	0.41
25:1Z:95:ALA:O	25:1Z:99:LYS:HG2	2.19	0.41
33:1h:48:GLY:HA3	41:1p:55:HIS:NE2	2.36	0.41
34:1i:86:LYS:HE3	34:1i:86:LYS:HB2	1.88	0.41
37:1l:25:LYS:O	37:1l:25:LYS:HD3	2.20	0.41
1:1A:1:FME:O	1:1A:5:LEU:N	2.40	0.41
4:1D:54:GLN:NE2	4:1D:56:PRO:HD3	2.34	0.41
4:1D:72:MET:HE3	4:1D:408:GLY:O	2.20	0.41
4:1D:157:HIS:HE1	4:1D:416:ALA:HA	1.84	0.41
4:1D:264:GLY:C	4:1D:287:ILE:HD11	2.45	0.41
4:1D:415:VAL:HG21	8:1H:205:SER:OG	2.20	0.41
5:1E:145:LEU:HA	6:1F:139:ARG:NH2	2.36	0.41
6:1F:118:LEU:HD13	6:1F:122:CYS:SG	2.60	0.41
6:1F:280:ILE:HG12	6:1F:280:ILE:H	1.43	0.41
7:1G:52:CYS:N	48:1G:803:FES:S1	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:169:GLN:HG2	8:1H:174:MET:CG	2.51	0.41
8:1H:199:ASP:CG	8:1H:200:LEU:N	2.78	0.41
9:1I:2:TYR:CD1	43:1r:103:TRP:HB2	2.55	0.41
12:1L:244:SER:OG	12:1L:299:LYS:HE2	2.21	0.41
12:1L:306:THR:OG1	12:1L:307:SER:N	2.54	0.41
13:1M:177:LEU:HD22	33:1h:94:LEU:HD21	2.02	0.41
13:1M:412:ILE:HA	13:1M:416:ARG:HB2	2.03	0.41
14:1N:1:FME:HG3	14:1N:46:LYS:HZ2	1.85	0.41
14:1N:322:GLN:HA	29:1d:49:ARG:CZ	2.49	0.41
15:1O:64:GLY:O	28:1c:3:TYR:HA	2.20	0.41
15:1O:320:LYS:HZ3	28:1c:11:SER:C	2.29	0.41
16:1P:29:PHE:CE2	16:1P:176:ASP:HA	2.55	0.41
17:1Q:55:TRP:CZ2	17:1Q:108:ARG:HB2	2.55	0.41
25:1Z:98:MET:HG3	25:1Z:104:TRP:CE3	2.55	0.41
30:1e:20:GLN:HG2	30:1e:36:GLU:OE2	2.21	0.41
34:1i:103:ILE:HD13	41:1p:15:ARG:HE	1.85	0.41
34:1i:127:HIS:HD2	40:1o:84:HIS:HD2	1.68	0.41
38:1m:39:ARG:O	38:1m:43:LYS:HG2	2.20	0.41
38:1m:68:THR:O	38:1m:72:SER:OG	2.22	0.41
39:1n:26:LEU:HD22	39:1n:29:TRP:CD1	2.56	0.41
39:1n:94:GLU:HA	39:1n:97:LYS:HD2	2.01	0.41
40:1o:117:ARG:HD2	40:1o:117:ARG:C	2.45	0.41
2:1B:37:VAL:HG21	46:1B:202:PC1:H382	2.03	0.41
4:1D:4:TRP:N	13:1M:138:ASN:O	2.54	0.41
4:1D:51:PHE:HD2	4:1D:64:LEU:HD12	1.86	0.41
4:1D:395:GLY:HA3	4:1D:423:ILE:HD13	2.01	0.41
6:1F:103:GLY:HA3	6:1F:333:ALA:HB1	2.02	0.41
6:1F:242:PHE:CE2	6:1F:252:GLY:HA3	2.56	0.41
6:1F:367:GLU:HG2	7:1G:96:PHE:O	2.20	0.41
7:1G:249:ARG:NH1	7:1G:251:LEU:HD21	2.36	0.41
9:1I:8:ARG:HA	9:1I:8:ARG:HD3	1.96	0.41
9:1I:75:GLU:HG3	9:1I:105:ARG:HD2	2.02	0.41
11:1K:34:GLU:O	11:1K:37:MET:HG3	2.20	0.41
11:1K:96:LEU:HD11	14:1N:121:GLY:HA3	2.02	0.41
12:1L:159:HIS:CE1	39:1n:95:CYS:HB3	2.54	0.41
12:1L:295:GLN:HG3	12:1L:304:PHE:CE2	2.48	0.41
13:1M:120:ILE:HG23	14:1N:255:PRO:HB3	2.01	0.41
14:1N:175:LEU:HD22	14:1N:296:LEU:HD11	2.02	0.41
20:1U:64:ASP:OD1	39:1n:17:ARG:HD2	2.21	0.41
23:1X:70:PHE:HA	23:1X:73:ILE:CG2	2.51	0.41
29:1d:111:GLU:OE1	29:1d:111:GLU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:56:TRP:CE3	33:1h:85:LYS:HG2	2.55	0.41
33:1h:111:ARG:HG3	33:1h:123:TYR:HE2	1.85	0.41
35:1j:59:TRP:CH2	40:1o:99:LYS:HB2	2.56	0.41
36:1k:89:SER:OG	36:1k:90:GLN:OE1	2.28	0.41
38:1m:29:ARG:HA	38:1m:32:GLN:OE1	2.21	0.41
40:1o:100:GLU:O	40:1o:104:GLU:HG3	2.21	0.41
41:1p:75:GLU:OE1	41:1p:75:GLU:N	2.53	0.41
1:1A:27:LEU:HG	1:1A:29:ALA:N	2.33	0.41
3:1C:52:ILE:HG13	3:1C:53:HIS:O	2.20	0.41
3:1C:96:LEU:HD11	3:1C:124:TYR:CE2	2.55	0.41
4:1D:59:HIS:CD2	47:1D:501:U10:H3M3	2.56	0.41
4:1D:159:LEU:CD1	47:1D:501:U10:H8	2.49	0.41
5:1E:98:TYR:HB2	5:1E:137:PHE:HD1	1.86	0.41
5:1E:215:ALA:O	5:1E:217:LEU:HD23	2.21	0.41
7:1G:197:GLY:H	7:1G:265:ASP:CG	2.29	0.41
7:1G:239:VAL:HG13	7:1G:251:LEU:HB2	2.01	0.41
9:1I:8:ARG:CZ	43:1r:111:TYR:HB2	2.51	0.41
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	2.01	0.41
10:1J:135:PHE:HD1	10:1J:135:PHE:HA	1.73	0.41
12:1L:125:LEU:O	12:1L:129:MET:HG2	2.20	0.41
12:1L:264:TYR:CG	12:1L:322:PRO:HG3	2.56	0.41
12:1L:350:LEU:HD13	12:1L:362:LEU:HD21	2.03	0.41
13:1M:71:TRP:O	13:1M:74:PRO:HD2	2.21	0.41
13:1M:294:MET:SD	13:1M:319:HIS:CE1	3.14	0.41
16:1P:136:ASN:ND2	16:1P:291:ASP:HA	2.36	0.41
16:1P:300:LEU:HB3	16:1P:305:ILE:HD11	2.02	0.41
17:1Q:59:PHE:N	17:1Q:59:PHE:HD1	2.18	0.41
20:1T:54:MET:SD	20:1T:76:ILE:HG21	2.61	0.41
20:1U:14:ARG:NH1	35:1j:11:TYR:CZ	2.89	0.41
21:1V:95:ARG:HD2	21:1V:96:TRP:N	2.36	0.41
22:1W:84:ILE:O	22:1W:88:MET:HG3	2.20	0.41
23:1X:44:LEU:HD12	23:1X:44:LEU:HA	1.88	0.41
24:1Y:90:PHE:HD2	24:1Y:90:PHE:O	2.04	0.41
25:1Z:111:PHE:HE1	30:1e:64:GLU:HG3	1.86	0.41
26:1a:21:MET:HA	26:1a:24:ALA:HB3	2.02	0.41
26:1a:31:ASN:HB2	26:1a:34:LYS:O	2.21	0.41
46:1d:201:PC1:H2	46:1d:201:PC1:H222	1.33	0.41
30:1e:85:LEU:HD11	30:1e:91:TYR:CD1	2.55	0.41
32:1g:106:PRO:HB2	32:1g:108:MET:SD	2.61	0.41
35:1j:11:TYR:C	35:1j:11:TYR:CD2	2.97	0.41
39:1n:149:ARG:NE	39:1n:149:ARG:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:108:LEU:HD23	40:1o:108:LEU:HA	1.97	0.41
1:1A:77:TRP:HB2	10:1J:144:ALA:HB2	2.02	0.41
2:1B:34:ASP:HB2	2:1B:173:LEU:HB2	2.03	0.41
4:1D:143:GLU:OE2	4:1D:310:ILE:HD12	2.21	0.41
5:1E:48:LEU:HD23	5:1E:48:LEU:HA	1.91	0.41
6:1F:30:ASP:HA	44:1s:39:ARG:HD2	2.02	0.41
6:1F:33:LEU:HD22	6:1F:37:GLN:HE22	1.86	0.41
6:1F:101:GLU:OE1	6:1F:184:TYR:OH	2.34	0.41
6:1F:145:GLU:OE1	6:1F:145:GLU:N	2.43	0.41
6:1F:434:ALA:HA	6:1F:437:HIS:CE1	2.56	0.41
7:1G:147:LYS:O	7:1G:208:LEU:HA	2.21	0.41
7:1G:254:MET:HA	7:1G:260:GLU:O	2.20	0.41
9:1I:13:ASP:OD1	9:1I:15:LYS:N	2.53	0.41
12:1L:68:TRP:CE3	12:1L:69:MET:HE1	2.55	0.41
12:1L:336:LYS:HE2	12:1L:336:LYS:HB2	1.95	0.41
12:1L:373:LEU:HD22	12:1L:431:PHE:CE2	2.52	0.41
13:1M:231:LEU:HA	13:1M:235:LEU:HG	2.03	0.41
13:1M:294:MET:HA	13:1M:294:MET:HE3	2.01	0.41
14:1N:92:PRO:O	14:1N:96:THR:HG23	2.20	0.41
15:1O:50:HIS:HA	15:1O:123:VAL:HG13	2.03	0.41
16:1P:206:TYR:HD1	16:1P:207:ILE:H	1.69	0.41
18:1R:10:LYS:HD3	18:1R:10:LYS:N	2.34	0.41
22:1W:80:ASP:O	22:1W:84:ILE:HG13	2.19	0.41
23:1X:15:GLN:C	23:1X:15:GLN:CD	2.88	0.41
24:1Y:37:ALA:O	24:1Y:40:ILE:HG22	2.21	0.41
24:1Y:57:ARG:O	24:1Y:61:THR:OG1	2.31	0.41
28:1c:45:ARG:HH22	29:1d:17:GLU:HA	1.85	0.41
34:1i:106:GLY:HA3	34:1i:118:LEU:CD2	2.50	0.41
38:1m:53:PRO:HD2	39:1n:132:TRP:CD1	2.55	0.41
39:1n:15:VAL:HG12	39:1n:63:LEU:HD21	2.03	0.41
40:1o:30:PHE:HE2	40:1o:103:ARG:HD2	1.85	0.41
1:1A:1:FME:HA	1:1A:1:FME:HE3	2.03	0.41
1:1A:22:PHE:HD2	1:1A:23:TRP:CD1	2.38	0.41
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.50	0.41
2:1B:93:THR:HG23	2:1B:96:MET:HB2	2.01	0.41
2:1B:119:CYS:HA	2:1B:124:GLY:HA3	2.03	0.41
4:1D:415:VAL:HA	4:1D:418:ILE:HG13	2.02	0.41
47:1D:501:U10:O2	47:1D:501:U10:C3M	2.69	0.41
5:1E:217:LEU:HD12	6:1F:55:TRP:CH2	2.51	0.41
6:1F:132:ARG:NH1	44:1s:66:PRO:HD3	2.36	0.41
6:1F:261:HIS:NE2	6:1F:341:THR:OG1	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:1F:501:FMN:H4'	49:1F:501:FMN:H1'2	1.78	0.41
7:1G:162:PHE:CZ	7:1G:198:ASN:HB2	2.56	0.41
7:1G:558:ASP:OD2	42:1q:144:TYR:OH	2.29	0.41
8:1H:92:PRO:HD3	8:1H:255:TYR:HD1	1.86	0.41
8:1H:117:LEU:HD12	10:1J:68:PHE:CD1	2.56	0.41
8:1H:156:MET:HE2	8:1H:156:MET:HB3	1.68	0.41
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.55	0.41
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.21	0.41
12:1L:69:MET:HE2	12:1L:69:MET:N	2.36	0.41
12:1L:132:VAL:HA	12:1L:258:PHE:HE2	1.85	0.41
12:1L:196:TRP:CZ2	13:1M:379:LEU:HD11	2.56	0.41
12:1L:552:LEU:HA	12:1L:556:ILE:HB	2.03	0.41
12:1L:554:ASP:OD1	13:1M:213:HIS:HE1	2.04	0.41
12:1L:580:GLN:OE1	12:1L:580:GLN:N	2.53	0.41
13:1M:54:LEU:HA	33:1h:93:ILE:HD12	2.03	0.41
13:1M:89:THR:O	13:1M:93:LYS:HG3	2.21	0.41
13:1M:175:ASN:HD22	33:1h:97:GLU:HG3	1.86	0.41
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.86	0.41
13:1M:200:ILE:O	13:1M:204:MET:HG2	2.20	0.41
13:1M:201:MET:O	13:1M:201:MET:HE3	2.21	0.41
13:1M:225:ILE:HD13	13:1M:331:ASN:HD21	1.85	0.41
13:1M:392:THR:HG22	38:1m:104:PHE:CE1	2.56	0.41
14:1N:29:ILE:H	14:1N:29:ILE:HG12	1.66	0.41
14:1N:247:THR:O	14:1N:251:MET:HE2	2.21	0.41
15:1O:223:TYR:CD1	15:1O:234:VAL:HG12	2.56	0.41
16:1P:68:ILE:HD12	16:1P:70:PHE:CE2	2.56	0.41
16:1P:81:ILE:O	16:1P:85:VAL:HG22	2.20	0.41
16:1P:288:HIS:ND1	16:1P:288:HIS:O	2.54	0.41
20:1U:11:ILE:O	20:1U:15:VAL:HG12	2.21	0.41
20:1U:54:MET:HE1	20:1U:76:ILE:HD12	2.03	0.41
21:1V:68:GLU:HB3	21:1V:74:GLY:O	2.21	0.41
24:1Y:40:ILE:HD12	24:1Y:40:ILE:HA	1.84	0.41
25:1Z:104:TRP:CE2	30:1e:78:ILE:HD11	2.55	0.41
25:1Z:137:THR:OG1	25:1Z:138:TYR:N	2.54	0.41
26:1a:9:ILE:HD12	26:1a:10:ALA:N	2.36	0.41
26:1a:21:MET:O	26:1a:25:HIS:N	2.32	0.41
26:1a:25:HIS:O	26:1a:29:PHE:N	2.46	0.41
26:1a:59:ARG:HH21	26:1a:61:HIS:CD2	2.39	0.41
30:1e:21:SER:N	30:1e:36:GLU:OE1	2.54	0.41
30:1e:85:LEU:HD12	30:1e:86:ILE:HD13	2.03	0.41
32:1g:64:PHE:O	32:1g:69:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:36:VAL:O	33:1h:40:ILE:HG12	2.20	0.41
34:1i:19:ARG:O	34:1i:23:LYS:HG2	2.21	0.41
34:1i:79:TRP:HH2	41:1p:43:PRO:HG2	1.85	0.41
34:1i:82:HIS:CD2	41:1p:44:VAL:HG21	2.55	0.41
35:1j:29:SER:O	35:1j:32:MET:HG2	2.21	0.41
38:1m:44:ARG:NH2	39:1n:139:LEU:HD22	2.36	0.41
39:1n:27:GLU:HB3	39:1n:36:TYR:CE1	2.56	0.41
41:1p:152:ARG:HE	41:1p:152:ARG:HB3	1.58	0.41
42:1q:61:TRP:CD1	42:1q:61:TRP:N	2.89	0.41
44:1s:74:ARG:CZ	44:1s:74:ARG:HB2	2.50	0.41
2:1B:71:ARG:NE	2:1B:72:PHE:HE2	2.19	0.41
2:1B:128:TYR:HD1	3:1C:194:PHE:HB2	1.85	0.41
4:1D:146:ARG:HG3	4:1D:150:HIS:CE1	2.56	0.41
4:1D:158:ALA:O	4:1D:163:ALA:N	2.54	0.41
6:1F:306:LEU:O	6:1F:307:ILE:HD13	2.20	0.41
7:1G:172:LEU:HD23	7:1G:172:LEU:HA	1.85	0.41
8:1H:140:ILE:HG21	10:1J:65:LEU:CD1	2.51	0.41
8:1H:196:ALA:HB3	8:1H:274:ARG:HB2	2.03	0.41
9:1I:42:PHE:HD2	43:1r:7:ILE:HG23	1.86	0.41
12:1L:19:ILE:HA	12:1L:19:ILE:HD13	1.77	0.41
12:1L:49:VAL:CG1	12:1L:50:PRO:HD3	2.41	0.41
15:1O:51:PHE:HD1	15:1O:51:PHE:HA	1.80	0.41
15:1O:92:ASN:O	15:1O:96:LEU:CB	2.68	0.41
15:1O:210:PHE:HD1	15:1O:211:LEU:HD13	1.83	0.41
15:1O:238:ILE:HA	15:1O:241:LEU:HD12	2.04	0.41
16:1P:111:VAL:C	16:1P:114:PRO:HD2	2.45	0.41
17:1Q:31:LYS:HD3	17:1Q:31:LYS:HA	1.95	0.41
18:1R:75:LEU:HB3	18:1R:93:GLN:HG2	2.03	0.41
22:1W:23:ARG:HB2	22:1W:27:GLU:OE2	2.21	0.41
22:1W:103:ILE:HD13	22:1W:103:ILE:HA	1.81	0.41
23:1X:81:PHE:HD2	23:1X:106:PHE:CZ	2.39	0.41
24:1Y:7:LYS:HE3	24:1Y:7:LYS:HB2	1.88	0.41
25:1Z:111:PHE:CE1	30:1e:64:GLU:HG3	2.55	0.41
28:1c:45:ARG:NH2	29:1d:17:GLU:HA	2.36	0.41
29:1d:3:SER:HA	29:1d:8:ARG:CZ	2.51	0.41
32:1g:88:TRP:NE1	41:1p:65:ARG:O	2.50	0.41
38:1m:65:ILE:HD12	38:1m:66:ARG:N	2.36	0.41
3:1C:145:HIS:CD2	3:1C:146:PRO:HD2	2.56	0.40
3:1C:204:GLU:N	17:1Q:50:ASN:OD1	2.54	0.40
4:1D:27:HIS:HA	4:1D:29:LYS:HZ1	1.86	0.40
5:1E:51:LEU:O	5:1E:54:ALA:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:145:LEU:HD11	5:1E:153:MET:SD	2.60	0.40
5:1E:217:LEU:HD23	5:1E:217:LEU:H	1.86	0.40
6:1F:42:TRP:CE3	6:1F:120:GLU:HG3	2.56	0.40
6:1F:43:TYR:CD2	6:1F:43:TYR:C	2.99	0.40
6:1F:93:LEU:HD23	6:1F:94:VAL:N	2.36	0.40
6:1F:193:ILE:HG23	6:1F:215:VAL:HG12	2.03	0.40
7:1G:231:MET:HB3	7:1G:266:LYS:HE3	2.02	0.40
8:1H:104:PHE:HA	10:1J:54:LEU:HD22	2.02	0.40
8:1H:236:ALA:O	8:1H:240:ILE:HG22	2.21	0.40
10:1J:102:CYS:SG	10:1J:103:MET:N	2.94	0.40
10:1J:152:TRP:CE3	10:1J:152:TRP:HA	2.56	0.40
11:1K:12:PHE:CE1	11:1K:36:MET:CG	3.04	0.40
12:1L:81:LYS:HG2	12:1L:83:ASP:OD1	2.20	0.40
12:1L:96:VAL:HG21	12:1L:333:ALA:HB1	2.02	0.40
12:1L:176:ARG:HH12	13:1M:405:LEU:H	1.68	0.40
12:1L:183:VAL:HA	12:1L:186:MET:SD	2.61	0.40
12:1L:212:PRO:O	12:1L:216:LEU:HG	2.21	0.40
12:1L:293:ILE:HD13	12:1L:422:TYR:HD1	1.85	0.40
12:1L:380:LEU:HD11	12:1L:423:SER:CB	2.51	0.40
12:1L:596:MET:HA	12:1L:599:MET:HB2	2.03	0.40
13:1M:47:GLU:HG2	41:1p:89:MET:HE1	2.03	0.40
14:1N:120:GLN:O	14:1N:176:ARG:NH2	2.54	0.40
17:1Q:95:PHE:CD1	17:1Q:98:LYS:HE2	2.56	0.40
20:1T:48:VAL:O	20:1T:52:MET:SD	2.79	0.40
20:1U:24:LYS:HZ2	36:1k:41:ARG:HD3	1.85	0.40
21:1V:35:GLY:HA2	21:1V:44:ARG:NH2	2.35	0.40
22:1W:99:GLN:HA	22:1W:99:GLN:OE1	2.21	0.40
24:1Y:75:ILE:HA	24:1Y:78:GLN:HG2	2.02	0.40
30:1e:53:LYS:NZ	30:1e:54:GLU:HG3	2.36	0.40
31:1f:46:ARG:HH12	31:1f:48:LEU:HA	1.86	0.40
32:1g:49:LYS:HE3	32:1g:49:LYS:CA	2.47	0.40
38:1m:44:ARG:HH22	39:1n:139:LEU:HB2	1.86	0.40
40:1o:110:ARG:HH12	40:1o:114:ARG:NH1	2.19	0.40
41:1p:34:LYS:HD2	41:1p:35:ILE:HG13	2.02	0.40
1:1A:56:PHE:HD1	1:1A:57:LEU:N	2.19	0.40
1:1A:110:GLY:HA2	10:1J:169:MET:HE1	2.03	0.40
2:1B:60:MET:HE3	4:1D:167:PHE:HZ	1.85	0.40
2:1B:94:ASN:ND2	2:1B:131:SER:HA	2.37	0.40
3:1C:40:VAL:HG22	43:1r:69:MET:HB3	2.03	0.40
3:1C:174:LEU:HA	3:1C:184:VAL:O	2.21	0.40
3:1C:181:LYS:HD2	16:1P:174:ARG:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:105:ARG:HH21	9:1I:117:ILE:HB	1.86	0.40
4:1D:147:LEU:HD22	4:1D:218:PHE:HE2	1.87	0.40
4:1D:176:LYS:HE3	4:1D:214:PHE:CD2	2.56	0.40
5:1E:33:ALA:O	5:1E:36:LYS:HG3	2.21	0.40
5:1E:34:ILE:HG22	5:1E:46:ALA:HB1	2.02	0.40
5:1E:105:THR:OG1	48:1E:301:FES:S2	2.79	0.40
5:1E:126:ILE:HG21	5:1E:132:THR:HA	2.03	0.40
7:1G:188:GLU:HA	7:1G:188:GLU:OE2	2.20	0.40
7:1G:601:ARG:NH2	7:1G:614:ASP:OD2	2.53	0.40
8:1H:103:LEU:HD12	10:1J:54:LEU:HB3	2.02	0.40
8:1H:199:ASP:C	8:1H:201:THR:H	2.29	0.40
9:1I:48:ILE:HG23	9:1I:53:GLU:HB2	2.03	0.40
11:1K:90:VAL:HG23	11:1K:93:LEU:HB3	2.03	0.40
12:1L:35:TYR:O	12:1L:39:THR:HG23	2.21	0.40
12:1L:68:TRP:HB3	12:1L:69:MET:HE1	2.02	0.40
12:1L:178:GLY:HA2	12:1L:218:LEU:HD23	2.03	0.40
12:1L:594:THR:O	12:1L:598:SER:OG	2.33	0.40
13:1M:178:ILE:O	13:1M:182:TRP:N	2.34	0.40
14:1N:245:MET:HE3	14:1N:246:VAL:HA	2.02	0.40
14:1N:316:GLN:HG3	15:1O:302:ARG:NH1	2.35	0.40
16:1P:119:GLN:OE1	16:1P:119:GLN:C	2.64	0.40
16:1P:253:PHE:CD2	16:1P:255:PRO:HD3	2.56	0.40
17:1Q:57:MET:O	17:1Q:57:MET:HG3	2.21	0.40
19:1S:23:CYS:HB2	19:1S:60:VAL:O	2.22	0.40
21:1V:112:LYS:HE3	21:1V:112:LYS:HB3	1.87	0.40
22:1W:80:ASP:O	22:1W:83:VAL:HG12	2.21	0.40
24:1Y:60:PHE:CZ	24:1Y:103:ARG:HD3	2.57	0.40
26:1a:69:ILE:H	26:1a:69:ILE:HG13	1.78	0.40
28:1c:7:PRO:HA	28:1c:8:PRO:HD3	1.96	0.40
29:1d:84:ALA:O	29:1d:88:HIS:N	2.54	0.40
32:1g:106:PRO:O	32:1g:106:PRO:HD2	2.20	0.40
34:1i:7:GLU:H	34:1i:7:GLU:CD	2.26	0.40
34:1i:10:ARG:HA	34:1i:10:ARG:HD2	1.94	0.40
34:1i:21:TRP:HD1	39:1n:124:TRP:CE2	2.39	0.40
34:1i:49:PHE:HB3	34:1i:57:LYS:HE2	2.03	0.40
34:1i:84:TYR:CE1	34:1i:89:VAL:HG23	2.56	0.40
36:1k:44:TRP:C	36:1k:46:ARG:HD3	2.46	0.40
37:1l:66:HIS:ND1	37:1l:71:LEU:HB3	2.36	0.40
37:1l:156:TYR:HB2	40:1o:35:GLU:HA	2.03	0.40
41:1p:111:ALA:O	41:1p:115:ARG:HD3	2.22	0.40
41:1p:139:GLN:O	41:1p:143:SER:OG	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:166:LYS:HA	2:1B:169:ARG:CZ	2.50	0.40
6:1F:272:MET:SD	6:1F:273:SER:N	2.95	0.40
7:1G:220:TRP:NE1	9:1I:85:ALA:HB2	2.36	0.40
8:1H:189:THR:HG23	8:1H:234:MET:HG2	2.02	0.40
9:1I:176:ARG:HE	9:1I:176:ARG:HB3	1.73	0.40
10:1J:68:PHE:O	10:1J:71:THR:N	2.54	0.40
11:1K:73:LEU:HD23	14:1N:38:LEU:HD23	2.03	0.40
11:1K:95:LEU:CD1	14:1N:51:ARG:HG2	2.51	0.40
13:1M:259:TYR:HH	38:1m:108:ARG:HE	1.60	0.40
13:1M:401:MET:SD	13:1M:405:LEU:HD11	2.61	0.40
14:1N:95:MET:HE3	14:1N:148:SER:O	2.21	0.40
14:1N:107:GLY:HA2	14:1N:111:PHE:O	2.22	0.40
14:1N:109:SER:C	14:1N:111:PHE:N	2.79	0.40
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	2.02	0.40
14:1N:231:SER:O	14:1N:234:TRP:HD1	2.05	0.40
15:1O:49:ARG:HH11	15:1O:114:HIS:CG	2.40	0.40
16:1P:131:HIS:HB3	16:1P:165:ILE:HD12	2.03	0.40
19:1S:16:ARG:HD3	19:1S:16:ARG:HA	1.92	0.40
23:1X:103:GLN:HE21	23:1X:118:ARG:CZ	2.35	0.40
53:1a:101:CDL:H511	43:1r:7:ILE:HD11	2.03	0.40
27:1b:13:ALA:HB3	27:1b:14:LYS:HE2	2.04	0.40
32:1g:114:ASP:H	32:1g:117:LYS:NZ	2.18	0.40
34:1i:22:LEU:HA	34:1i:22:LEU:HD13	1.97	0.40
35:1j:18:THR:O	35:1j:21:GLN:HG2	2.21	0.40
39:1n:26:LEU:HD22	39:1n:29:TRP:HD1	1.86	0.40
39:1n:43:MET:SD	39:1n:46:ARG:HB2	2.61	0.40
39:1n:168:HIS:NE2	39:1n:169:ILE:HG23	2.36	0.40
40:1o:15:GLU:CD	40:1o:16:PRO:HD2	2.47	0.40
41:1p:99:GLN:O	41:1p:102:VAL:HG22	2.21	0.40
3:1C:56:GLY:HA2	3:1C:59:PRO:HD2	2.03	0.40
4:1D:270:ARG:HE	4:1D:270:ARG:HB2	1.71	0.40
4:1D:346:ILE:HD13	7:1G:117:GLN:HG2	2.03	0.40
5:1E:104:THR:HG23	6:1F:349:ARG:NE	2.27	0.40
6:1F:90:PRO:HB3	6:1F:132:ARG:HD3	2.03	0.40
6:1F:259:SER:HB3	6:1F:335:ILE:HD12	2.04	0.40
6:1F:275:PRO:HD3	6:1F:316:LEU:HG	2.03	0.40
7:1G:189:LYS:HE3	7:1G:190:MET:H	1.87	0.40
7:1G:668:ILE:HG23	7:1G:691:VAL:HG11	2.04	0.40
7:1G:704:CYS:HB2	9:1I:103:SER:HA	2.02	0.40
9:1I:18:THR:HA	27:1b:12:TRP:HE1	1.87	0.40
11:1K:12:PHE:CE1	11:1K:36:MET:HG2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:148:GLY:HA3	12:1L:175:ASN:HD21	1.86	0.40
12:1L:154:LEU:HD23	12:1L:154:LEU:HA	1.96	0.40
12:1L:176:ARG:HH22	13:1M:403:THR:HB	1.87	0.40
12:1L:241:THR:HG22	12:1L:299:LYS:HE3	2.02	0.40
12:1L:392:LYS:HZ1	12:1L:416:THR:HG23	1.86	0.40
12:1L:483:PRO:HA	35:1j:53:TYR:HB2	2.03	0.40
13:1M:119:TYR:CE1	13:1M:160:LEU:HD12	2.56	0.40
13:1M:388:TRP:HD1	29:1d:120:ARG:O	2.04	0.40
14:1N:104:MET:HE2	14:1N:104:MET:HB2	1.89	0.40
15:1O:309:ASN:N	15:1O:314:ASP:OD2	2.55	0.40
17:1Q:22:LEU:HD21	22:1W:81:LEU:HB3	2.03	0.40
19:1S:16:ARG:HB2	19:1S:68:TYR:O	2.21	0.40
19:1S:17:GLU:CB	19:1S:51:PRO:HG2	2.51	0.40
20:1U:50:ILE:HD12	20:1U:51:ILE:HD13	2.04	0.40
20:1U:60:PHE:HE2	20:1U:79:TYR:HE2	1.69	0.40
21:1V:6:LYS:HD3	21:1V:6:LYS:H	1.86	0.40
21:1V:22:ARG:HD2	21:1V:25:ILE:HD11	2.03	0.40
21:1V:76:ILE:HD12	21:1V:76:ILE:HA	1.86	0.40
22:1W:114:ARG:HA	22:1W:114:ARG:NH1	2.37	0.40
23:1X:18:LYS:H	23:1X:18:LYS:HG2	1.64	0.40
23:1X:39:ASN:OD1	25:1Z:73:PRO:HB2	2.21	0.40
24:1Y:80:ARG:C	24:1Y:81:GLU:HG3	2.45	0.40
25:1Z:89:GLU:OE1	25:1Z:128:ARG:NH1	2.55	0.40
34:1i:18:ARG:HD2	39:1n:170:VAL:O	2.21	0.40
34:1i:35:PRO:O	34:1i:35:PRO:CD	2.68	0.40
34:1i:100:LYS:HB3	41:1p:14:ARG:HH12	1.85	0.40
35:1j:7:ILE:O	35:1j:7:ILE:CG2	2.69	0.40
35:1j:51:PHE:CE2	40:1o:91:HIS:HB2	2.57	0.40
36:1k:50:TRP:CD1	36:1k:50:TRP:H	2.40	0.40
37:1l:94:THR:OG1	37:1l:95:PRO:HD2	2.21	0.40
39:1n:104:ASP:OD1	39:1n:104:ASP:N	2.55	0.40
1:1A:43:PRO:HB3	8:1H:126:LYS:HG2	2.03	0.40
1:1A:54:LYS:NZ	4:1D:71:GLU:HG2	2.36	0.40
2:1B:93:THR:HA	2:1B:132:VAL:HA	2.03	0.40
3:1C:53:HIS:CG	3:1C:54:PRO:HD2	2.57	0.40
3:1C:162:PHE:CZ	4:1D:88:GLU:HB2	2.56	0.40
4:1D:57:ALA:HA	47:1D:501:U10:O5	2.22	0.40
4:1D:347:HIS:CG	7:1G:121:MET:HE1	2.56	0.40
5:1E:175:GLU:HG2	5:1E:180:LYS:HD3	2.02	0.40
6:1F:337:MET:HE2	6:1F:337:MET:H	1.86	0.40
7:1G:35:MET:HE3	7:1G:35:MET:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:594:ARG:CZ	22:1W:125:GLY:HA2	2.51	0.40
7:1G:647:GLU:HA	7:1G:650:LYS:CE	2.51	0.40
8:1H:192:GLU:OE2	8:1H:193:THR:HG23	2.21	0.40
8:1H:202:GLU:HB3	8:1H:204:GLU:OE2	2.21	0.40
9:1I:29:GLU:HA	9:1I:32:ARG:HB2	2.04	0.40
10:1J:27:ILE:HD11	10:1J:28:TYR:CE2	2.56	0.40
11:1K:30:LEU:HA	11:1K:33:LEU:HB3	2.04	0.40
12:1L:437:PHE:O	36:1k:51:ARG:NH1	2.54	0.40
13:1M:293:HIS:CD2	13:1M:319:HIS:HD2	2.40	0.40
13:1M:331:ASN:OD1	13:1M:331:ASN:C	2.64	0.40
14:1N:23:SER:O	30:1e:1:PRO:HB3	2.22	0.40
16:1P:97:ARG:HD3	16:1P:97:ARG:HA	1.80	0.40
18:1R:3:ARG:HE	18:1R:11:VAL:HG11	1.87	0.40
19:1S:17:GLU:O	19:1S:18:ILE:HD13	2.21	0.40
31:1f:6:ILE:H	31:1f:6:ILE:HG13	1.66	0.40
31:1f:12:VAL:O	31:1f:15:LEU:HG	2.22	0.40
31:1f:42:LEU:HA	31:1f:42:LEU:HD12	1.74	0.40
31:1f:45:LYS:HD3	31:1f:45:LYS:N	2.32	0.40
33:1h:114:MET:HE1	33:1h:122:TRP:N	2.36	0.40
34:1i:24:ASP:CB	39:1n:120:LYS:HD3	2.51	0.40
34:1i:60:ILE:HD13	34:1i:60:ILE:HA	1.86	0.40
38:1m:13:LEU:HD21	38:1m:18:ASP:HA	2.03	0.40
41:1p:90:GLN:O	41:1p:93:ARG:HG2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	95 (84%)	16 (14%)	2 (2%)	6	26
2	1B	153/258 (59%)	137 (90%)	15 (10%)	1 (1%)	18	47

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1C	207/264 (78%)	186 (90%)	20 (10%)	1 (0%)	24	54
4	1D	427/476 (90%)	390 (91%)	37 (9%)	0	100	100
5	1E	212/249 (85%)	193 (91%)	18 (8%)	1 (0%)	24	54
6	1F	430/464 (93%)	408 (95%)	21 (5%)	1 (0%)	43	71
7	1G	697/727 (96%)	645 (92%)	48 (7%)	4 (1%)	21	50
8	1H	316/318 (99%)	291 (92%)	23 (7%)	2 (1%)	21	50
9	1I	174/239 (73%)	166 (95%)	8 (5%)	0	100	100
10	1J	173/175 (99%)	162 (94%)	10 (6%)	1 (1%)	21	50
11	1K	96/98 (98%)	87 (91%)	9 (9%)	0	100	100
12	1L	604/606 (100%)	543 (90%)	59 (10%)	2 (0%)	36	65
13	1M	457/459 (100%)	436 (95%)	20 (4%)	1 (0%)	43	71
14	1N	345/347 (99%)	320 (93%)	24 (7%)	1 (0%)	36	65
15	1O	318/357 (89%)	300 (94%)	18 (6%)	0	100	100
16	1P	340/377 (90%)	315 (93%)	23 (7%)	2 (1%)	21	50
17	1Q	127/175 (73%)	113 (89%)	14 (11%)	0	100	100
18	1R	94/123 (76%)	85 (90%)	9 (10%)	0	100	100
19	1S	85/99 (86%)	73 (86%)	12 (14%)	0	100	100
20	1T	83/156 (53%)	74 (89%)	9 (11%)	0	100	100
20	1U	84/156 (54%)	76 (90%)	8 (10%)	0	100	100
21	1V	113/116 (97%)	109 (96%)	4 (4%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	7 (6%)	0	100	100
23	1X	169/172 (98%)	153 (90%)	16 (10%)	0	100	100
24	1Y	137/141 (97%)	128 (93%)	9 (7%)	0	100	100
25	1Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
26	1a	68/70 (97%)	65 (96%)	3 (4%)	0	100	100
27	1b	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
28	1c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	49 (89%)	6 (11%)	0	100	100
32	1g	98/154 (64%)	88 (90%)	8 (8%)	2 (2%)	6	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
33	1h	136/189 (72%)	120 (88%)	16 (12%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	60 (87%)	9 (13%)	0	100	100
36	1k	79/98 (81%)	74 (94%)	5 (6%)	0	100	100
37	1l	154/186 (83%)	139 (90%)	15 (10%)	0	100	100
38	1m	126/129 (98%)	119 (94%)	7 (6%)	0	100	100
39	1n	170/179 (95%)	154 (91%)	15 (9%)	1 (1%)	21	50
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
41	1p	171/176 (97%)	163 (95%)	8 (5%)	0	100	100
42	1q	143/145 (99%)	135 (94%)	8 (6%)	0	100	100
43	1r	90/114 (79%)	85 (94%)	5 (6%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
All	All	8194/9744 (84%)	7564 (92%)	608 (7%)	22 (0%)	37	65

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	1C	121	VAL
7	1G	416	THR
7	1G	460	ARG
7	1G	650	LYS
8	1H	170	GLU
13	1M	390	ASN
39	1n	148	PRO
1	1A	109	LYS
2	1B	49	THR
7	1G	186	TYR
10	1J	116	ILE
16	1P	174	ARG
32	1g	64	PHE
6	1F	249	ARG
12	1L	551	SER
12	1L	72	GLN
1	1A	44	MET
5	1E	215	ALA
32	1g	63	PHE
14	1N	110	PRO
8	1H	208	VAL

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Mol	Chain	Res	Type
16	1P	23	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	92 (93%)	7 (7%)	13	39
2	1B	131/212 (62%)	117 (89%)	14 (11%)	6	23
3	1C	190/227 (84%)	179 (94%)	11 (6%)	18	45
4	1D	371/405 (92%)	342 (92%)	29 (8%)	11	37
5	1E	183/207 (88%)	170 (93%)	13 (7%)	13	39
6	1F	346/368 (94%)	329 (95%)	17 (5%)	22	49
7	1G	588/610 (96%)	548 (93%)	40 (7%)	14	40
8	1H	274/274 (100%)	258 (94%)	16 (6%)	18	45
9	1I	151/201 (75%)	143 (95%)	8 (5%)	20	47
10	1J	140/140 (100%)	130 (93%)	10 (7%)	13	39
11	1K	84/84 (100%)	76 (90%)	8 (10%)	8	29
12	1L	539/539 (100%)	505 (94%)	34 (6%)	16	42
13	1M	408/408 (100%)	389 (95%)	19 (5%)	23	50
14	1N	310/310 (100%)	295 (95%)	15 (5%)	23	50
15	1O	283/307 (92%)	269 (95%)	14 (5%)	22	49
16	1P	296/323 (92%)	270 (91%)	26 (9%)	9	31
17	1Q	117/152 (77%)	111 (95%)	6 (5%)	21	48
18	1R	79/97 (81%)	75 (95%)	4 (5%)	21	48
19	1S	77/82 (94%)	73 (95%)	4 (5%)	21	48
20	1T	79/133 (59%)	75 (95%)	4 (5%)	21	48
20	1U	79/133 (59%)	71 (90%)	8 (10%)	7	25
21	1V	100/101 (99%)	94 (94%)	6 (6%)	17	43
22	1W	107/112 (96%)	102 (95%)	5 (5%)	23	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	1X	153/154 (99%)	148 (97%)	5 (3%)	33	57
24	1Y	101/102 (99%)	96 (95%)	5 (5%)	22	49
25	1Z	123/124 (99%)	115 (94%)	8 (6%)	15	42
26	1a	58/58 (100%)	52 (90%)	6 (10%)	7	24
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	39
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	41
29	1d	107/109 (98%)	99 (92%)	8 (8%)	12	38
30	1e	87/94 (93%)	85 (98%)	2 (2%)	44	63
31	1f	54/113 (48%)	52 (96%)	2 (4%)	30	55
32	1g	92/129 (71%)	86 (94%)	6 (6%)	15	42
33	1h	121/158 (77%)	118 (98%)	3 (2%)	42	62
34	1i	119/120 (99%)	114 (96%)	5 (4%)	26	52
35	1j	62/84 (74%)	58 (94%)	4 (6%)	15	42
36	1k	63/76 (83%)	60 (95%)	3 (5%)	23	50
37	1l	141/161 (88%)	130 (92%)	11 (8%)	11	37
38	1m	113/114 (99%)	109 (96%)	4 (4%)	32	56
39	1n	156/160 (98%)	151 (97%)	5 (3%)	34	58
40	1o	110/120 (92%)	105 (96%)	5 (4%)	24	51
41	1p	154/156 (99%)	150 (97%)	4 (3%)	40	61
42	1q	131/131 (100%)	125 (95%)	6 (5%)	24	50
43	1r	85/98 (87%)	80 (94%)	5 (6%)	18	44
44	1s	44/351 (12%)	43 (98%)	1 (2%)	44	63
All	All	7219/8272 (87%)	6795 (94%)	424 (6%)	19	44

All (424) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	9	THR
1	1A	49	LEU
1	1A	52	SER
1	1A	53	MET
1	1A	73	LEU
1	1A	94	LEU
1	1A	96	ILE

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Mol	Chain	Res	Type
2	1B	29	VAL
2	1B	44	SER
2	1B	49	THR
2	1B	52	LEU
2	1B	54	CYS
2	1B	74	VAL
2	1B	93	THR
2	1B	128	TYR
2	1B	133	VAL
2	1B	137	ASP
2	1B	140	VAL
2	1B	152	THR
2	1B	168	LYS
2	1B	173	LEU
3	1C	7	THR
3	1C	21	GLN
3	1C	44	CYS
3	1C	71	GLN
3	1C	107	VAL
3	1C	109	THR
3	1C	111	THR
3	1C	151	ILE
3	1C	168	LEU
3	1C	172	VAL
3	1C	174	LEU
4	1D	41	ASP
4	1D	44	VAL
4	1D	45	SER
4	1D	62	LEU
4	1D	68	LEU
4	1D	72	MET
4	1D	95	THR
4	1D	97	LEU
4	1D	111	MET
4	1D	123	GLU
4	1D	145	THR
4	1D	159	LEU
4	1D	161	ILE
4	1D	165	THR
4	1D	199	VAL
4	1D	203	LEU
4	1D	209	ASP

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Mol	Chain	Res	Type
4	1D	215	SER
4	1D	219	SER
4	1D	244	VAL
4	1D	246	THR
4	1D	253	TYR
4	1D	263	SER
4	1D	284	ASP
4	1D	285	VAL
4	1D	312	SER
4	1D	376	VAL
4	1D	389	CYS
4	1D	415	VAL
5	1E	24	THR
5	1E	47	VAL
5	1E	53	LEU
5	1E	60	TRP
5	1E	75	VAL
5	1E	78	MET
5	1E	91	ASN
5	1E	102	VAL
5	1E	108	CYS
5	1E	126	ILE
5	1E	145	LEU
5	1E	148	CYS
5	1E	203	THR
6	1F	54	ASP
6	1F	63	SER
6	1F	86	SER
6	1F	136	ILE
6	1F	151	VAL
6	1F	167	CYS
6	1F	250	ASN
6	1F	266	CYS
6	1F	280	ILE
6	1F	287	VAL
6	1F	311	VAL
6	1F	314	THR
6	1F	318	ASP
6	1F	320	ASP
6	1F	336	VAL
6	1F	367	GLU
6	1F	435	LEU

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Mol	Chain	Res	Type
7	1G	41	CYS
7	1G	57	VAL
7	1G	65	VAL
7	1G	81	THR
7	1G	93	VAL
7	1G	107	ILE
7	1G	123	PHE
7	1G	138	GLU
7	1G	141	ASN
7	1G	151	THR
7	1G	157	THR
7	1G	174	THR
7	1G	183	VAL
7	1G	195	LEU
7	1G	209	THR
7	1G	215	PHE
7	1G	216	THR
7	1G	222	THR
7	1G	227	SER
7	1G	236	SER
7	1G	242	THR
7	1G	254	MET
7	1G	263	ILE
7	1G	288	LYS
7	1G	313	ASN
7	1G	323	VAL
7	1G	339	ASP
7	1G	356	THR
7	1G	371	VAL
7	1G	375	ASP
7	1G	400	LEU
7	1G	408	LEU
7	1G	413	VAL
7	1G	417	TYR
7	1G	462	ASP
7	1G	483	VAL
7	1G	588	THR
7	1G	615	THR
7	1G	631	VAL
7	1G	661	LEU
8	1H	9	LEU
8	1H	32	GLN

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Mol	Chain	Res	Type
8	1H	61	LEU
8	1H	76	ILE
8	1H	102	VAL
8	1H	125	SER
8	1H	152	SER
8	1H	173	TRP
8	1H	200	LEU
8	1H	213	VAL
8	1H	241	LEU
8	1H	248	ASP
8	1H	266	LEU
8	1H	276	SER
8	1H	289	LEU
8	1H	298	LEU
9	1I	26	LEU
9	1I	93	THR
9	1I	106	THR
9	1I	107	THR
9	1I	122	CYS
9	1I	129	ASP
9	1I	143	THR
9	1I	174	LEU
10	1J	17	PHE
10	1J	44	VAL
10	1J	66	VAL
10	1J	68	PHE
10	1J	79	TYR
10	1J	95	SER
10	1J	102	CYS
10	1J	126	VAL
10	1J	130	THR
10	1J	160	SER
11	1K	10	MET
11	1K	43	MET
11	1K	47	ILE
11	1K	61	ILE
11	1K	69	CYS
11	1K	84	THR
11	1K	88	ASP
11	1K	95	LEU
12	1L	9	LEU
12	1L	41	SER

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Mol	Chain	Res	Type
12	1L	49	VAL
12	1L	65	ASN
12	1L	84	TYR
12	1L	86	SER
12	1L	92	VAL
12	1L	99	SER
12	1L	104	SER
12	1L	110	SER
12	1L	127	THR
12	1L	129	MET
12	1L	131	LEU
12	1L	159	HIS
12	1L	253	VAL
12	1L	260	LEU
12	1L	308	SER
12	1L	329	ILE
12	1L	340	PHE
12	1L	346	ILE
12	1L	349	SER
12	1L	396	ILE
12	1L	419	THR
12	1L	481	THR
12	1L	484	LEU
12	1L	489	THR
12	1L	502	LEU
12	1L	510	TYR
12	1L	519	THR
12	1L	575	ILE
12	1L	577	VAL
12	1L	590	SER
12	1L	593	ILE
12	1L	598	SER
13	1M	15	THR
13	1M	36	LEU
13	1M	55	THR
13	1M	101	LEU
13	1M	109	THR
13	1M	115	LEU
13	1M	116	ILE
13	1M	157	SER
13	1M	195	MET
13	1M	229	MET

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Mol	Chain	Res	Type
13	1M	289	SER
13	1M	299	VAL
13	1M	343	ILE
13	1M	349	GLN
13	1M	367	LEU
13	1M	373	ILE
13	1M	391	ILE
13	1M	431	THR
13	1M	447	LEU
14	1N	43	VAL
14	1N	70	LEU
14	1N	93	VAL
14	1N	95	MET
14	1N	140	SER
14	1N	161	SER
14	1N	217	MET
14	1N	226	THR
14	1N	240	ILE
14	1N	249	LEU
14	1N	282	MET
14	1N	299	SER
14	1N	303	THR
14	1N	308	THR
14	1N	335	LEU
15	1O	14	THR
15	1O	26	THR
15	1O	123	VAL
15	1O	161	CYS
15	1O	170	VAL
15	1O	195	THR
15	1O	217	LYS
15	1O	229	GLU
15	1O	243	CYS
15	1O	270	LEU
15	1O	283	THR
15	1O	293	PHE
15	1O	315	LYS
15	1O	317	ILE
16	1P	43	SER
16	1P	45	VAL
16	1P	47	VAL
16	1P	52	GLU

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Mol	Chain	Res	Type
16	1P	62	MET
16	1P	88	SER
16	1P	108	ASP
16	1P	109	VAL
16	1P	126	VAL
16	1P	140	LYS
16	1P	141	SER
16	1P	143	SER
16	1P	144	ARG
16	1P	148	SER
16	1P	151	VAL
16	1P	154	LYS
16	1P	208	VAL
16	1P	210	VAL
16	1P	272	VAL
16	1P	290	SER
16	1P	291	ASP
16	1P	315	ILE
16	1P	334	VAL
16	1P	338	LYS
16	1P	339	THR
16	1P	340	VAL
17	1Q	6	GLN
17	1Q	11	ILE
17	1Q	52	THR
17	1Q	69	LEU
17	1Q	123	SER
17	1Q	130	VAL
18	1R	20	ASP
18	1R	54	SER
18	1R	79	THR
18	1R	83	THR
19	1S	41	VAL
19	1S	47	ASN
19	1S	80	ASN
19	1S	94	LEU
20	1T	7	THR
20	1T	19	LEU
20	1T	40	LEU
20	1T	44	SER
20	1U	16	LEU
20	1U	18	VAL

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Mol	Chain	Res	Type
20	1U	26	ASP
20	1U	30	LEU
20	1U	32	VAL
20	1U	60	PHE
20	1U	61	GLU
20	1U	65	ILE
21	1V	8	THR
21	1V	68	GLU
21	1V	70	GLN
21	1V	94	LEU
21	1V	110	GLN
21	1V	115	ILE
22	1W	32	VAL
22	1W	50	PHE
22	1W	70	ASN
22	1W	110	THR
22	1W	126	HIS
23	1X	8	THR
23	1X	12	LEU
23	1X	40	LYS
23	1X	110	VAL
23	1X	157	LEU
24	1Y	15	THR
24	1Y	74	CYS
24	1Y	84	ASP
24	1Y	114	CYS
24	1Y	132	TRP
25	1Z	20	ASP
25	1Z	30	LEU
25	1Z	62	ILE
25	1Z	110	VAL
25	1Z	114	THR
25	1Z	117	VAL
25	1Z	133	ILE
25	1Z	141	ILE
26	1a	5	ILE
26	1a	11	VAL
26	1a	12	MET
26	1a	38	VAL
26	1a	50	ARG
26	1a	57	VAL
27	1b	19	VAL

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Mol	Chain	Res	Type
27	1b	29	ILE
27	1b	35	SER
27	1b	56	LEU
27	1b	80	LEU
28	1c	3	TYR
28	1c	9	HIS
28	1c	43	LYS
29	1d	2	MET
29	1d	34	MET
29	1d	37	LEU
29	1d	41	SER
29	1d	44	ILE
29	1d	62	LEU
29	1d	67	SER
29	1d	96	SER
30	1e	63	VAL
30	1e	88	GLU
31	1f	16	VAL
31	1f	51	ASN
32	1g	36	ASN
32	1g	44	SER
32	1g	64	PHE
32	1g	74	SER
32	1g	76	PHE
32	1g	112	CYS
33	1h	47	ILE
33	1h	91	MET
33	1h	136	SER
34	1i	8	LYS
34	1i	33	VAL
34	1i	75	LEU
34	1i	103	ILE
34	1i	116	ILE
35	1j	24	GLN
35	1j	37	LEU
35	1j	40	PHE
35	1j	47	VAL
36	1k	21	TRP
36	1k	48	GLU
36	1k	63	VAL
37	1l	5	THR
37	1l	46	ASP

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Mol	Chain	Res	Type
37	1l	50	LEU
37	1l	69	LEU
37	1l	71	LEU
37	1l	83	MET
37	1l	92	SER
37	1l	96	VAL
37	1l	140	LEU
37	1l	147	THR
37	1l	149	GLU
38	1m	16	THR
38	1m	24	ILE
38	1m	120	LEU
38	1m	127	SER
39	1n	72	TYR
39	1n	107	HIS
39	1n	138	GLN
39	1n	150	THR
39	1n	169	ILE
40	1o	15	GLU
40	1o	19	LEU
40	1o	63	ILE
40	1o	83	GLN
40	1o	93	ASP
41	1p	3	SER
41	1p	81	ILE
41	1p	105	ILE
41	1p	116	GLU
42	1q	9	ARG
42	1q	20	LEU
42	1q	35	VAL
42	1q	55	PHE
42	1q	66	THR
42	1q	142	THR
43	1r	6	VAL
43	1r	9	LEU
43	1r	30	ILE
43	1r	55	THR
43	1r	70	SER
44	1s	41	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	38	ASN
3	1C	38	GLN
3	1C	200	ASN
4	1D	149	ASN
4	1D	201	GLN
4	1D	348	HIS
5	1E	112	ASN
5	1E	150	ASN
6	1F	37	GLN
6	1F	96	ASN
6	1F	148	ASN
6	1F	250	ASN
6	1F	257	ASN
6	1F	324	GLN
7	1G	36	GLN
7	1G	51	ASN
7	1G	392	ASN
7	1G	421	HIS
7	1G	441	GLN
7	1G	476	ASN
7	1G	546	GLN
12	1L	165	ASN
12	1L	506	ASN
13	1M	48	ASN
13	1M	220	HIS
13	1M	293	HIS
13	1M	331	ASN
13	1M	338	HIS
13	1M	415	GLN
13	1M	434	ASN
14	1N	63	GLN
15	1O	114	HIS
15	1O	184	GLN
15	1O	200	GLN
15	1O	251	GLN
15	1O	271	ASN
16	1P	8	HIS
16	1P	180	ASN
16	1P	306	GLN
17	1Q	6	GLN
17	1Q	44	ASN
20	1T	74	GLN
22	1W	48	HIS

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Mol	Chain	Res	Type
22	1W	58	GLN
23	1X	64	GLN
23	1X	103	GLN
23	1X	142	HIS
25	1Z	85	GLN
25	1Z	90	ASN
25	1Z	130	ASN
28	1c	9	HIS
29	1d	97	HIS
30	1e	20	GLN
30	1e	33	HIS
31	1f	39	ASN
32	1g	116	ASN
33	1h	143	ASN
34	1i	12	GLN
35	1j	16	GLN
37	1l	28	ASN
37	1l	136	ASN
39	1n	138	GLN
40	1o	84	HIS
41	1p	27	ASN
41	1p	54	GLN
41	1p	55	HIS
42	1q	135	GLN
43	1r	12	ASN
43	1r	35	GLN
43	1r	46	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	FME	1H	1	8	8,9,10	0.54	0	8,9,11	1.08	1 (12%)
10	FME	1J	1	10	8,9,10	0.55	0	8,9,11	0.95	1 (12%)
34	SAC	1i	1	-	7,8,9	0.56	0	7,9,11	1.16	1 (14%)
13	FME	1M	1	13	8,9,10	0.53	0	8,9,11	0.87	1 (12%)
12	FME	1L	1	12	8,9,10	0.56	0	8,9,11	0.97	1 (12%)
11	FME	1K	1	11	8,9,10	0.55	0	8,9,11	1.03	1 (12%)
1	FME	1A	1	1	8,9,10	0.56	0	8,9,11	0.98	1 (12%)
14	FME	1N	1	14	8,9,10	0.54	0	8,9,11	0.93	1 (12%)

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

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.97	117.12	124.77
8	1H	1	FME	O-C-CA	-2.73	117.74	124.77
1	1A	1	FME	O-C-CA	-2.59	118.11	124.77
12	1L	1	FME	O-C-CA	-2.56	118.18	124.77
11	1K	1	FME	O-C-CA	-2.53	118.27	124.77
14	1N	1	FME	O-C-CA	-2.48	118.38	124.77
10	1J	1	FME	O-C-CA	-2.46	118.45	124.77
13	1M	1	FME	O-C-CA	-2.29	118.88	124.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	1A	1	FME	O-C-CA-CB
8	1H	1	FME	O-C-CA-CB
10	1J	1	FME	N-CA-CB-CG
10	1J	1	FME	C-CA-CB-CG
11	1K	1	FME	O-C-CA-CB
12	1L	1	FME	O-C-CA-CB
13	1M	1	FME	N-CA-CB-CG
34	1i	1	SAC	O-C-CA-CB
11	1K	1	FME	N-CA-CB-CG
13	1M	1	FME	C-CA-CB-CG
34	1i	1	SAC	C-CA-N-C1A

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	1H	1	FME	1	0
34	1i	1	SAC	3	0
13	1M	1	FME	1	0
1	1A	1	FME	3	0
14	1N	1	FME	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 3 are monoatomic - leaving 21 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
48	FES	1G	803	7	0,4,4	-	-	-		
54	GTP	1O	401	55	33,34,34	0.60	0	50,54,54	0.62	0
45	SF4	1G	801	7	0,12,12	-	-	-		
53	CDL	1N	401	14	66,66,99	0.32	0	72,78,111	0.43	0
45	SF4	1I	202	9	0,12,12	-	-	-		
52	3PE	1M	501	-	37,37,50	0.31	0	40,42,55	0.38	0
46	PC1	1q	201	-	47,47,53	0.31	0	53,55,61	0.42	0
45	SF4	1G	802	7	0,12,12	-	-	-		
53	CDL	1a	101	26,42	60,60,99	0.33	0	66,72,111	0.43	0
58	EHZ	1W	201	-	31,36,37	0.20	0	36,44,47	1.35	1 (2%)
45	SF4	1B	201	2	0,12,12	-	-	-		
46	PC1	1d	201	29,30	38,38,53	0.30	0	44,46,61	0.38	0
49	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.67	1 (2%)
46	PC1	1B	202	2	33,33,53	0.33	0	39,41,61	0.33	0
56	NDP	1P	501	-	51,52,52	0.49	0	71,80,80	0.84	2 (2%)
45	SF4	1I	201	9	0,12,12	-	-	-		
45	SF4	1F	502	6	0,12,12	-	-	-		
48	FES	1E	301	5	0,4,4	-	-	-		
47	U10	1D	501	-	63,63,63	0.59	2 (3%)	78,79,79	0.76	4 (5%)
58	EHZ	1n	201	-	31,36,37	0.18	0	36,44,47	1.12	2 (5%)
51	MYR	1L	701	-	13,14,15	0.31	0	12,13,15	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	FES	1G	803	7	-	-	0/1/1/1
54	GTP	1O	401	55	-	1/22/38/38	0/3/3/3
45	SF4	1G	801	7	-	-	0/6/5/5
53	CDL	1N	401	14	-	25/76/76/110	-
52	3PE	1M	501	-	-	5/41/41/54	-
45	SF4	1I	202	9	-	-	0/6/5/5
46	PC1	1q	201	-	-	15/51/51/57	-
45	SF4	1G	802	7	-	-	0/6/5/5
53	CDL	1a	101	26,42	-	8/71/71/110	-
58	EHZ	1W	201	-	-	12/42/44/45	-
45	SF4	1B	201	2	-	-	0/6/5/5
46	PC1	1d	201	29,30	-	13/42/42/57	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
46	PC1	1B	202	2	-	11/37/37/57	-
56	NDP	1P	501	-	-	2/34/77/77	0/5/5/5
45	SF4	1I	201	9	-	-	0/6/5/5
45	SF4	1F	502	6	-	-	0/6/5/5
48	FES	1E	301	5	-	-	0/1/1/1
47	U10	1D	501	-	-	14/63/87/87	0/1/1/1
58	EHZ	1n	201	-	-	8/42/44/45	-
51	MYR	1L	701	-	-	0/12/12/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	1D	501	U10	C4-C5	-2.51	1.41	1.48
47	1D	501	U10	C4-C3	2.01	1.43	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1W	201	EHZ	C10-S1-C9	7.62	124.38	101.84
58	1n	201	EHZ	C10-S1-C9	5.94	119.42	101.84
56	1P	501	NDP	P2B-O2B-C2B	-4.93	110.26	123.43
56	1P	501	NDP	O4D-C1D-C2D	-2.81	100.60	106.62
47	1D	501	U10	O3-C3-C2	2.68	125.69	116.64
47	1D	501	U10	O4-C4-C5	-2.44	108.42	116.64
47	1D	501	U10	C4-C3-C2	-2.37	116.35	120.69
58	1n	201	EHZ	C14-C13-C12	2.10	115.89	112.39
49	1F	501	FMN	C4-N3-C2	-2.10	121.92	125.64
47	1D	501	U10	O4-C4-C3	2.05	131.40	123.64

There are no chirality outliers.

All (116) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C1-O11-P-O13
46	1B	202	PC1	C2-C1-O11-P
46	1B	202	PC1	O32-C31-O31-C3
46	1B	202	PC1	C32-C31-O31-C3
46	1d	201	PC1	C11-O13-P-O14
46	1d	201	PC1	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
46	1d	201	PC1	C22-C21-O21-C2
46	1d	201	PC1	O32-C31-O31-C3
46	1d	201	PC1	C32-C31-O31-C3
46	1q	201	PC1	C11-O13-P-O14
46	1q	201	PC1	C1-O11-P-O13
46	1q	201	PC1	O32-C31-O31-C3
46	1q	201	PC1	C32-C31-O31-C3
47	1D	501	U10	C34-C36-C37-C38
49	1F	501	FMN	N10-C1'-C2'-O2'
49	1F	501	FMN	N10-C1'-C2'-C3'
52	1M	501	3PE	C11-O13-P-O12
52	1M	501	3PE	C12-C11-O13-P
53	1N	401	CDL	CA2-OA2-PA1-OA4
53	1N	401	CDL	CA2-OA2-PA1-OA5
58	1W	201	EHZ	O1-C7-C8-C9
58	1W	201	EHZ	N2-C15-C16-C17
58	1W	201	EHZ	N2-C15-C16-O5
58	1W	201	EHZ	O4-C15-C16-C17
58	1W	201	EHZ	O2-C9-S1-C10
58	1W	201	EHZ	C8-C9-S1-C10
58	1n	201	EHZ	O1-C7-C8-C9
47	1D	501	U10	C12-C11-C9-C10
47	1D	501	U10	C12-C11-C9-C8
58	1n	201	EHZ	C13-C12-N1-C11
53	1N	401	CDL	O1-C1-CA2-OA2
47	1D	501	U10	C40-C39-C41-C42
47	1D	501	U10	C45-C44-C46-C47
47	1D	501	U10	C38-C39-C41-C42
47	1D	501	U10	C43-C44-C46-C47
47	1D	501	U10	C24-C26-C27-C28
58	1n	201	EHZ	O3-C12-N1-C11
53	1N	401	CDL	CB2-C1-CA2-OA2
47	1D	501	U10	C4-C3-O3-C3M
53	1N	401	CDL	CB5-C51-C52-C53
53	1N	401	CDL	C1-CA2-OA2-PA1
53	1N	401	CDL	C1-CB2-OB2-PB2
46	1B	202	PC1	C31-C32-C33-C34
53	1N	401	CDL	C74-C75-C76-C77
53	1N	401	CDL	C31-CA7-OA8-CA6
52	1M	501	3PE	C24-C25-C26-C27
53	1N	401	CDL	C14-C15-C16-C17
52	1M	501	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
53	1N	401	CDL	OA9-CA7-OA8-CA6
56	1P	501	NDP	O4D-C1D-N1N-C6N
53	1N	401	CDL	C57-C58-C59-C60
58	1W	201	EHZ	O4-C15-C16-O5
46	1q	201	PC1	O11-C1-C2-C3
47	1D	501	U10	C2-C3-O3-C3M
46	1d	201	PC1	C2-C1-O11-P
53	1a	101	CDL	CA7-C31-C32-C33
53	1N	401	CDL	OB5-CB3-CB4-OB6
46	1q	201	PC1	C3B-C3C-C3D-C3E
46	1d	201	PC1	C22-C23-C24-C25
58	1W	201	EHZ	C6-C7-C8-C9
58	1n	201	EHZ	C6-C7-C8-C9
53	1N	401	CDL	C52-C51-CB5-OB6
46	1q	201	PC1	O11-C1-C2-O21
47	1D	501	U10	C9-C11-C12-C13
46	1B	202	PC1	C12-C11-O13-P
46	1d	201	PC1	C12-C11-O13-P
46	1q	201	PC1	C12-C11-O13-P
58	1W	201	EHZ	C15-C16-C17-C19
53	1a	101	CDL	C12-C13-C14-C15
53	1N	401	CDL	CB4-CB3-OB5-PB2
46	1d	201	PC1	O13-C11-C12-N
46	1q	201	PC1	O13-C11-C12-N
53	1N	401	CDL	C72-C71-CB7-OB8
58	1W	201	EHZ	O3-C12-C13-C14
58	1W	201	EHZ	C15-C16-C17-C20
58	1n	201	EHZ	C19-C17-C20-O6
58	1W	201	EHZ	N1-C12-C13-C14
46	1B	202	PC1	C1-C2-C3-O31
46	1B	202	PC1	C11-O13-P-O14
46	1d	201	PC1	C11-O13-P-O11
46	1q	201	PC1	C1-O11-P-O14
53	1N	401	CDL	CA2-OA2-PA1-OA3
53	1a	101	CDL	CA3-OA5-PA1-OA3
46	1q	201	PC1	C24-C25-C26-C27
46	1d	201	PC1	C35-C36-C37-C38
46	1B	202	PC1	O21-C2-C3-O31
53	1a	101	CDL	OA6-CA4-CA6-OA8
46	1B	202	PC1	O21-C21-C22-C23
58	1n	201	EHZ	C2-C3-C4-C5
53	1N	401	CDL	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
58	1n	201	EHZ	C10-C11-N1-C12
52	1M	501	3PE	C2-C1-O11-P
53	1N	401	CDL	CA2-C1-CB2-OB2
56	1P	501	NDP	O4D-C4D-C5D-O5D
53	1N	401	CDL	OB5-CB3-CB4-CB6
53	1a	101	CDL	CA4-CA3-OA5-PA1
46	1q	201	PC1	C23-C24-C25-C26
46	1B	202	PC1	O22-C21-C22-C23
47	1D	501	U10	C5-C4-O4-C4M
58	1n	201	EHZ	C1-C21-C22-C23
53	1N	401	CDL	C72-C71-CB7-OB9
54	1O	401	GTP	PB-O3A-PA-O2A
46	1q	201	PC1	O21-C21-C22-C23
53	1N	401	CDL	C56-C57-C58-C59
46	1d	201	PC1	C39-C3A-C3B-C3C
53	1N	401	CDL	C12-C11-CA5-OA6
46	1q	201	PC1	C3-C2-O21-C21
47	1D	501	U10	C46-C47-C48-C49
53	1a	101	CDL	C13-C14-C15-C16
53	1N	401	CDL	C52-C51-CB5-OB7
46	1q	201	PC1	O22-C21-C22-C23
47	1D	501	U10	C36-C37-C38-C39
53	1N	401	CDL	C12-C11-CA5-OA7
46	1d	201	PC1	O31-C31-C32-C33
53	1a	101	CDL	C12-C11-CA5-OA6
53	1a	101	CDL	C72-C71-CB7-OB8

There are no ring outliers.

20 monomers are involved in 72 short contacts:

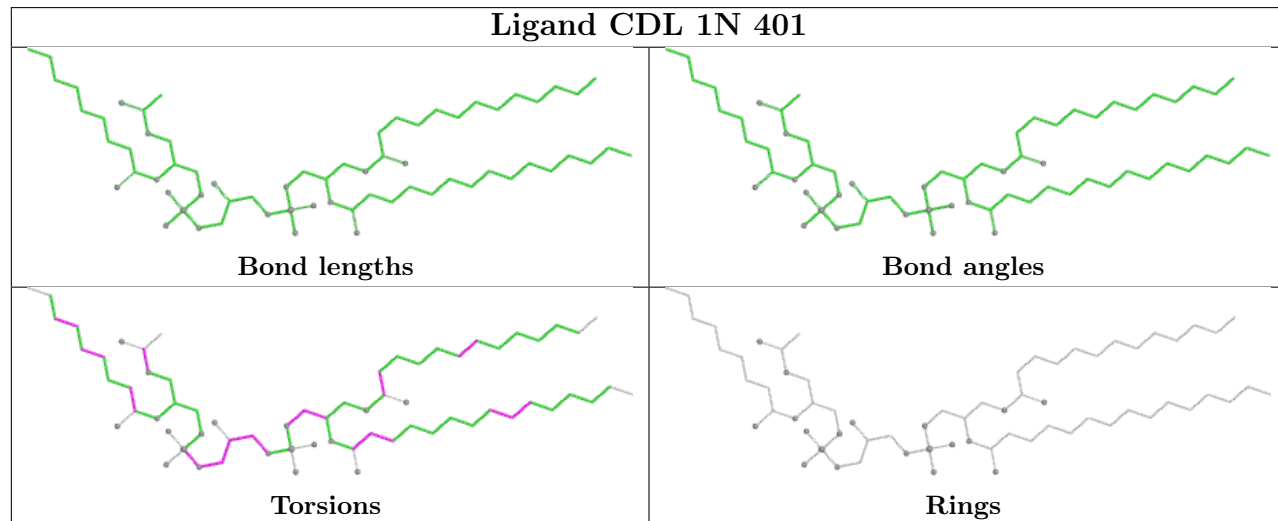
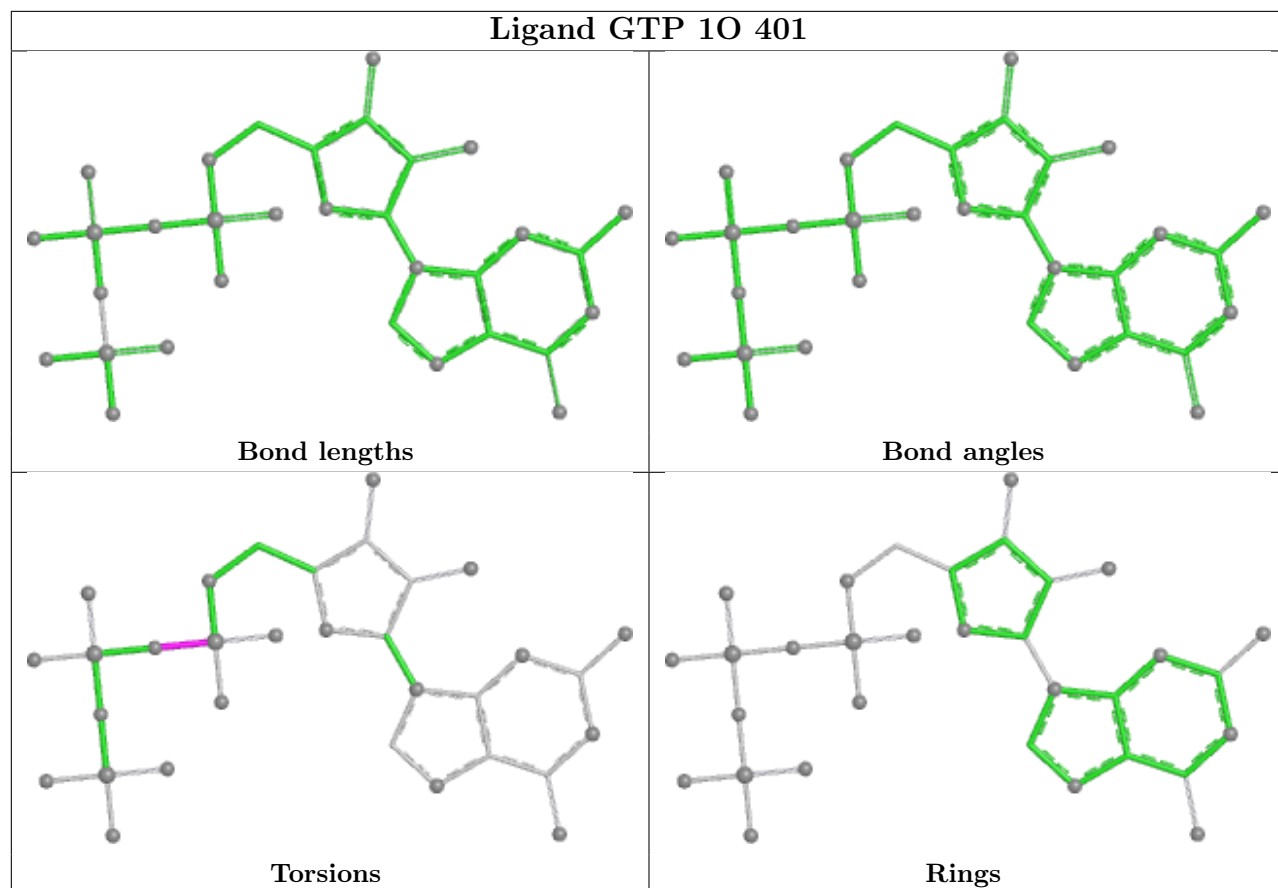
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	1G	803	FES	4	0
54	1O	401	GTP	3	0
45	1G	801	SF4	2	0
53	1N	401	CDL	8	0
45	1I	202	SF4	1	0
52	1M	501	3PE	2	0
46	1q	201	PC1	2	0
53	1a	101	CDL	6	0
58	1W	201	EHZ	1	0
45	1B	201	SF4	1	0
46	1d	201	PC1	6	0

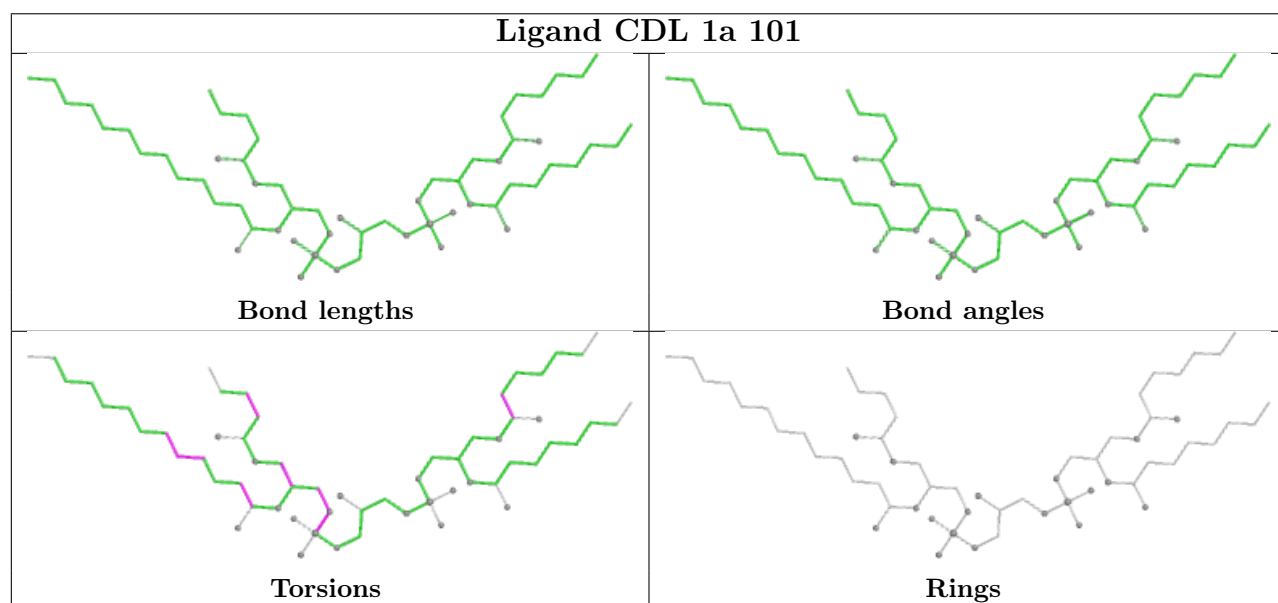
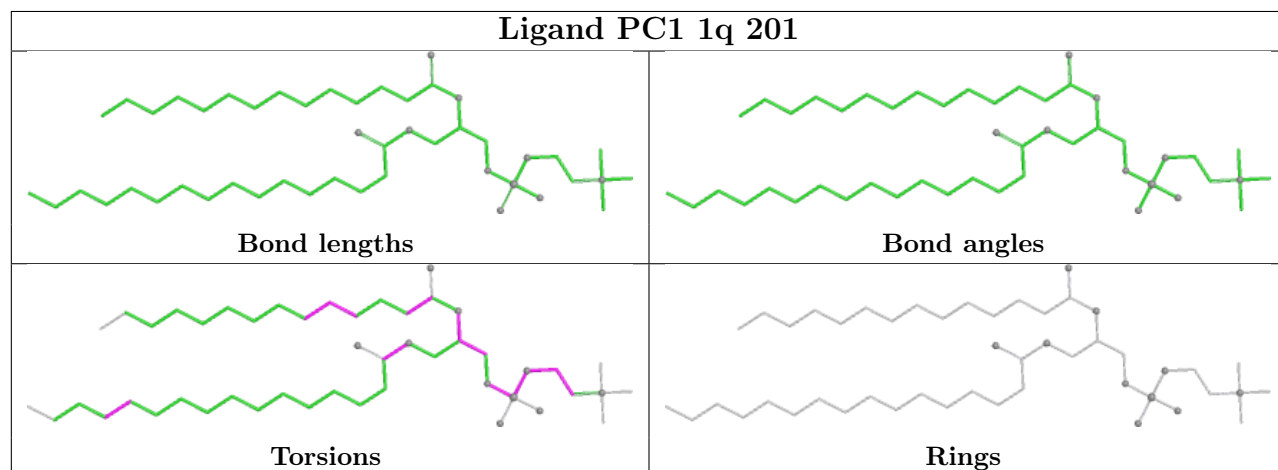
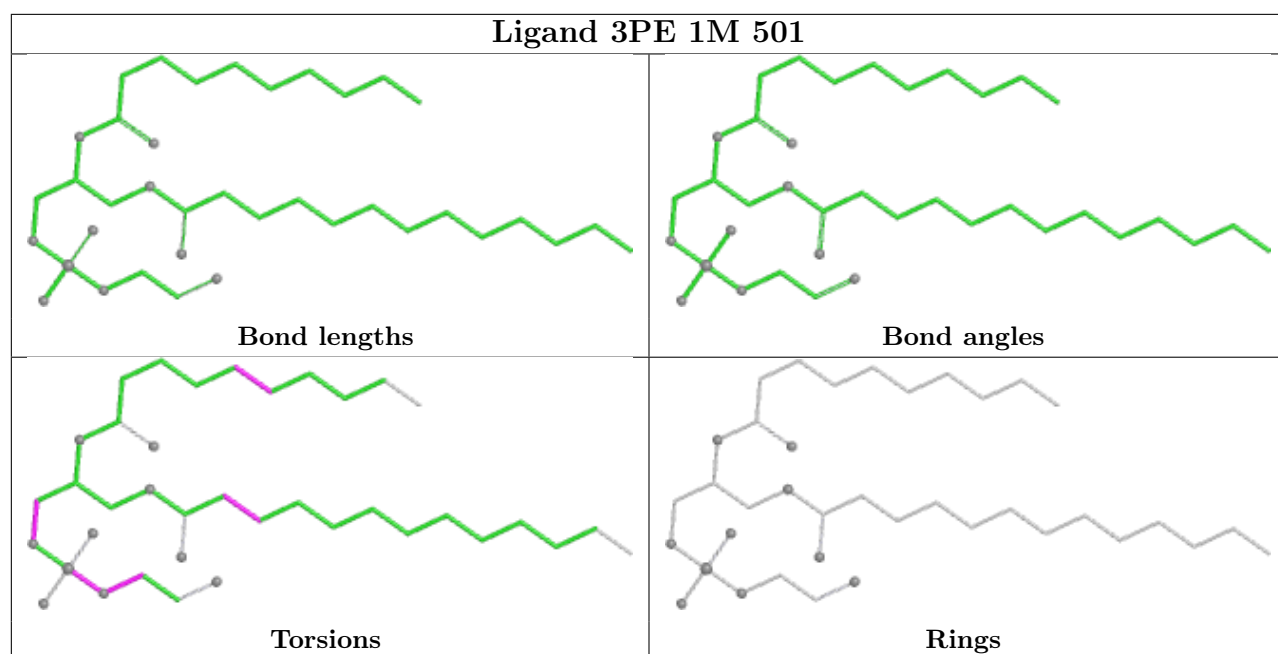
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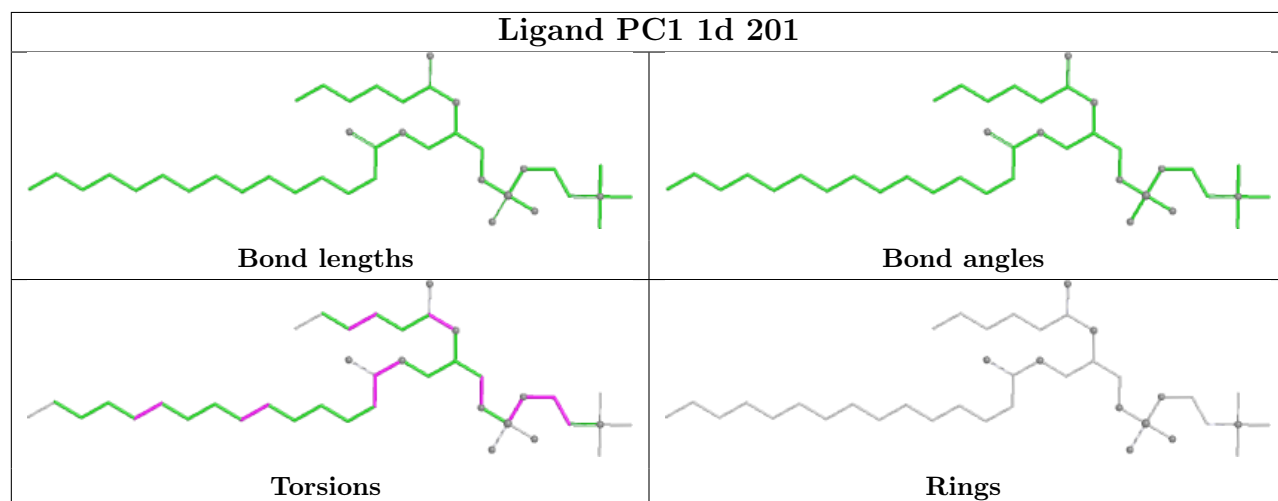
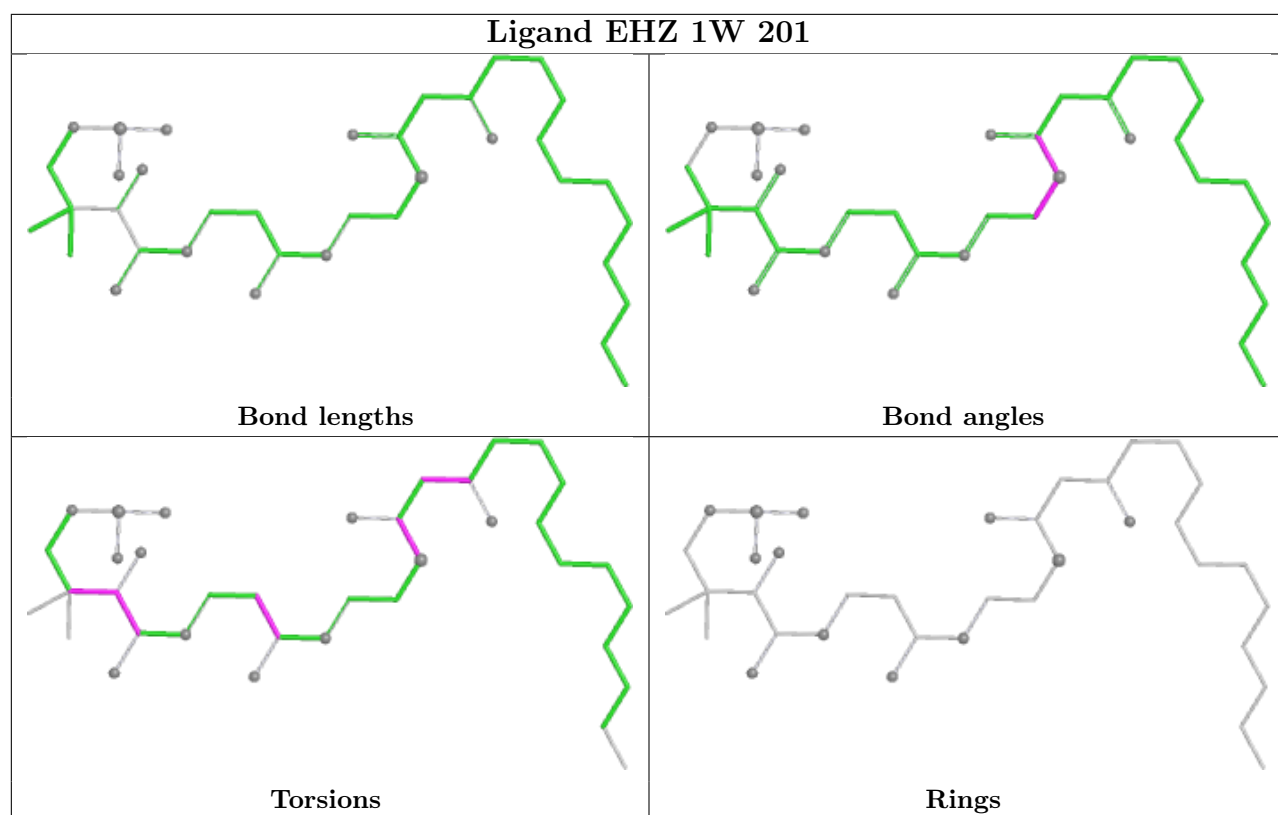
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	1F	501	FMN	1	0
46	1B	202	PC1	4	0
56	1P	501	NDP	6	0
45	1I	201	SF4	1	0
45	1F	502	SF4	1	0
48	1E	301	FES	1	0
47	1D	501	U10	19	0
58	1n	201	EHZ	1	0
51	1L	701	MYR	2	0

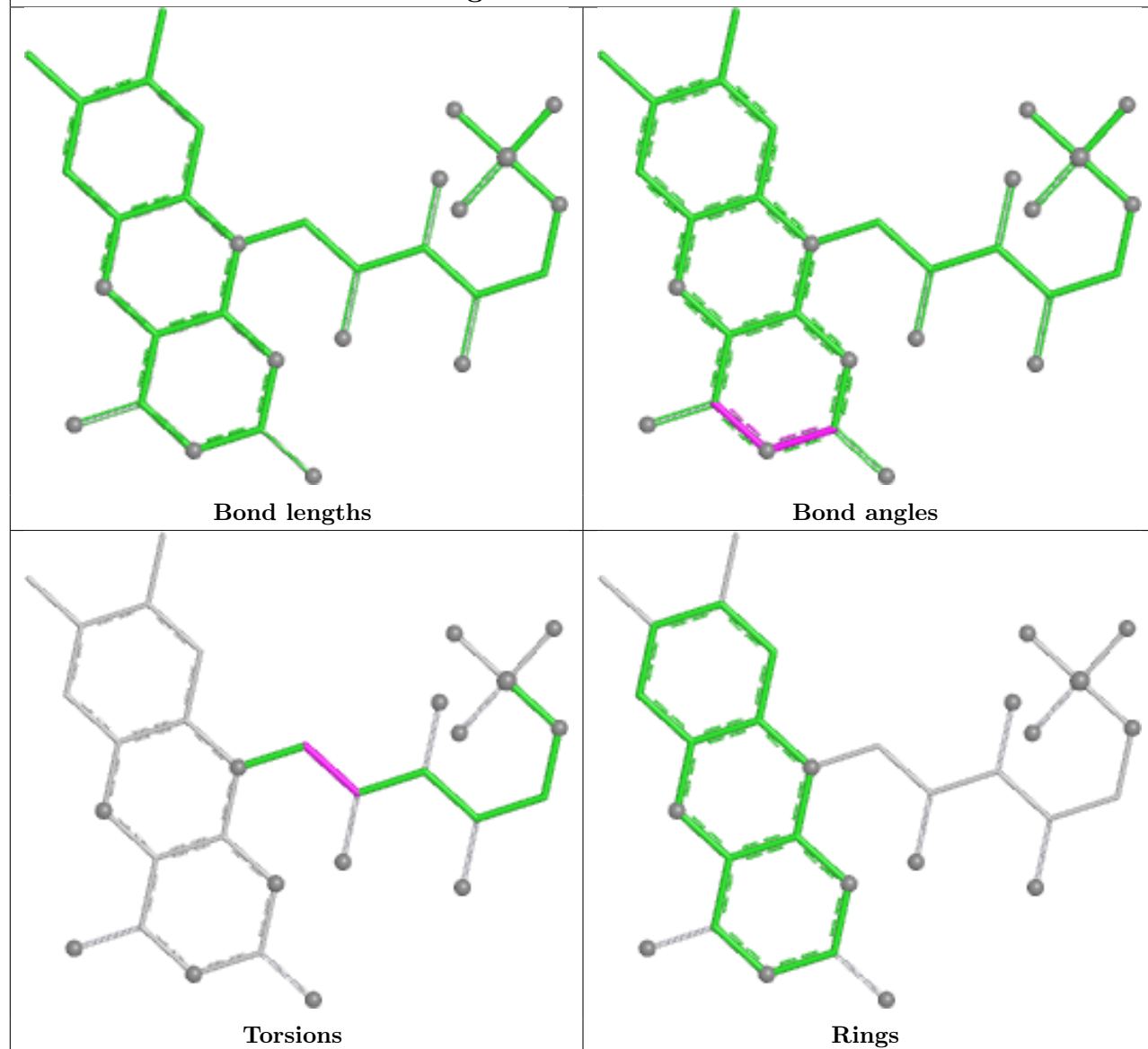
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



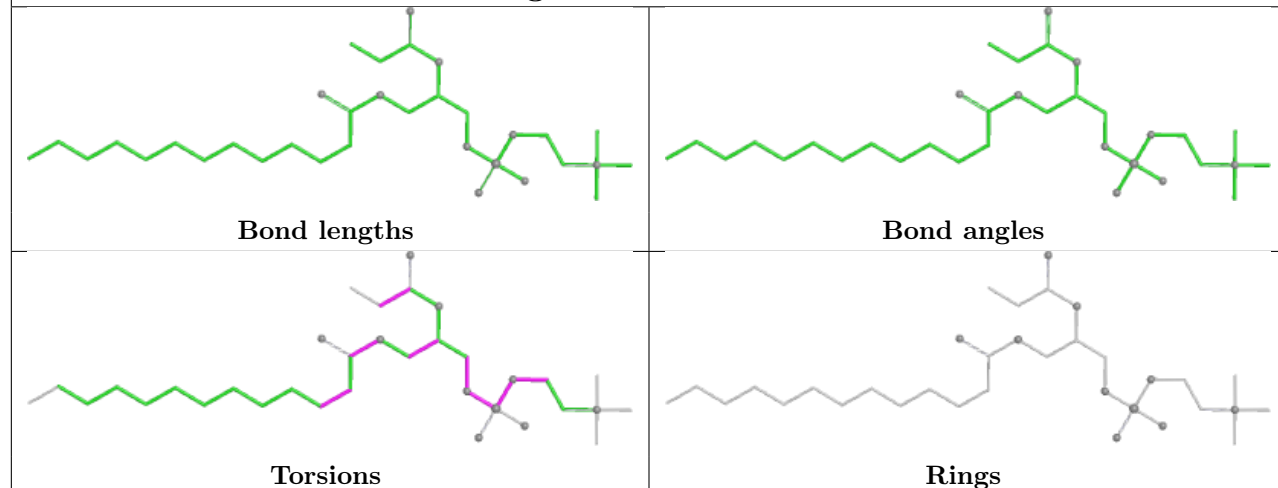


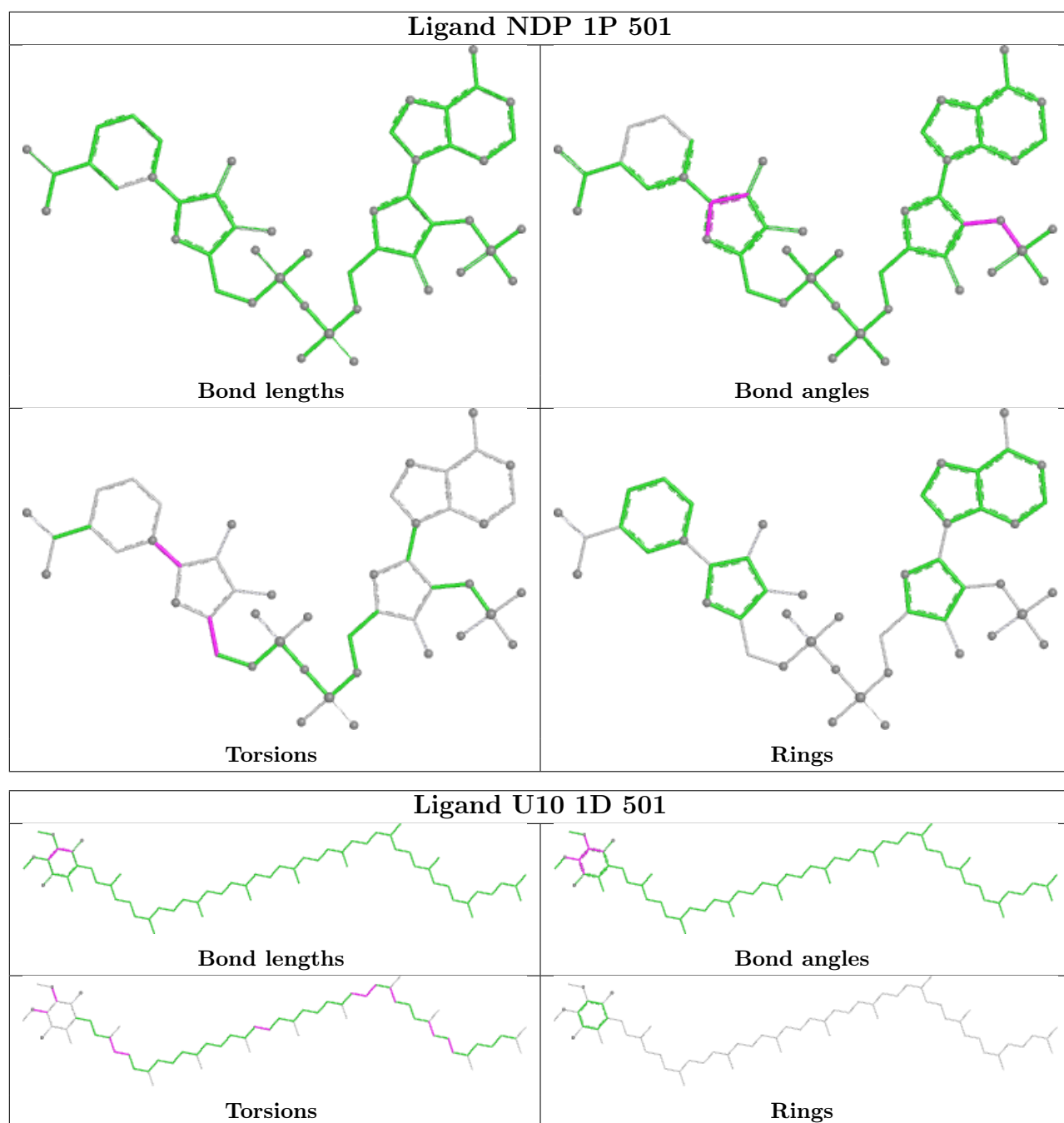


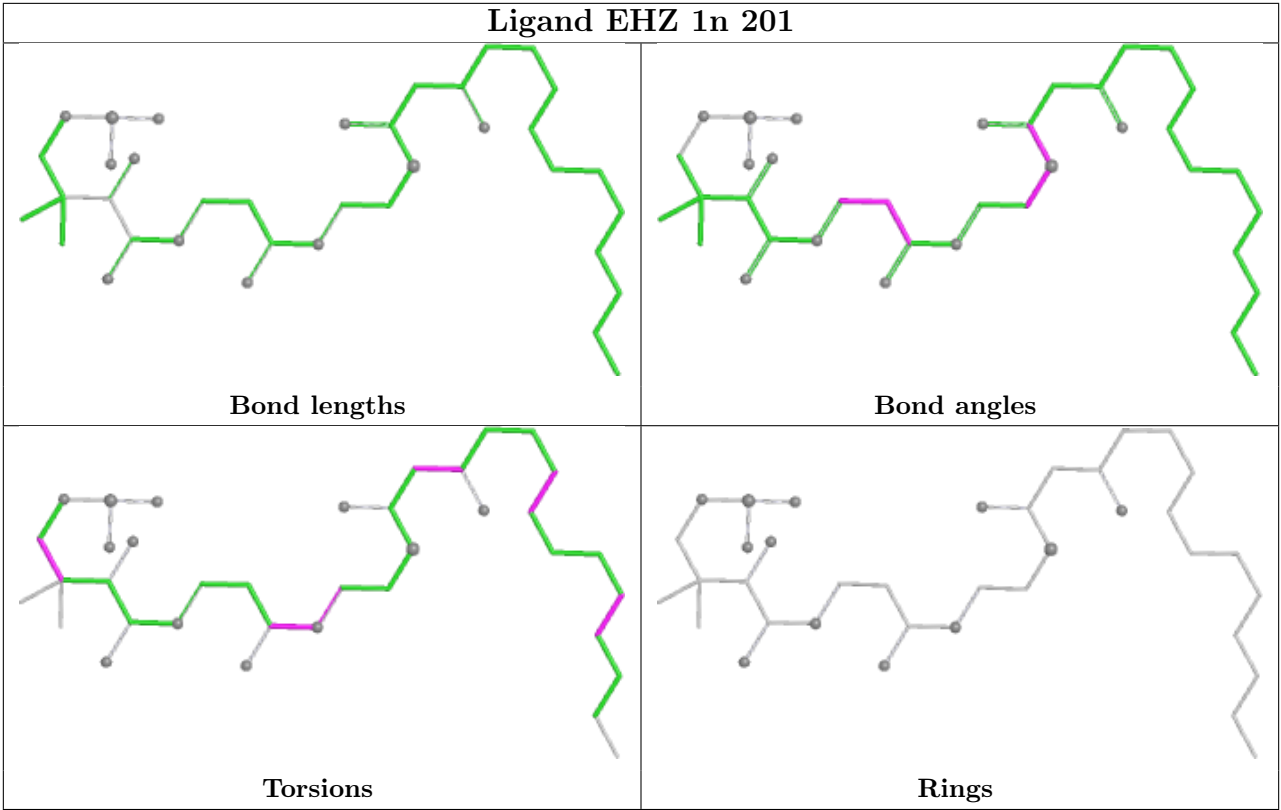
Ligand FMN 1F 501



Ligand PC1 1B 202







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	9.77
1	1i	1:SAC	C	2:GLY	N	3.19

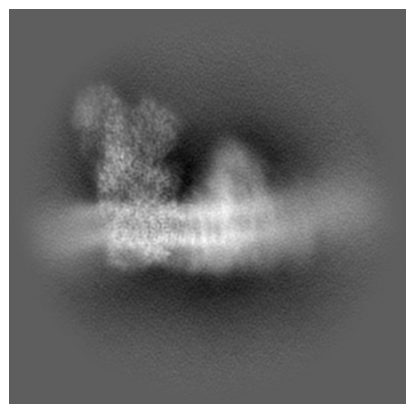
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42167. These allow visual inspection of the internal detail of the map and identification of artifacts.

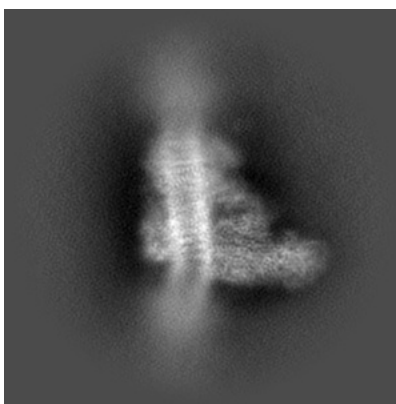
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

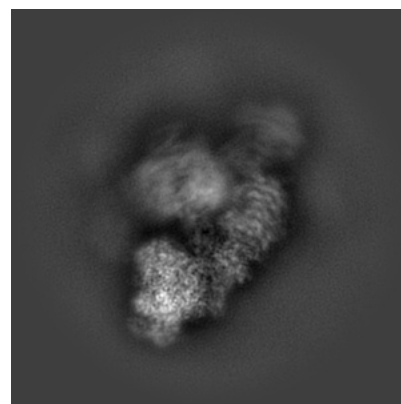
6.1.1 Primary map



X

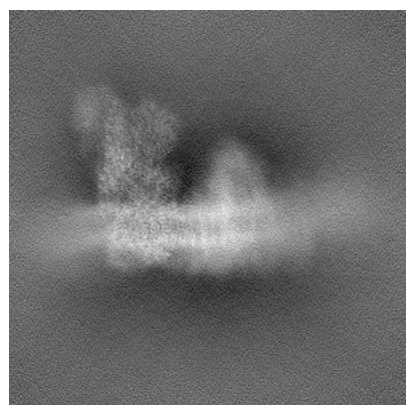


Y

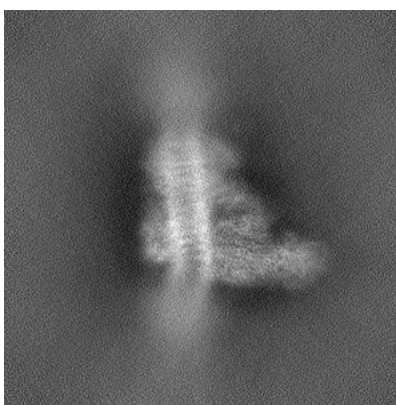


Z

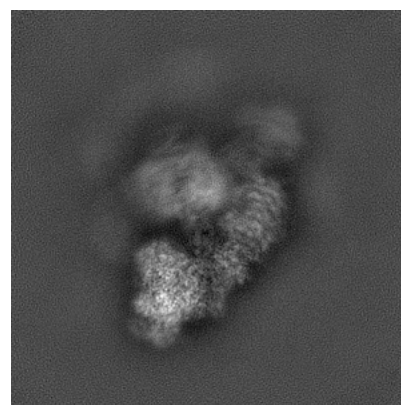
6.1.2 Raw map



X



Y

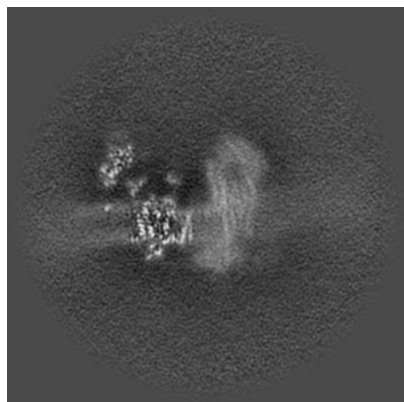


Z

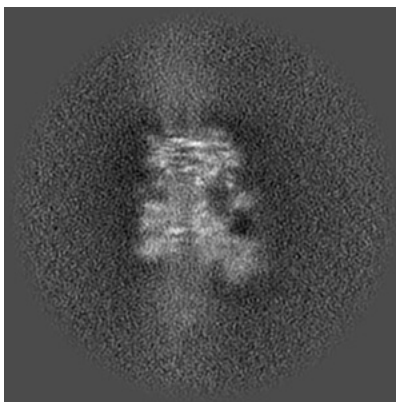
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

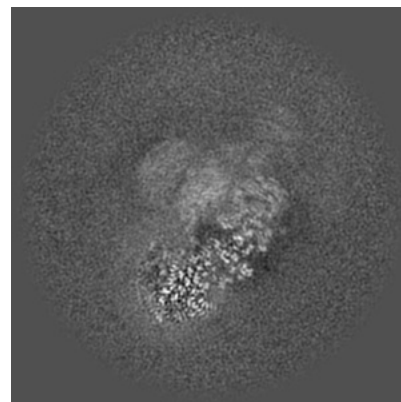
6.2.1 Primary map



X Index: 160

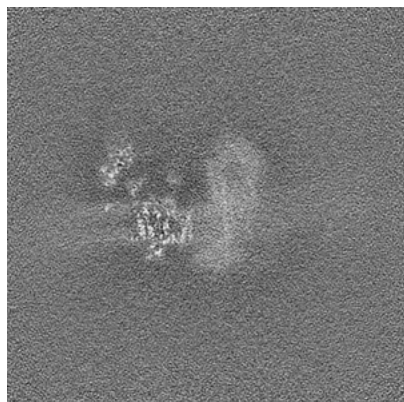


Y Index: 160

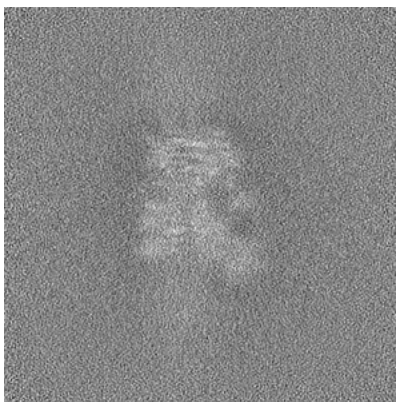


Z Index: 160

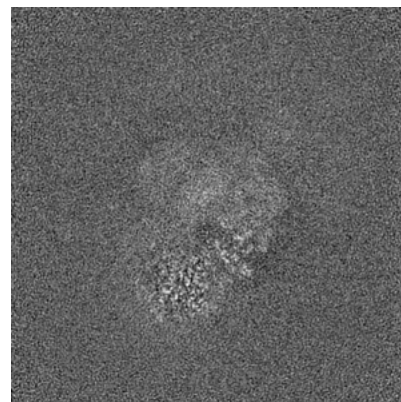
6.2.2 Raw map



X Index: 160



Y Index: 160

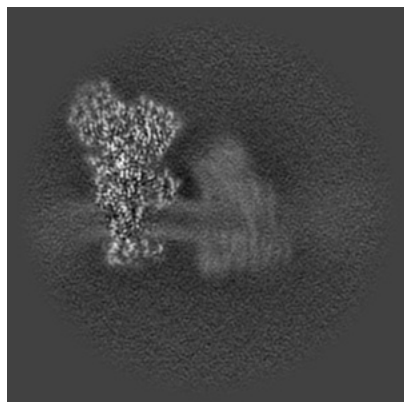


Z Index: 160

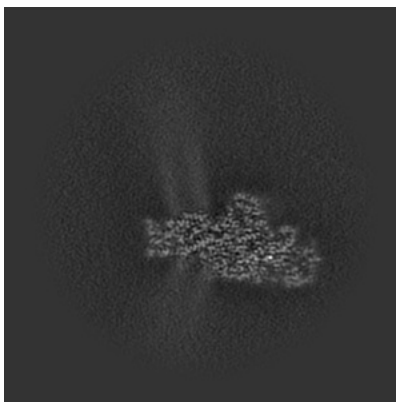
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

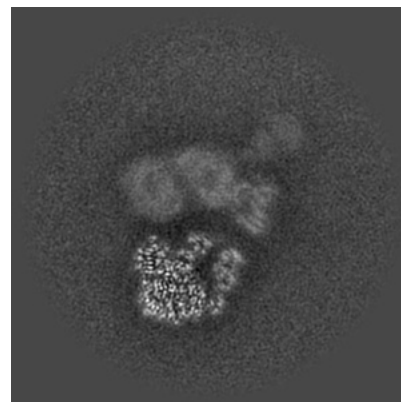
6.3.1 Primary map



X Index: 123

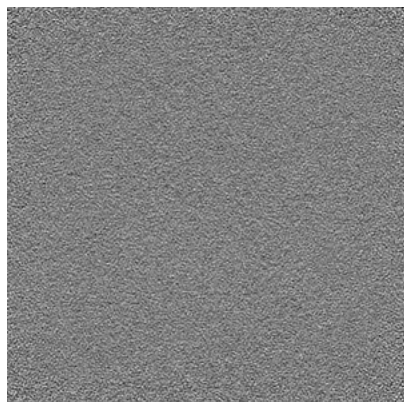


Y Index: 86

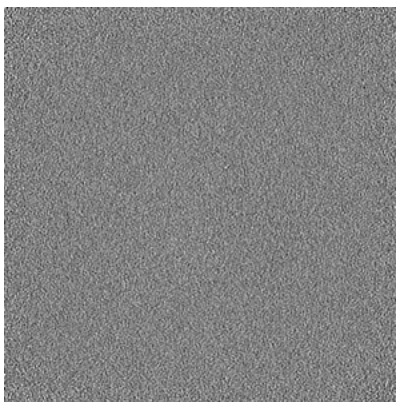


Z Index: 184

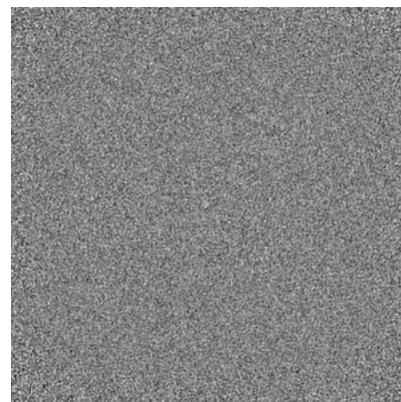
6.3.2 Raw map



X Index: 0



Y Index: 0

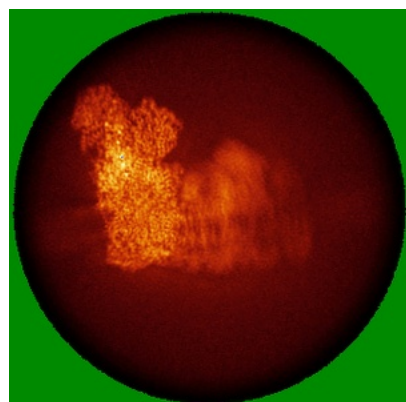


Z Index: 0

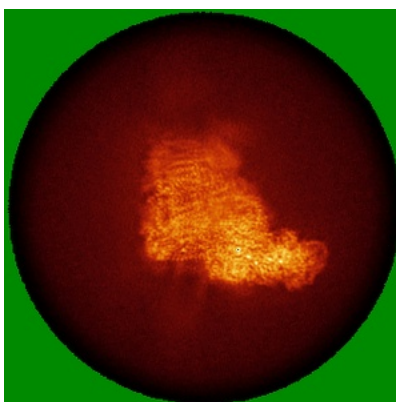
The images above show the largest variance slices of the map in three orthogonal directions.

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

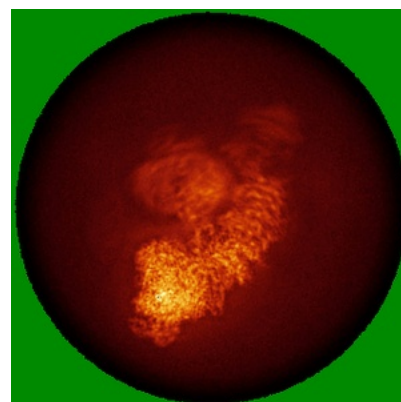
6.4.1 Primary map



X

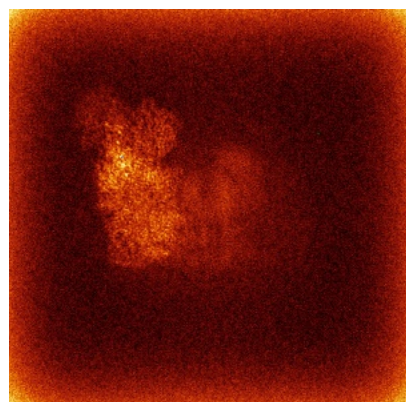


Y

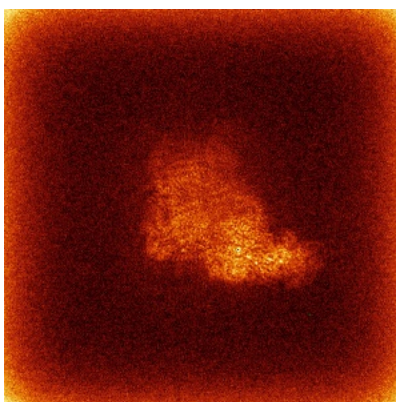


Z

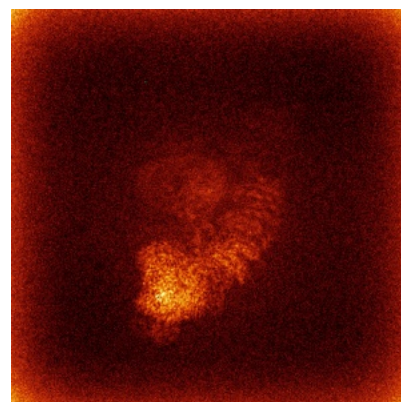
6.4.2 Raw map



X



Y

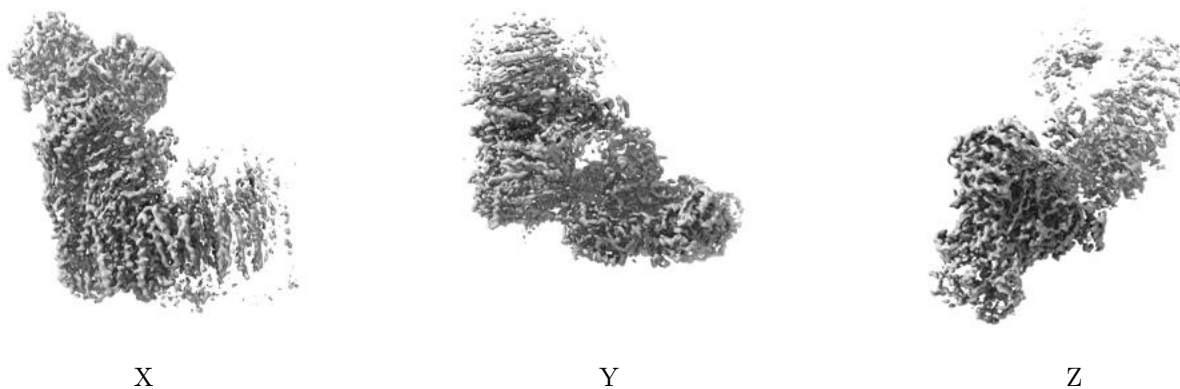


Z

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.

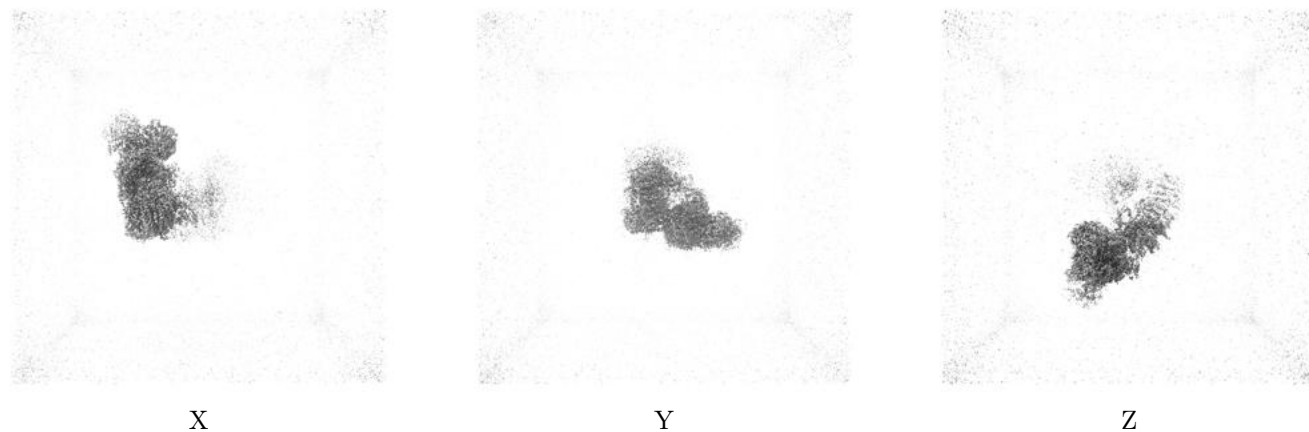
6.5 Orthogonal surface views [i](#)

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.

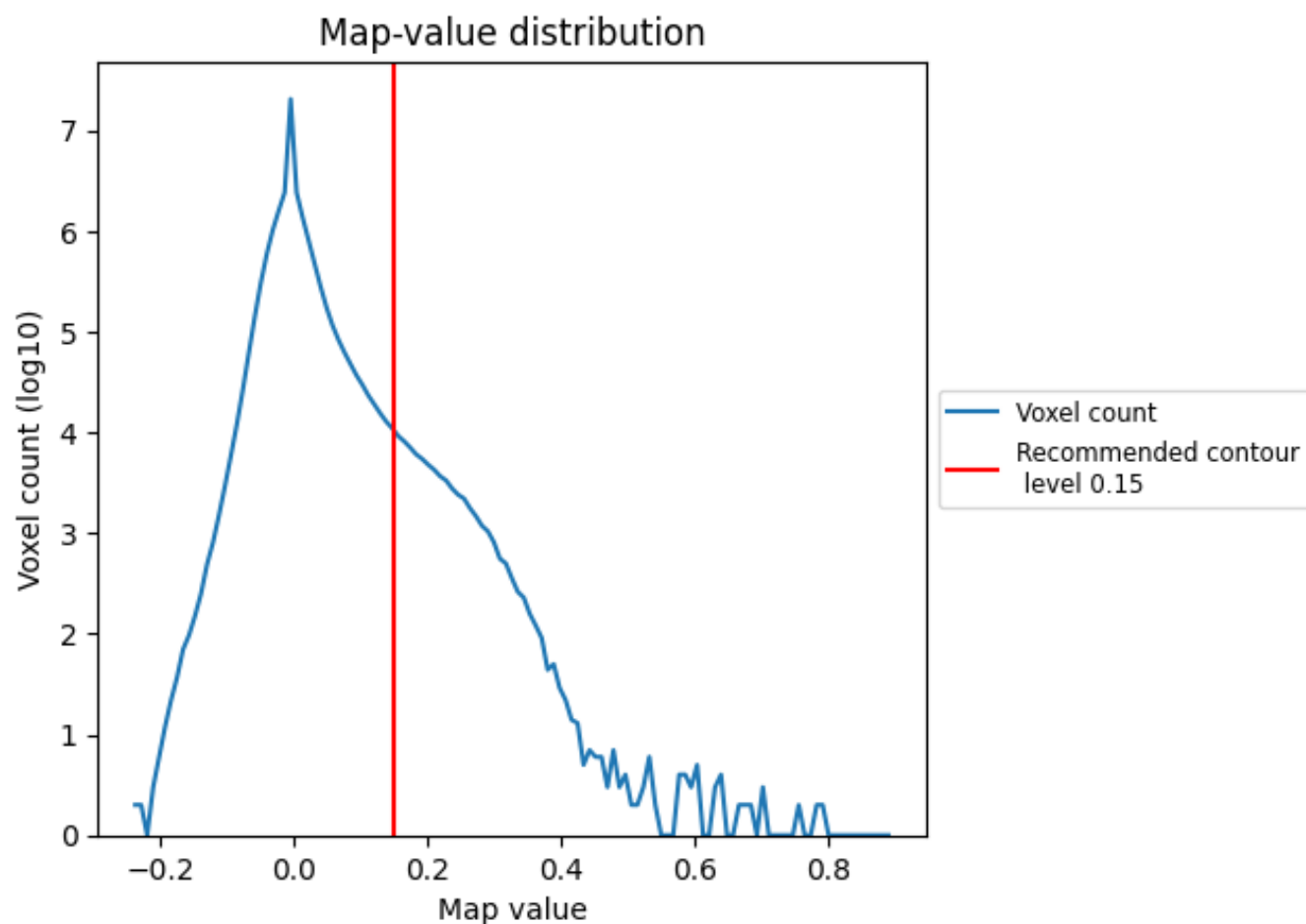
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

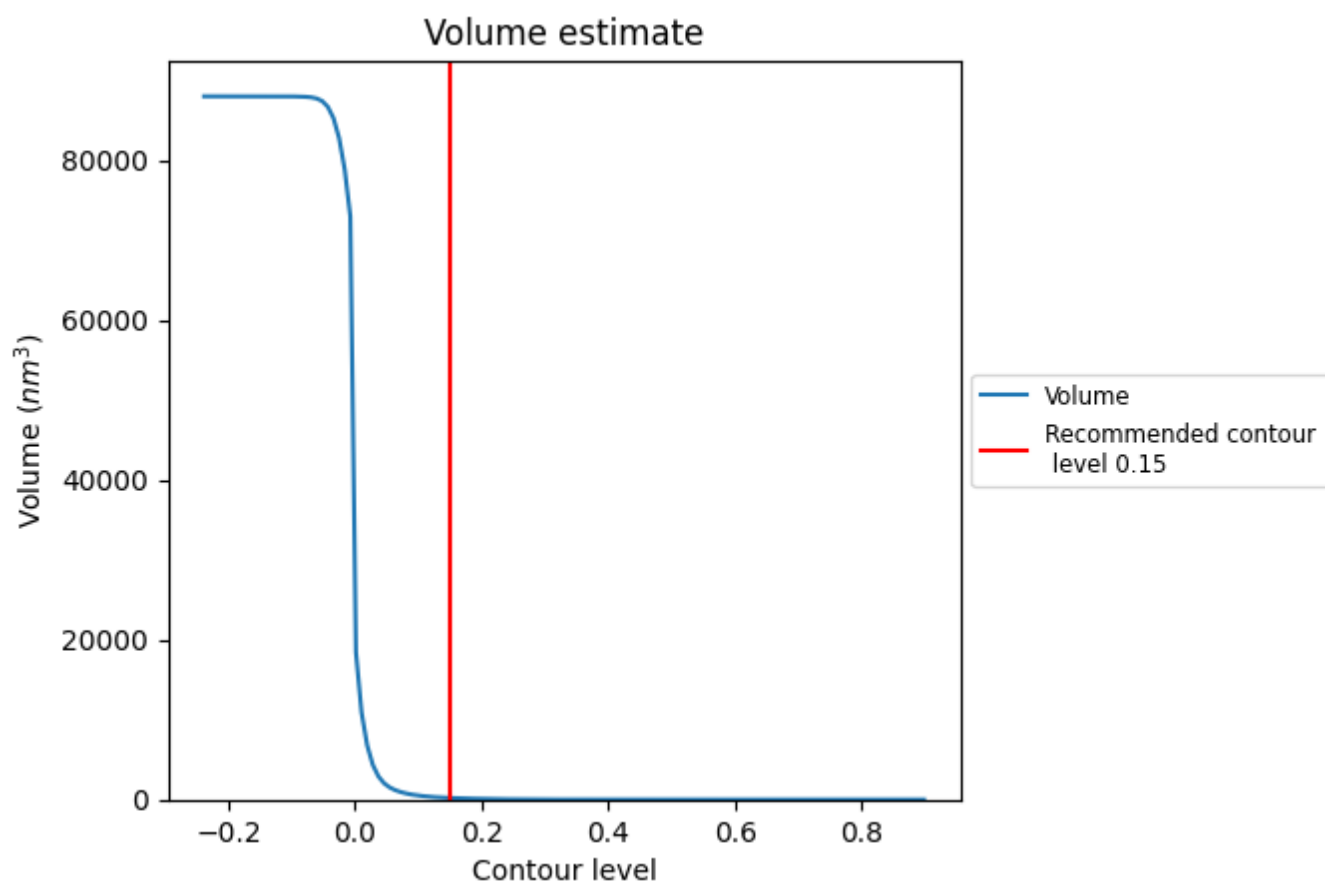
This section contains the results of statistical analysis of the map.

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.

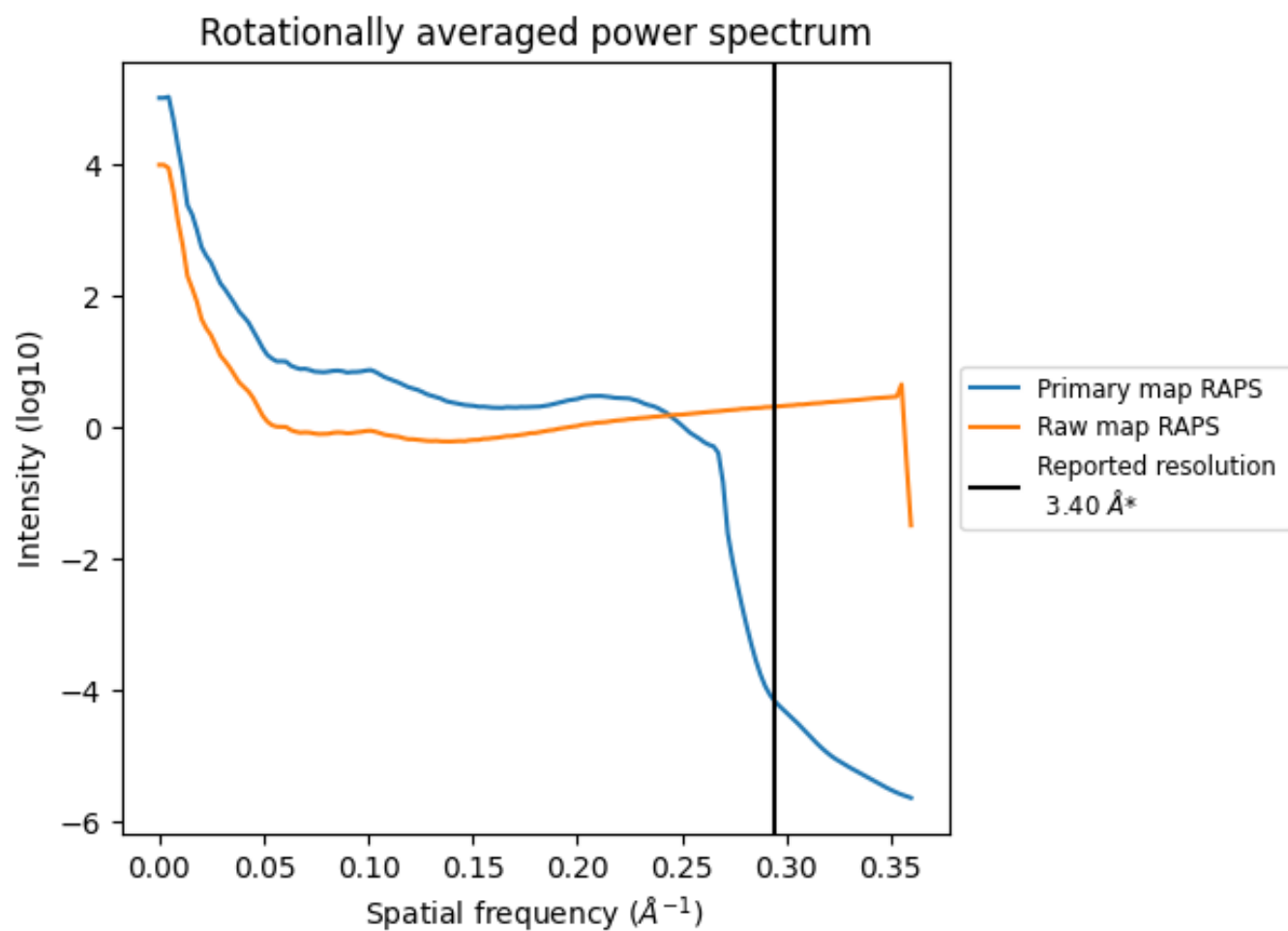
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 203 nm³; this corresponds to an approximate mass of 183 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 ⓘ

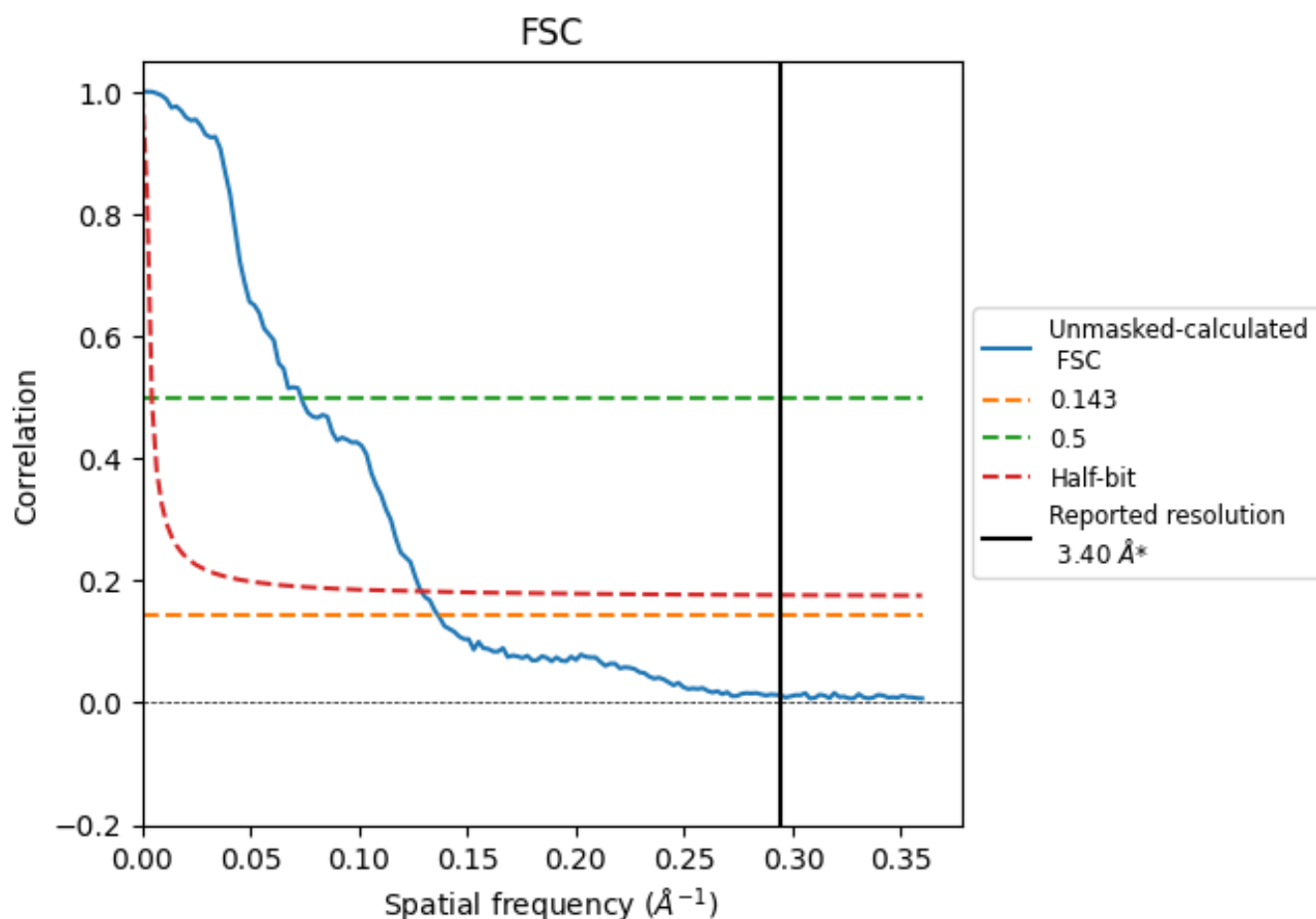


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

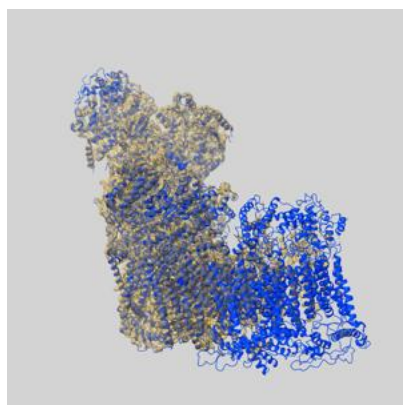
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.33	13.64	7.76

*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 7.33 differs from the reported value 3.4 by more than 10 %

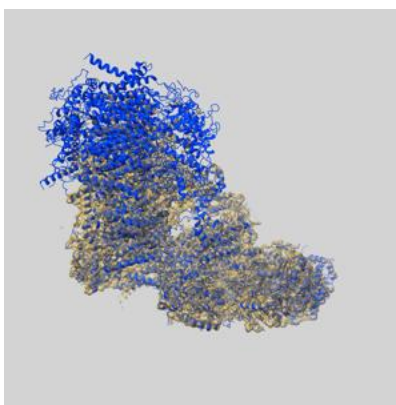
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-42167 and PDB model 8UEQ. Per-residue inclusion information can be found in section [3](#) on page [20](#).

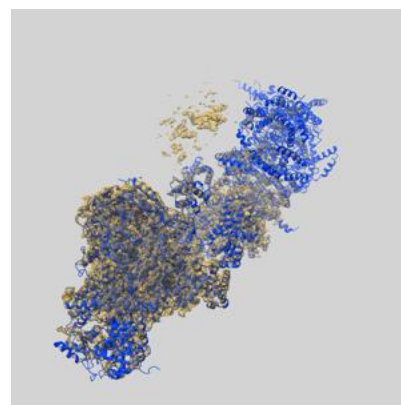
9.1 Map-model overlay [i](#)



X



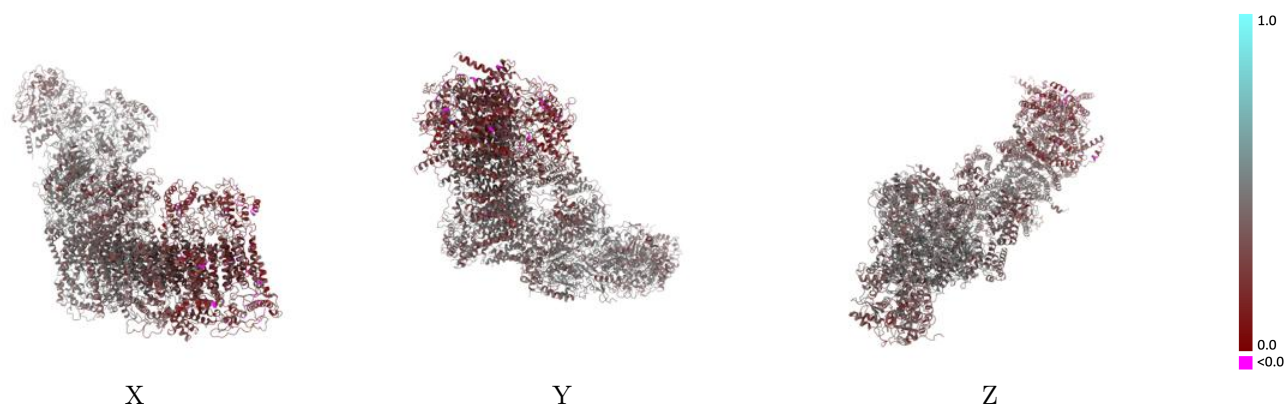
Y



Z

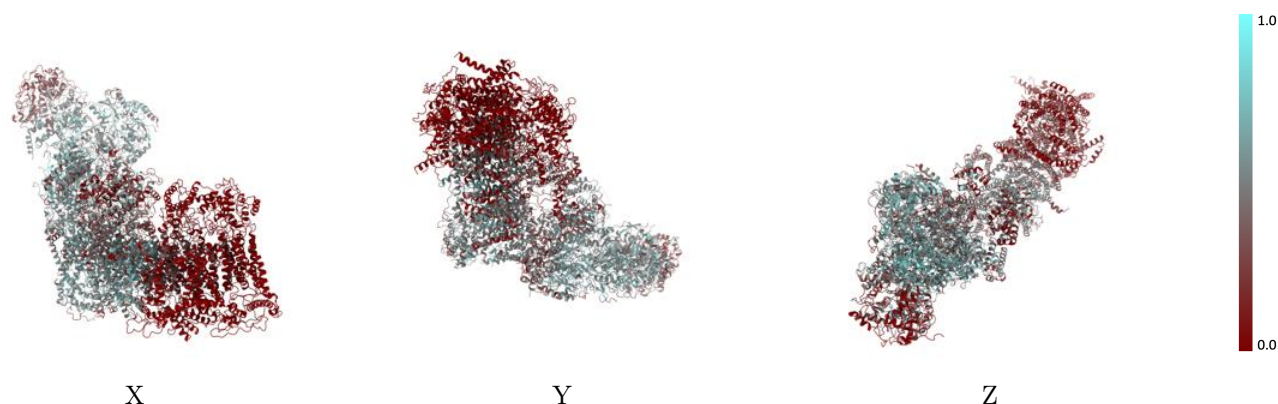
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



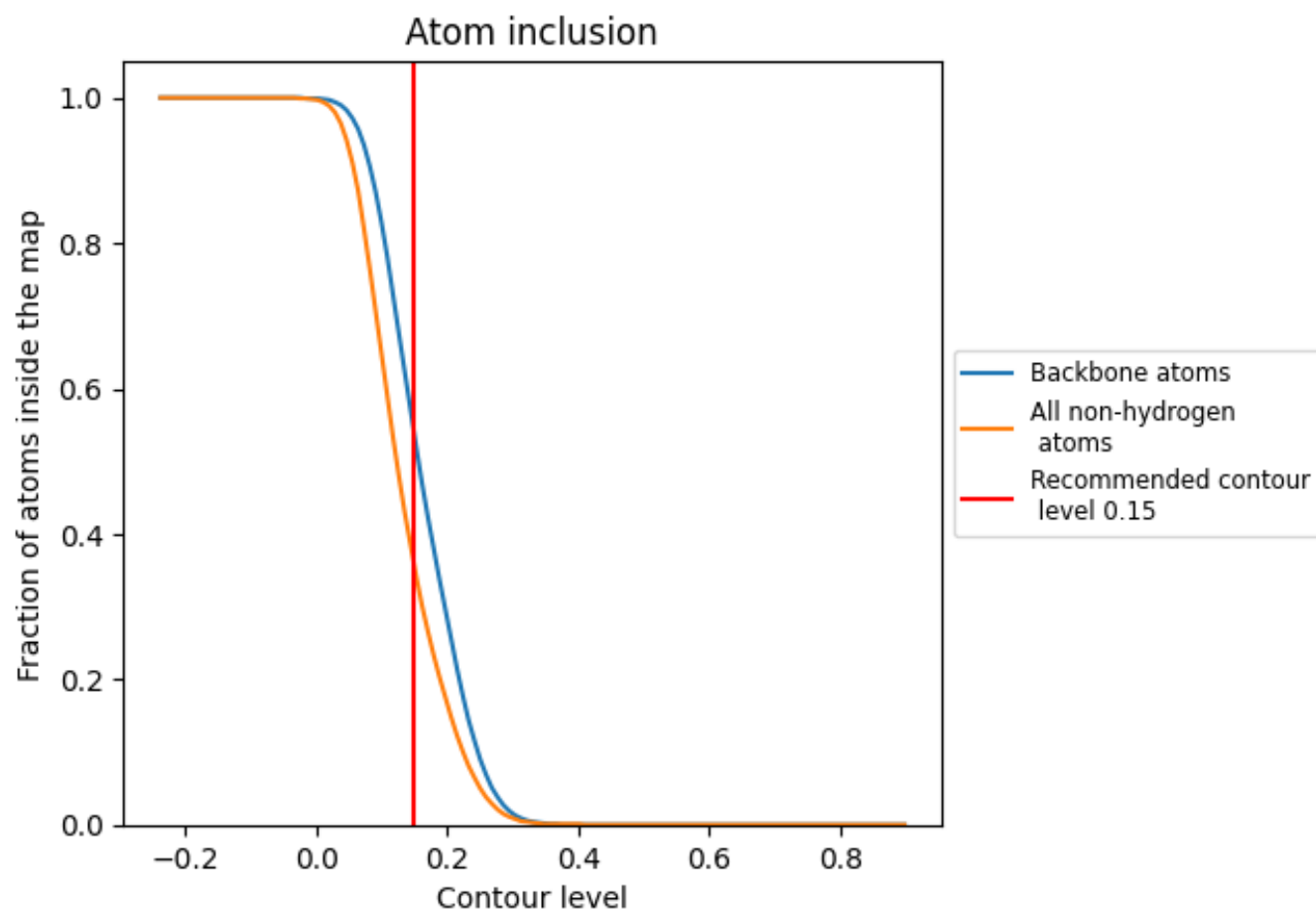
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 35% 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	 0.3540	 0.3660
1A	 0.3730	 0.3490
1B	 0.5570	 0.4360
1C	 0.5160	 0.4470
1D	 0.5310	 0.4200
1E	 0.2900	 0.3700
1F	 0.3130	 0.3700
1G	 0.5490	 0.4250
1H	 0.5340	 0.4130
1I	 0.6600	 0.4360
1J	 0.3670	 0.3700
1K	 0.4530	 0.3930
1L	 0.0860	 0.2640
1M	 0.3200	 0.3550
1N	 0.5210	 0.4200
1O	 0.2810	 0.3560
1P	 0.4190	 0.4130
1Q	 0.4350	 0.4370
1R	 0.4940	 0.4280
1S	 0.5020	 0.3930
1T	 0.2020	 0.3220
1U	 0.0020	 0.2440
1V	 0.4310	 0.3990
1W	 0.4090	 0.3910
1X	 0.4860	 0.3970
1Y	 0.2720	 0.3290
1Z	 0.5460	 0.4150
1a	 0.5650	 0.4070
1b	 0.4610	 0.4110
1c	 0.3420	 0.3590
1d	 0.4500	 0.4020
1e	 0.5160	 0.4190
1f	 0.2370	 0.3460
1g	 0.1060	 0.3090
1h	 0.2390	 0.3490



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Chain	Atom inclusion	Q-score
1i	 0.0060	 0.2390
1j	 0.0020	 0.2440
1k	 0.0020	 0.1830
1l	 0.0560	 0.2550
1m	 0.1060	 0.2740
1n	 0.0210	 0.2250
1o	 0.0040	 0.2250
1p	 0.0360	 0.2900
1q	 0.5810	 0.4250
1r	 0.5630	 0.4430
1s	 0.1560	 0.3570