



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 12:40 PM UTC

PDB ID : 8UEV / pdb_00008uev
EMDB ID : EMD-42172
Title : In-situ complex I, Deactive class04
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.70 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:

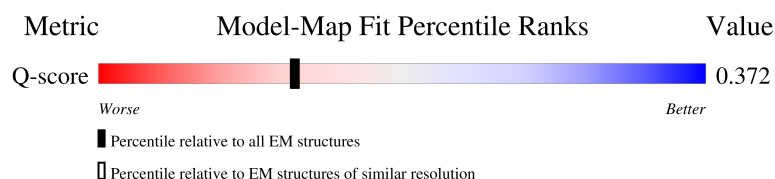
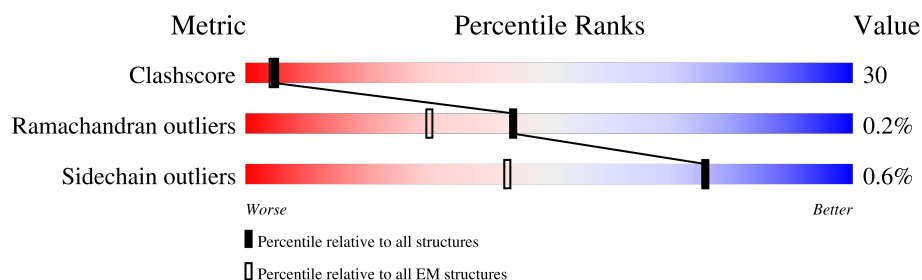
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.49

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 3.70 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	11569 (3.20 - 4.20)

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
46	SF4	1F	502	-	-	X	-
47	FES	1E	301	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67103 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1A	88	Total	C	N	O	S	0	0
			707	484	101	117	5		

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

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

- 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	297	Total	C	N	O	S	0	0
			2344	1571	363	389	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		
			1062	691	182	189	0	0

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

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

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

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

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

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

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

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

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

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

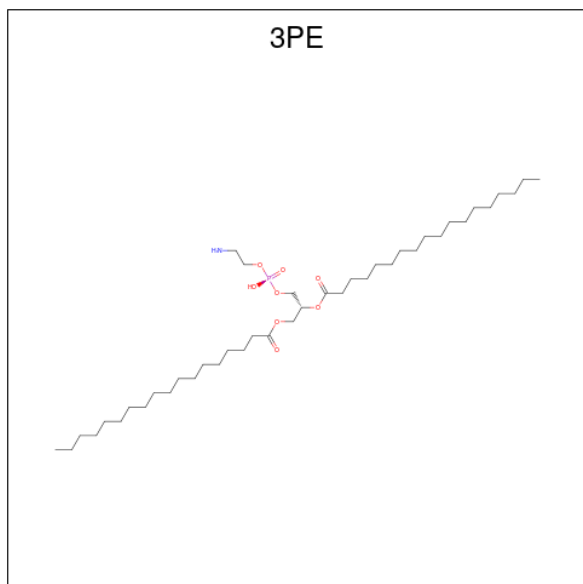
There is a discrepancy between the modelled and reference sequences:

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

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

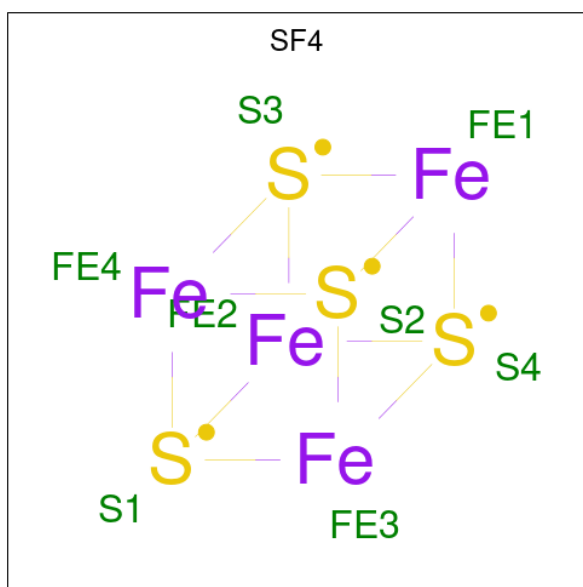
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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



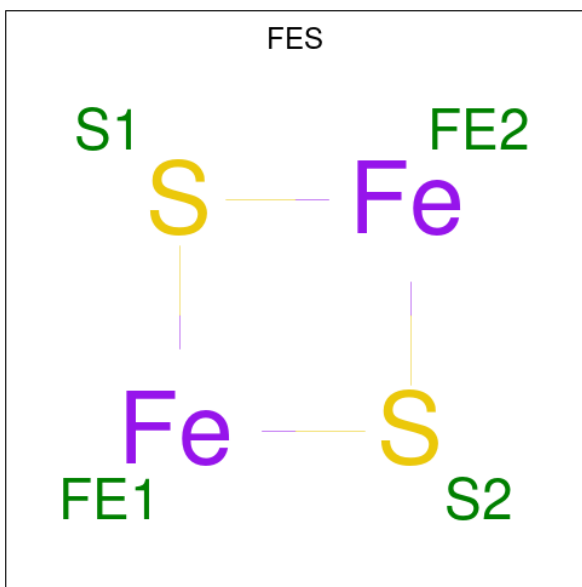
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



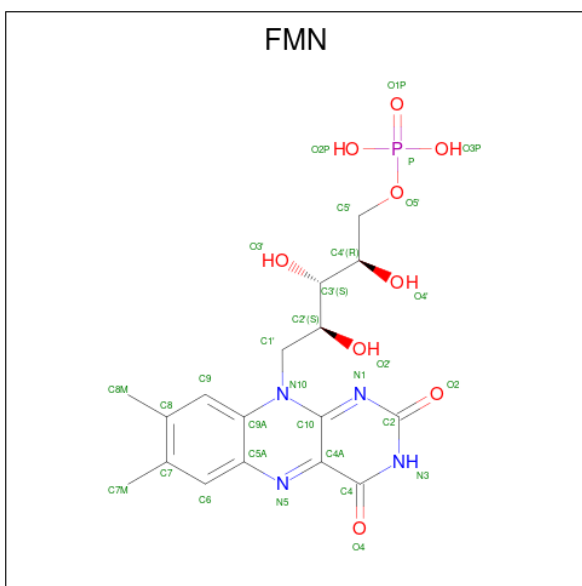
Mol	Chain	Residues	Atoms			AltConf
46	1B	1	Total	Fe	S	0
			8	4	4	
46	1F	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	

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



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

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

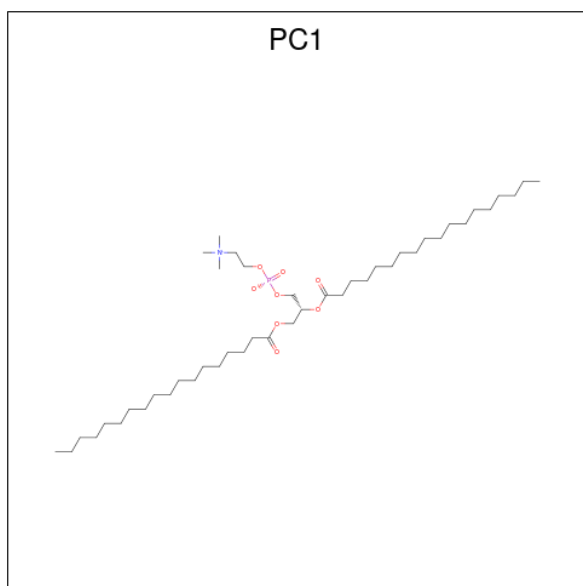


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

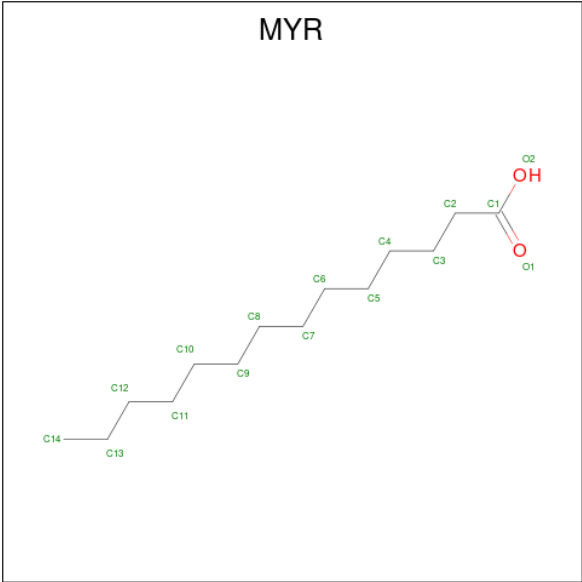
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

- Molecule 50 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



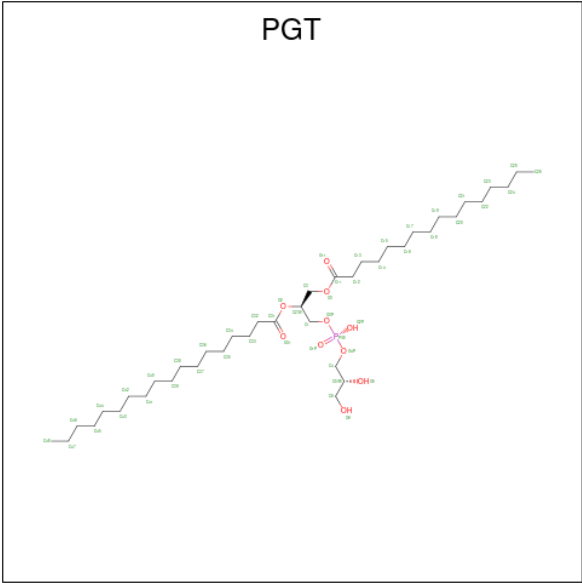
Mol	Chain	Residues	Atoms					AltConf
50	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 51 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



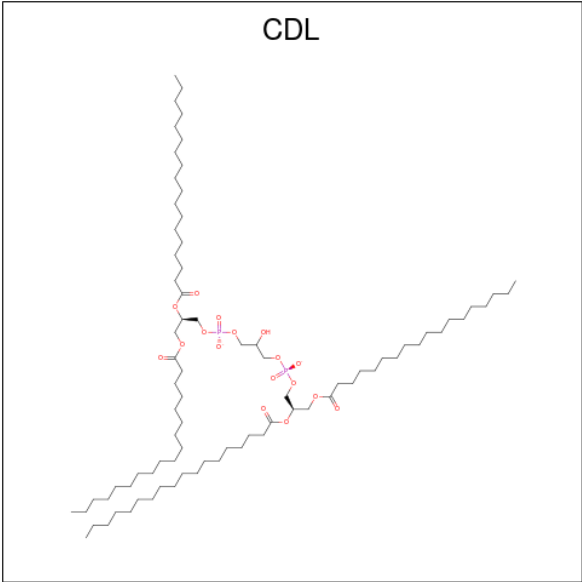
Mol	Chain	Residues	Atoms			AltConf
51	1L	1	Total	C	O	0
			15	14	1	

- Molecule 52 is (1S)-2-{\{[(2R)-2,3-DIHYDROXYPROPYL]OXY\}(HYDROXY)PHOSP HORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).



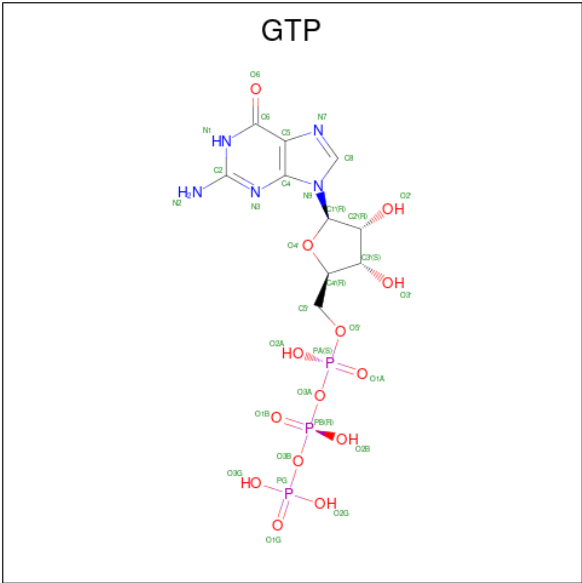
Mol	Chain	Residues	Atoms				AltConf
52	1M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 53 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
53	1N	1	77	58	17	2	0
53	1r	1	61	42	17	2	0

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

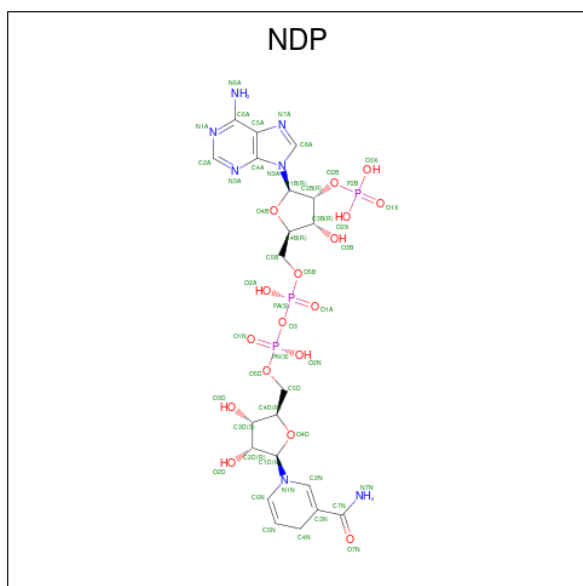


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
54	1O	1	32	10	5	14	3	0

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

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

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

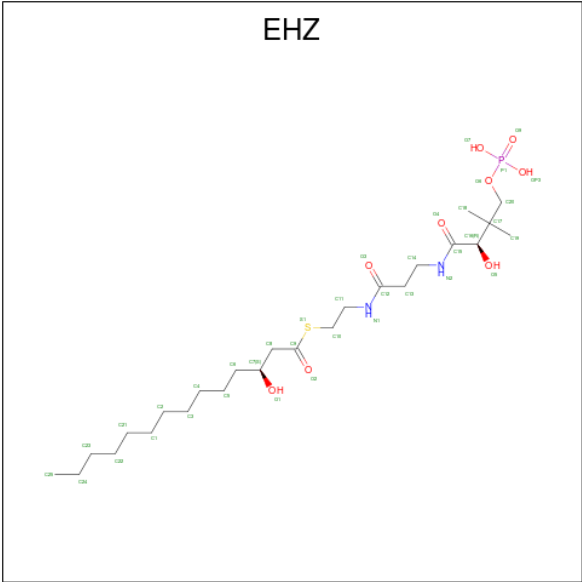


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

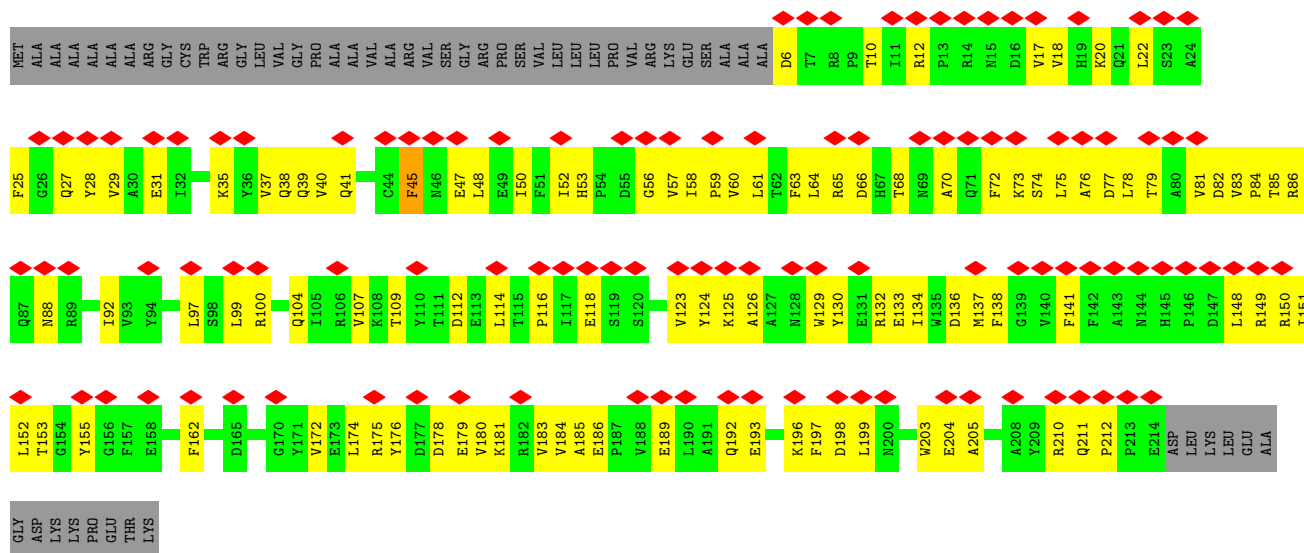
- Molecule 57 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

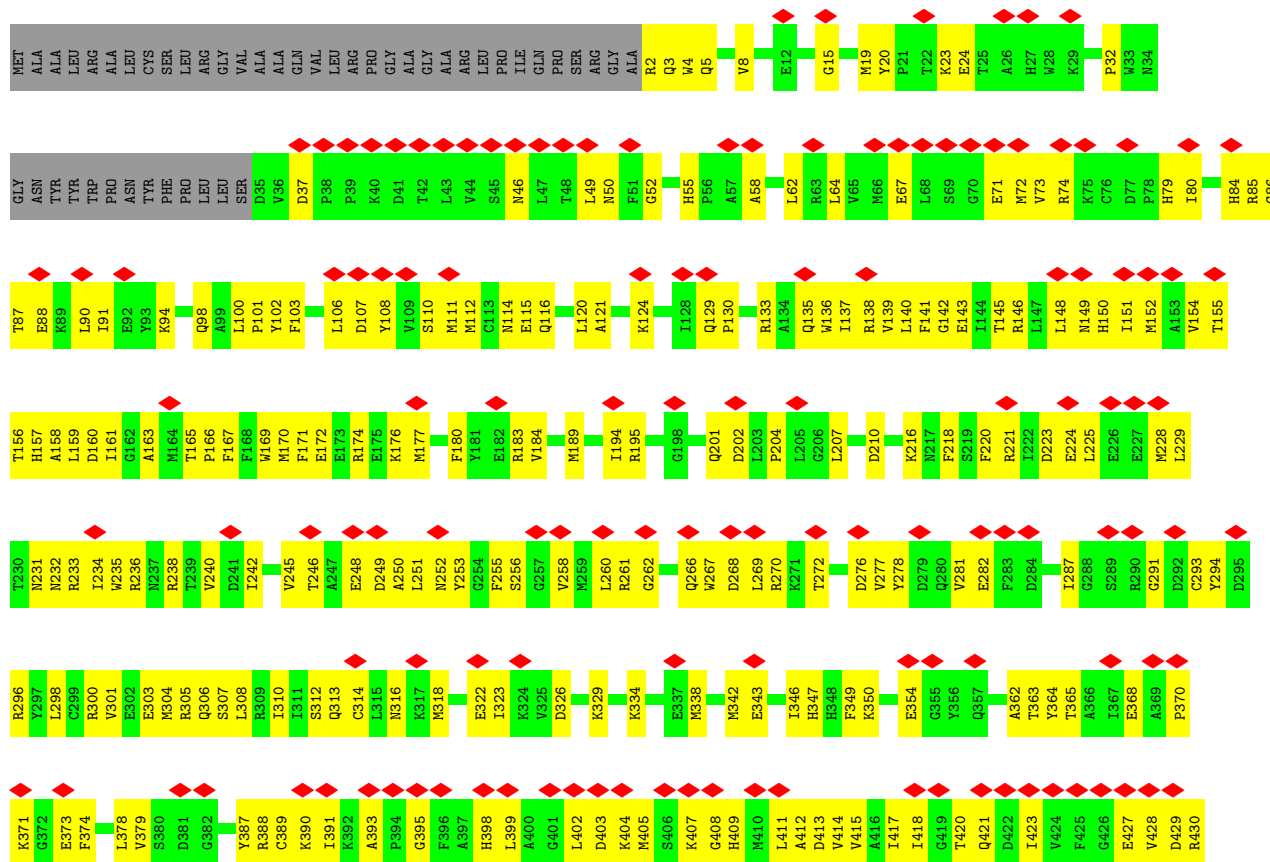
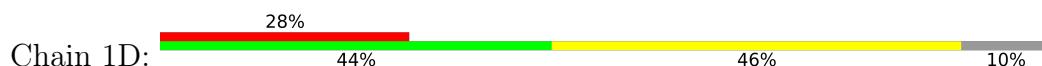
- Molecule 58 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



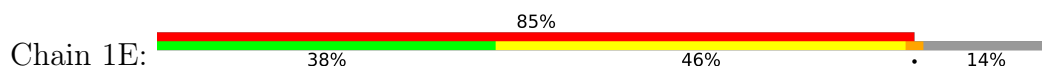
Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	



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

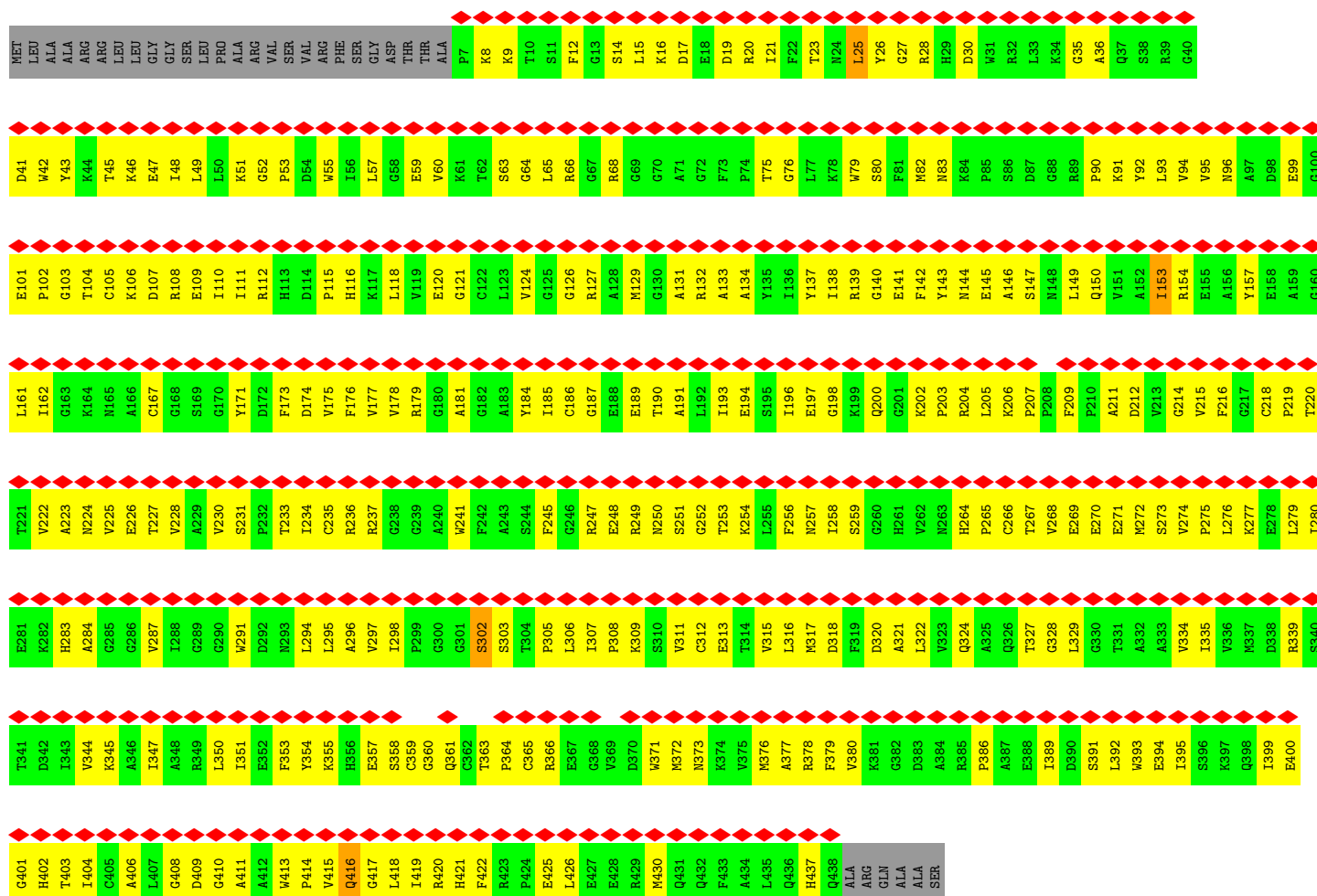


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

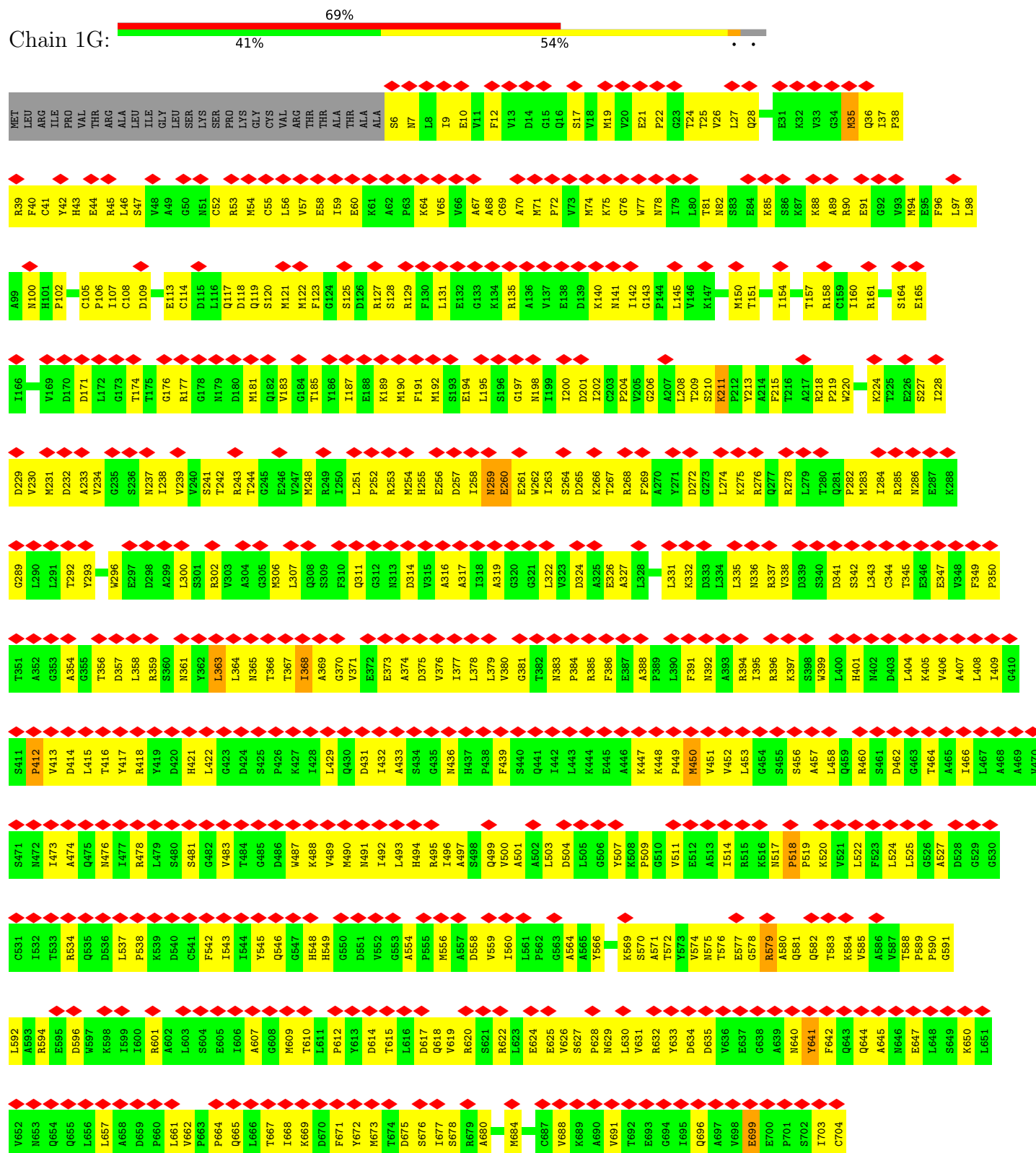




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

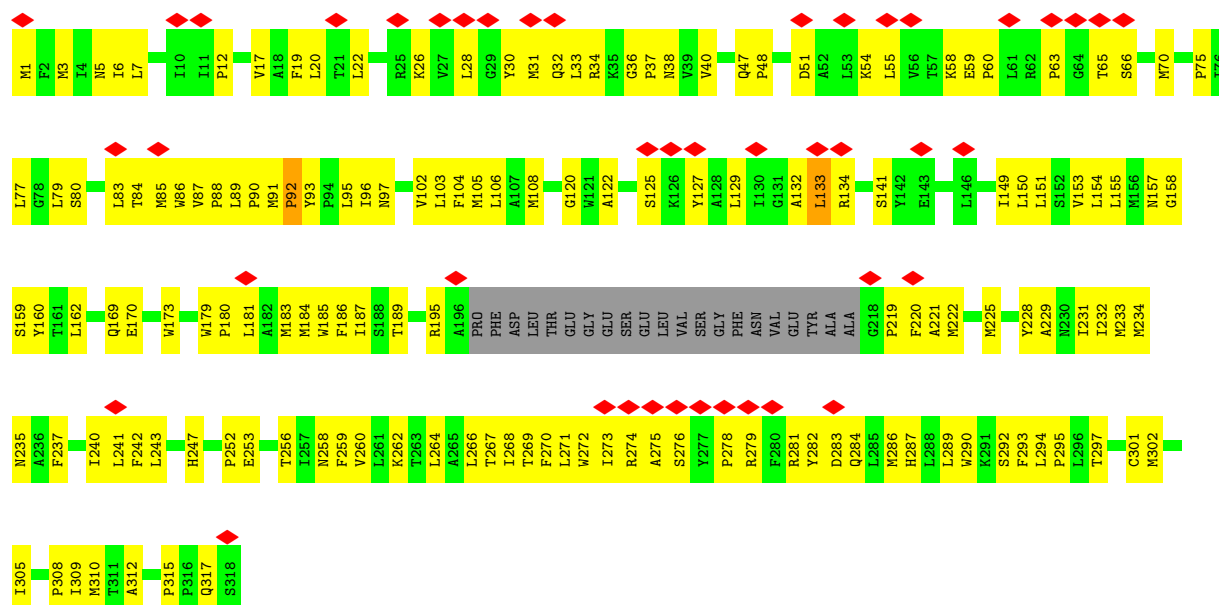


Chain 1G:

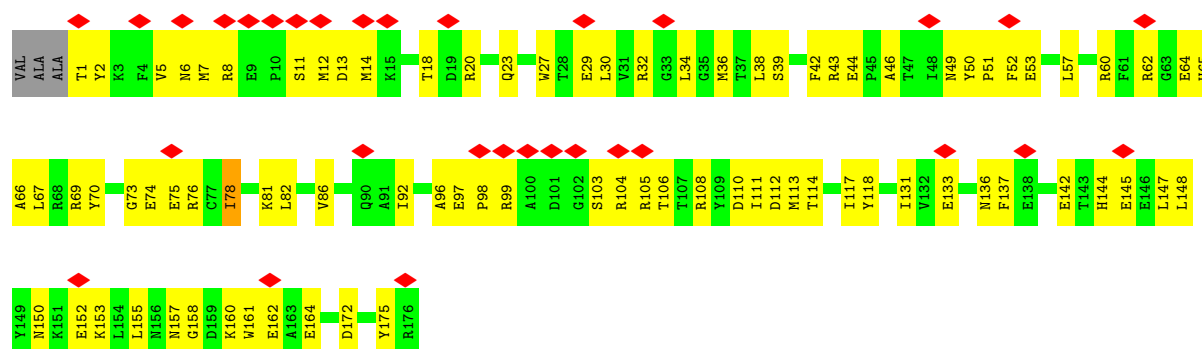
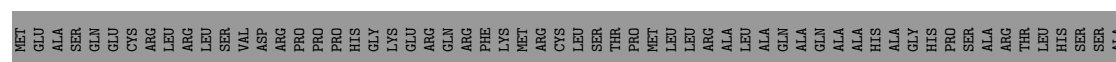


Chain 1H:

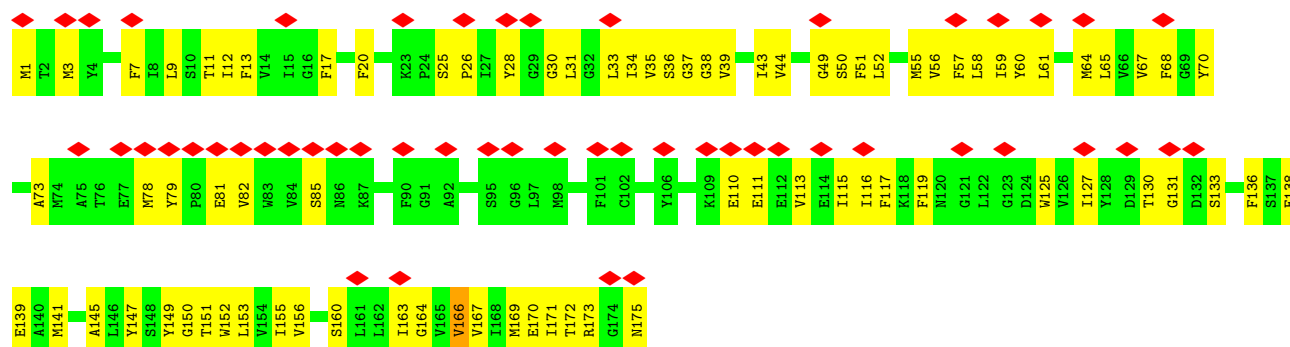




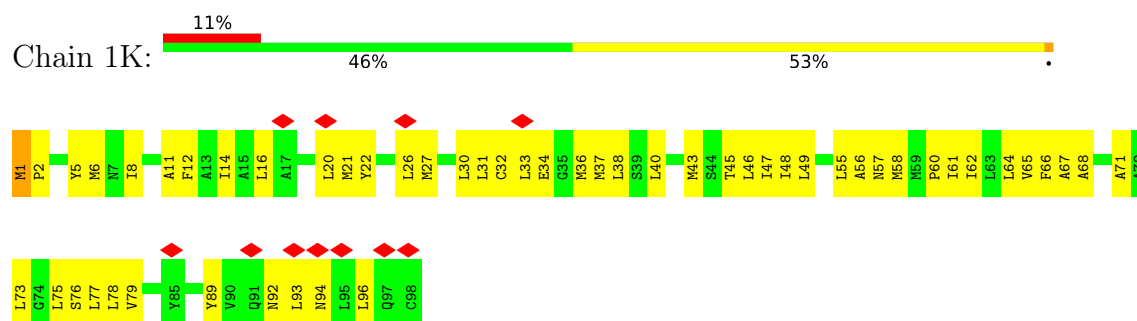
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



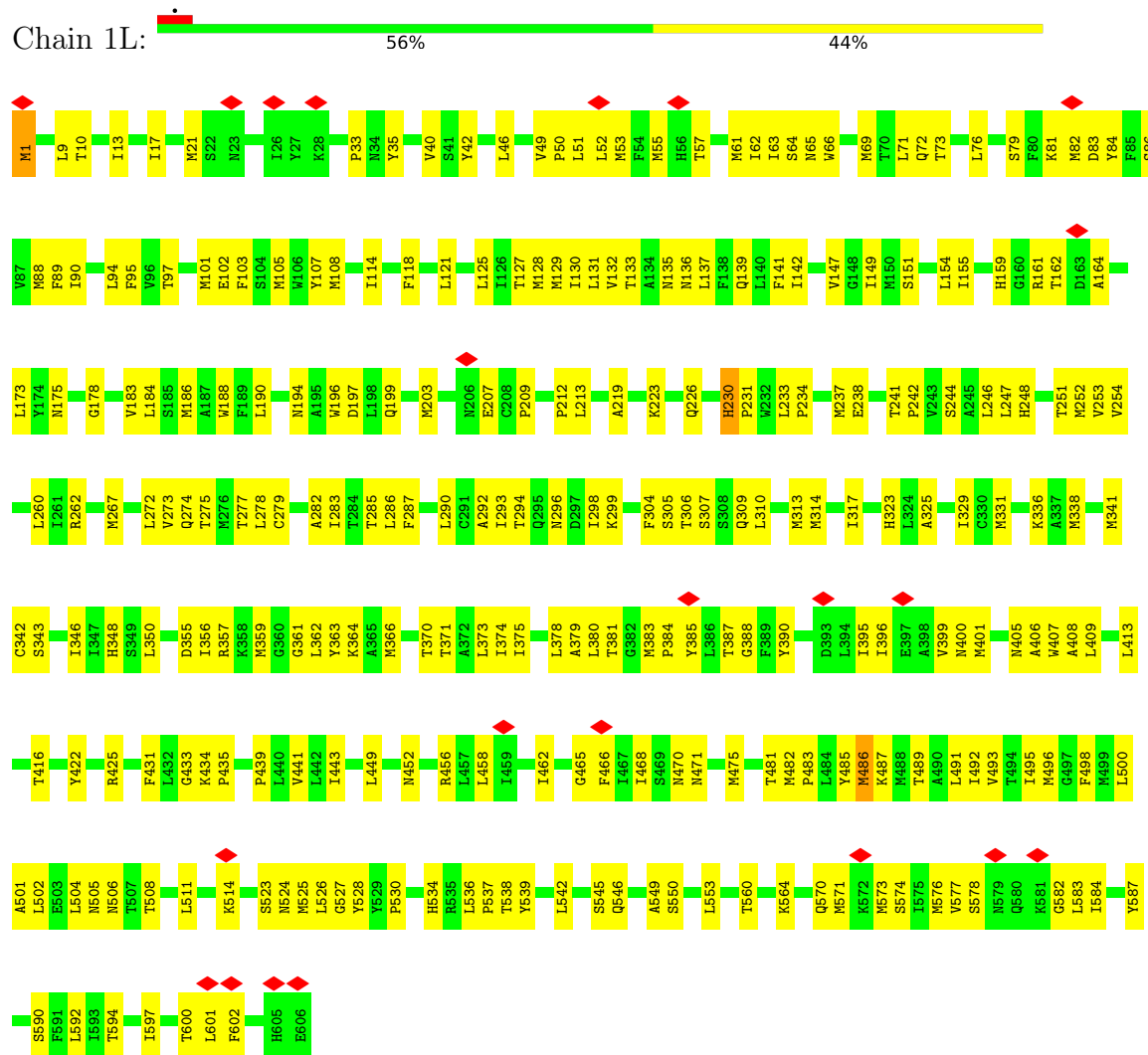
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6



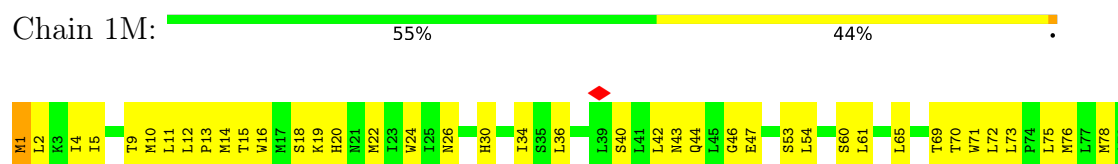
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

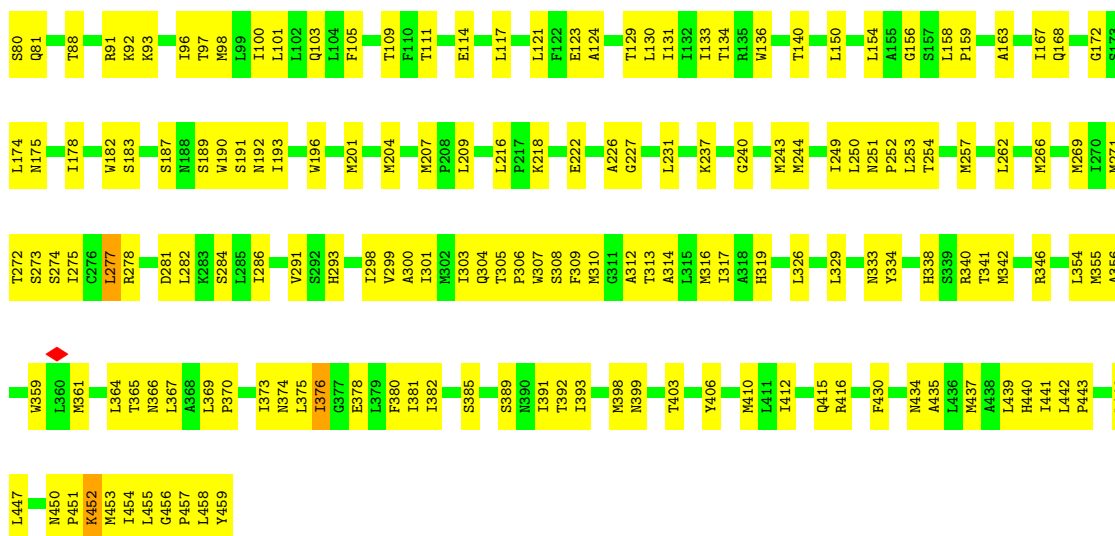


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

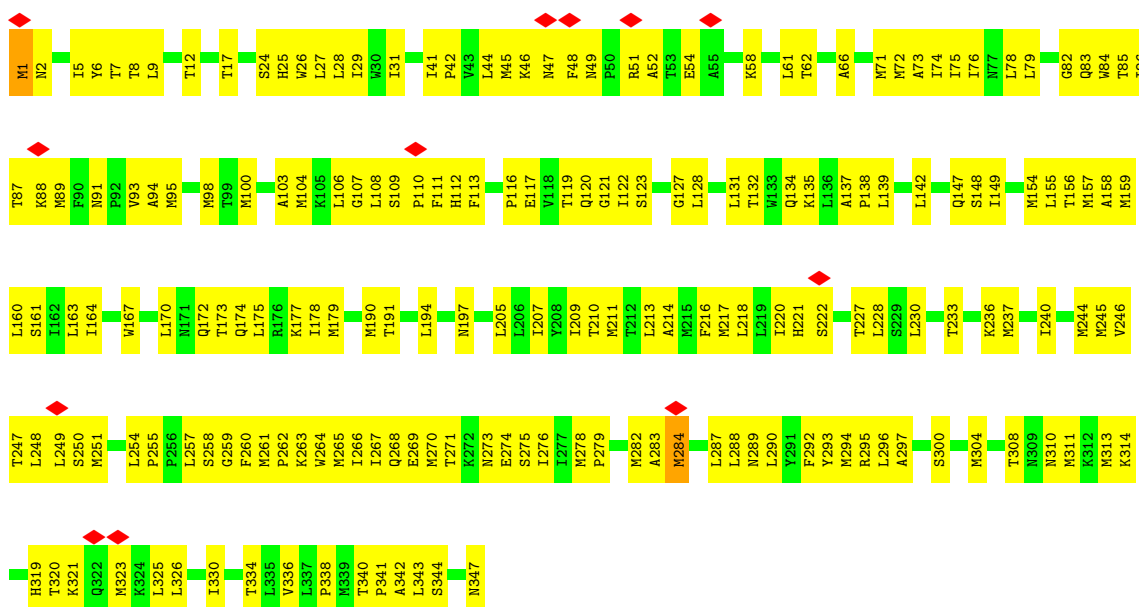


- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

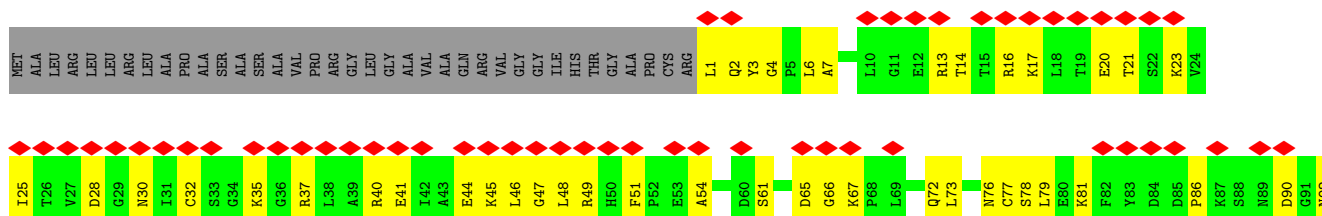


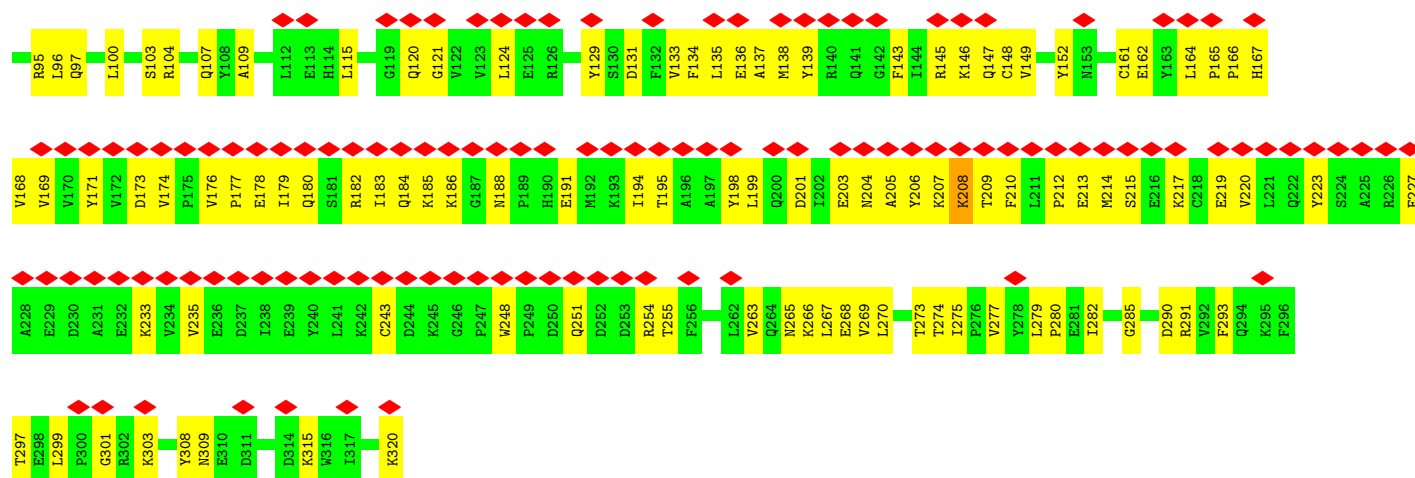


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

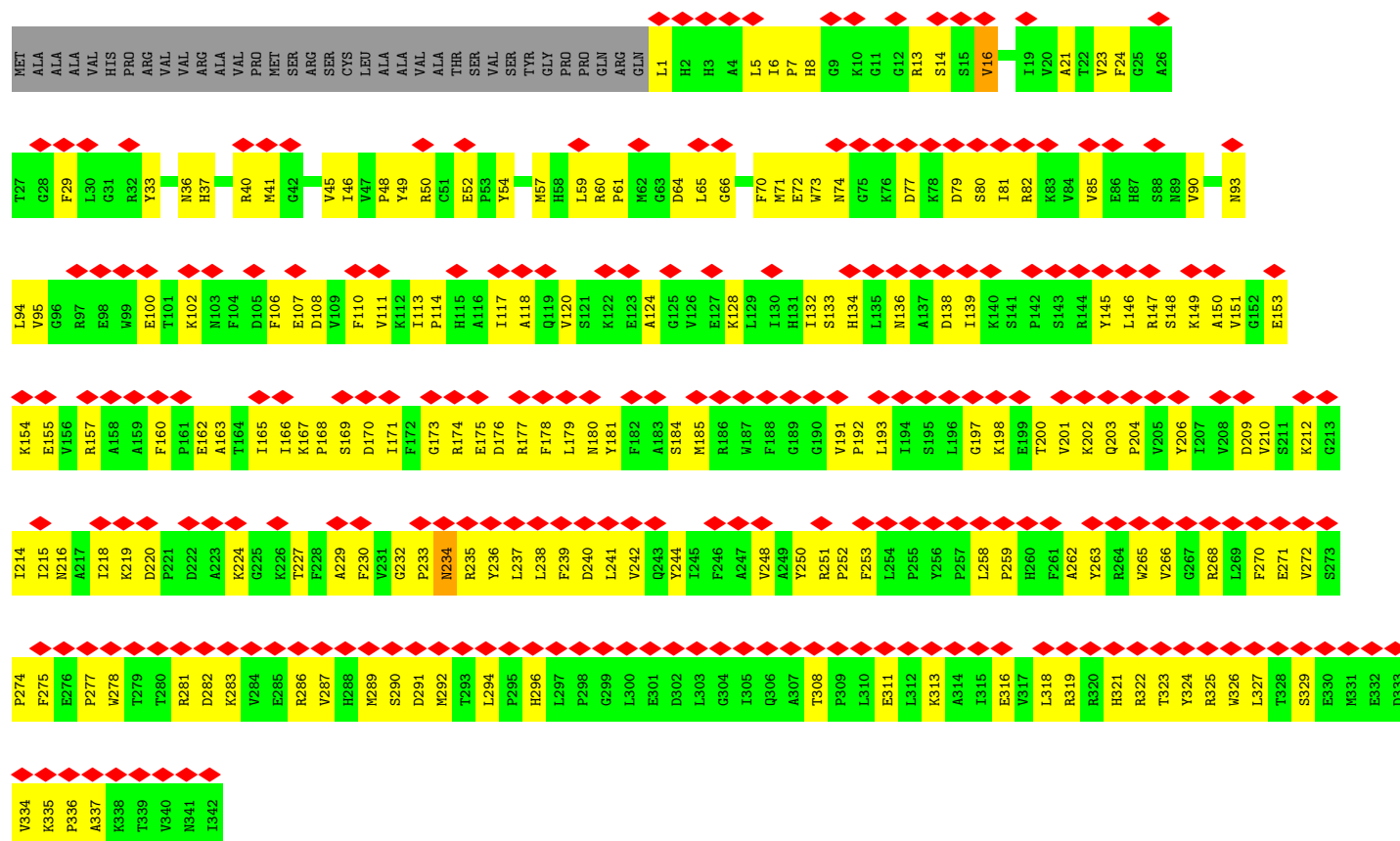


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



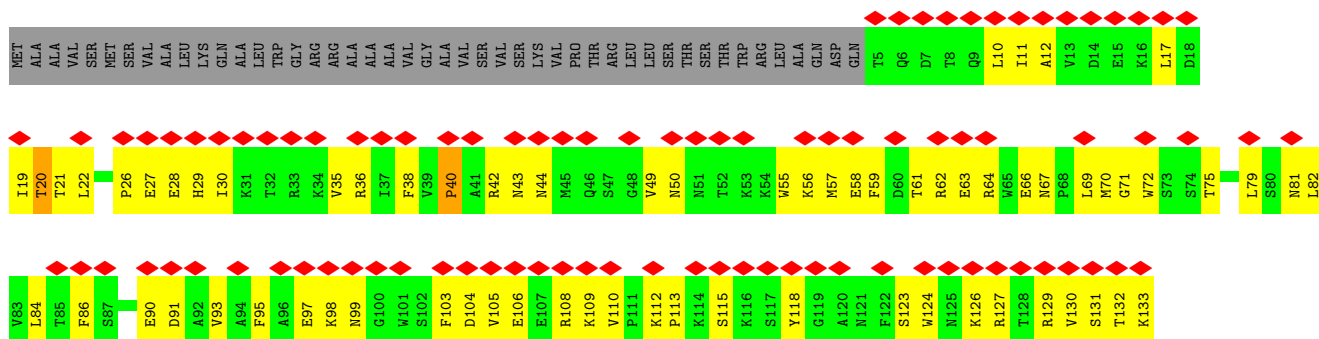


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



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

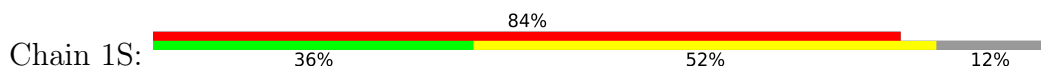




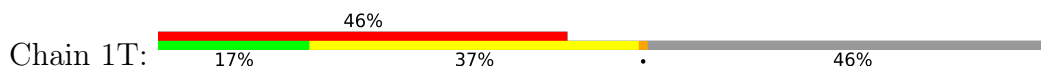
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



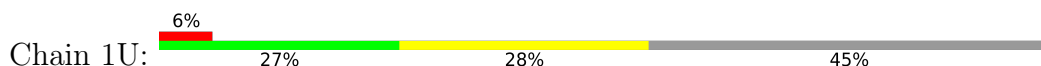
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

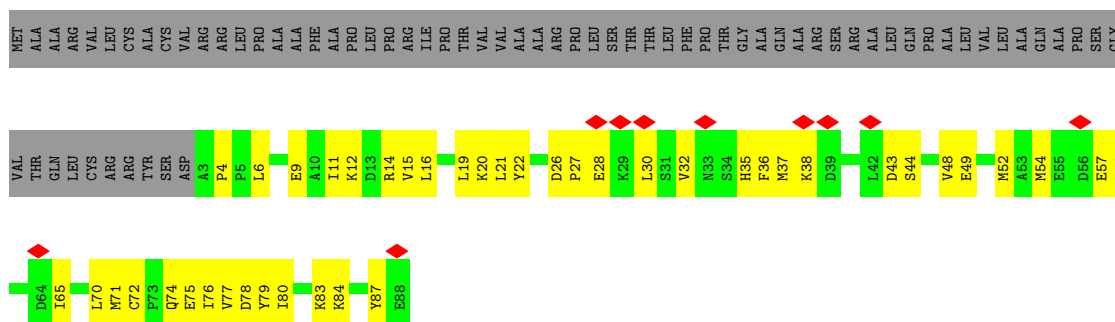


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

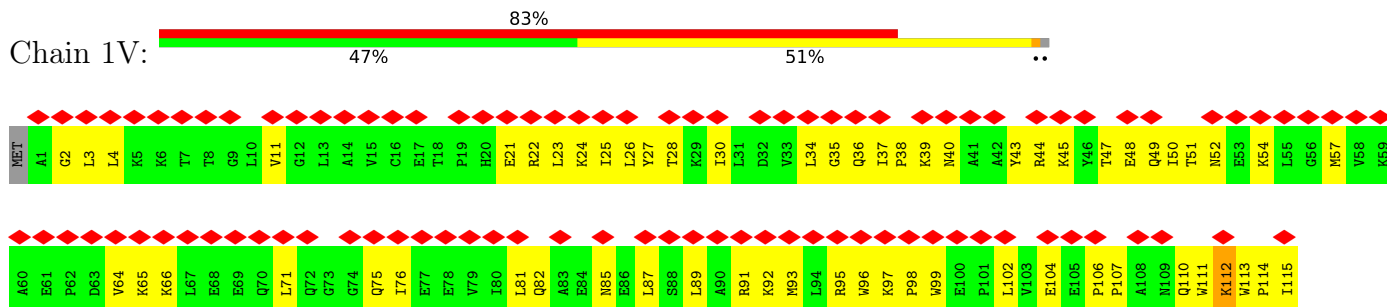


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

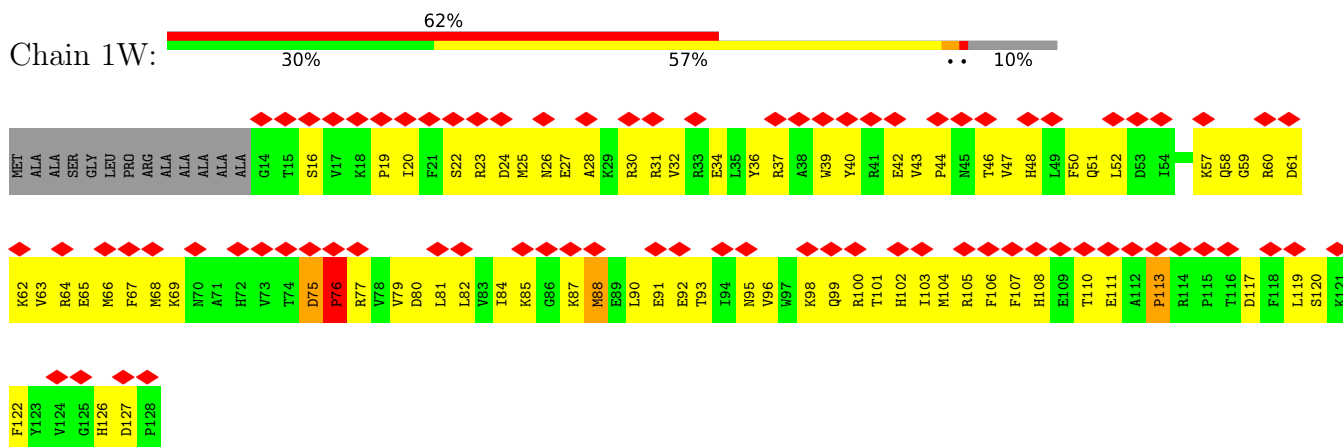




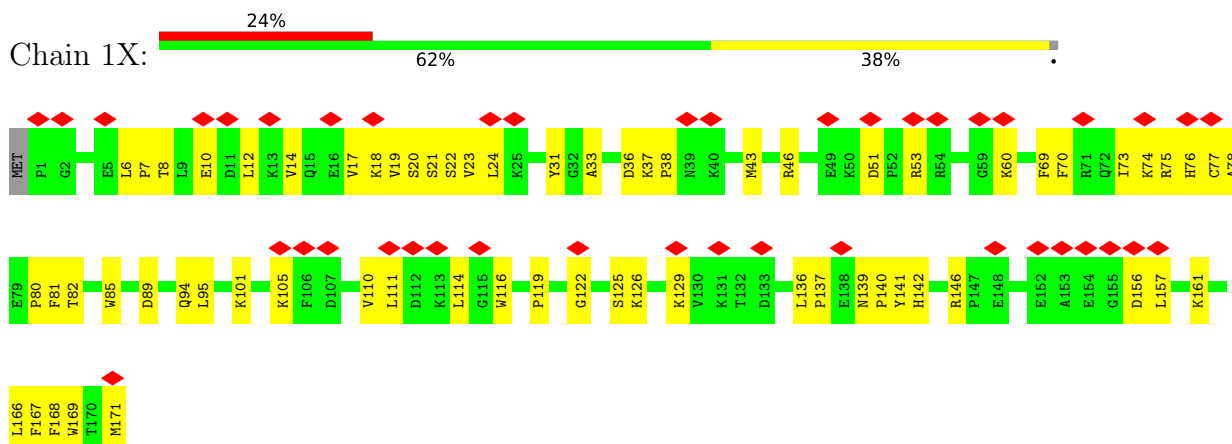
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



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

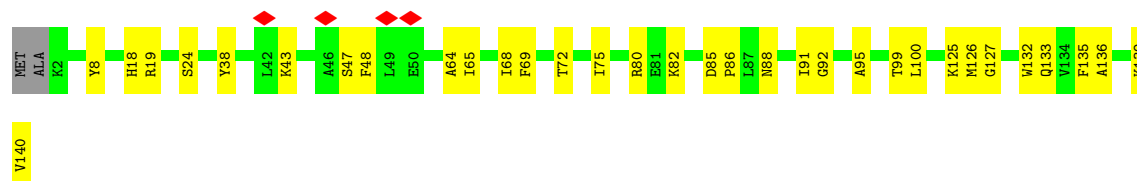


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



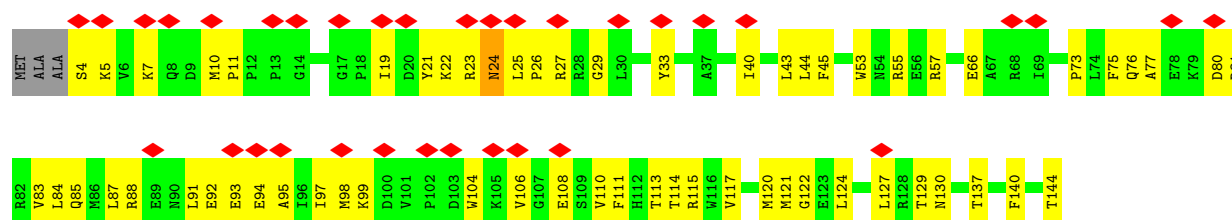
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y: 



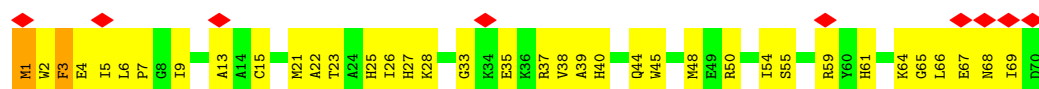
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z: 



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

Chain 1a: 

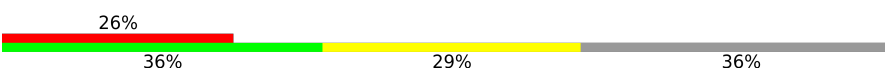


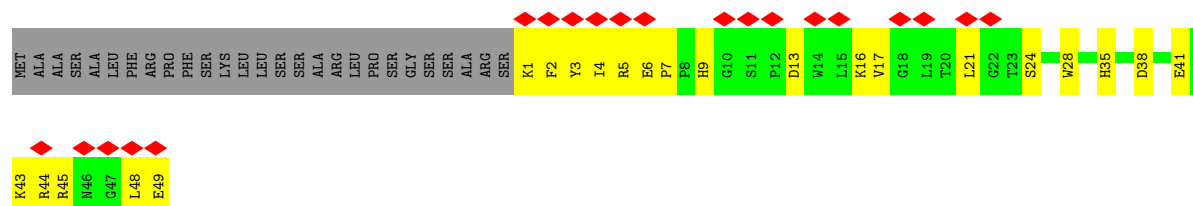
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain 1b: 

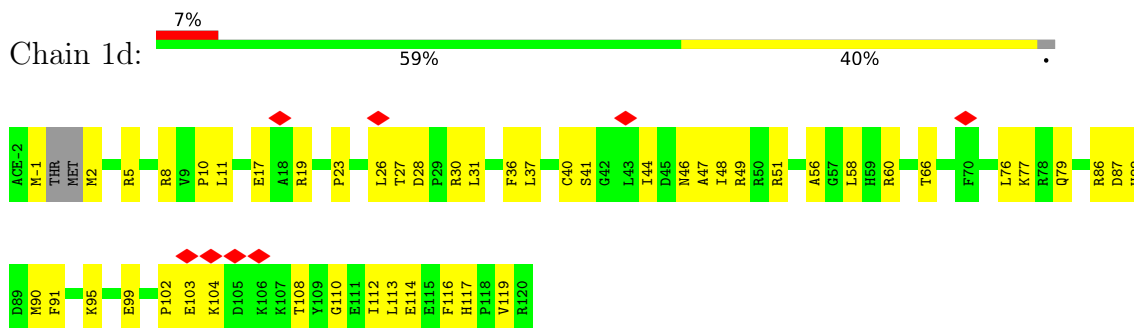


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

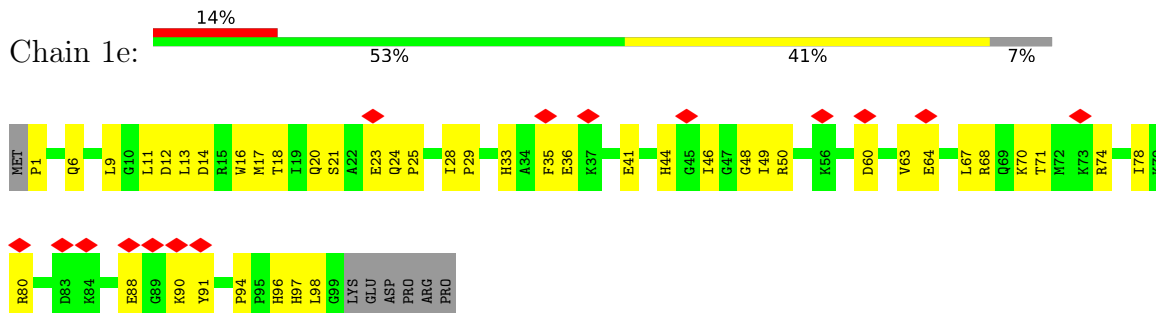
Chain 1c: 



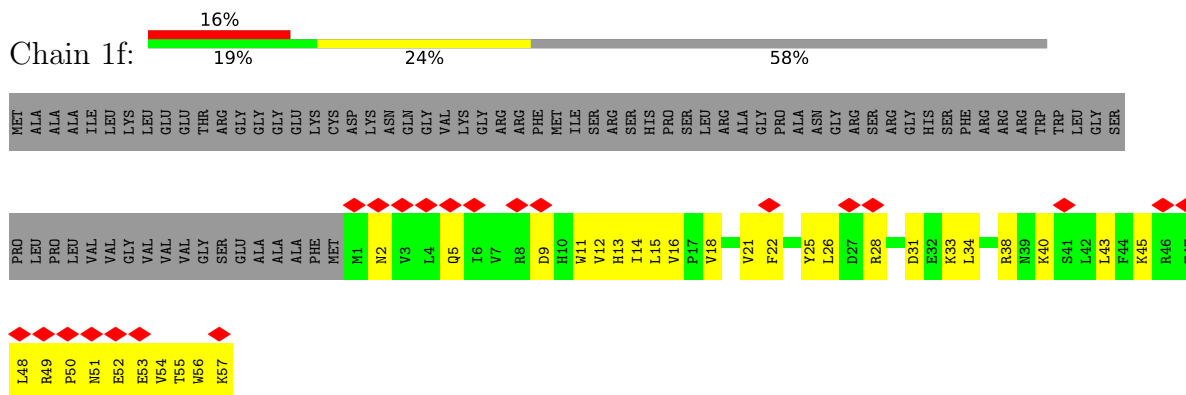
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



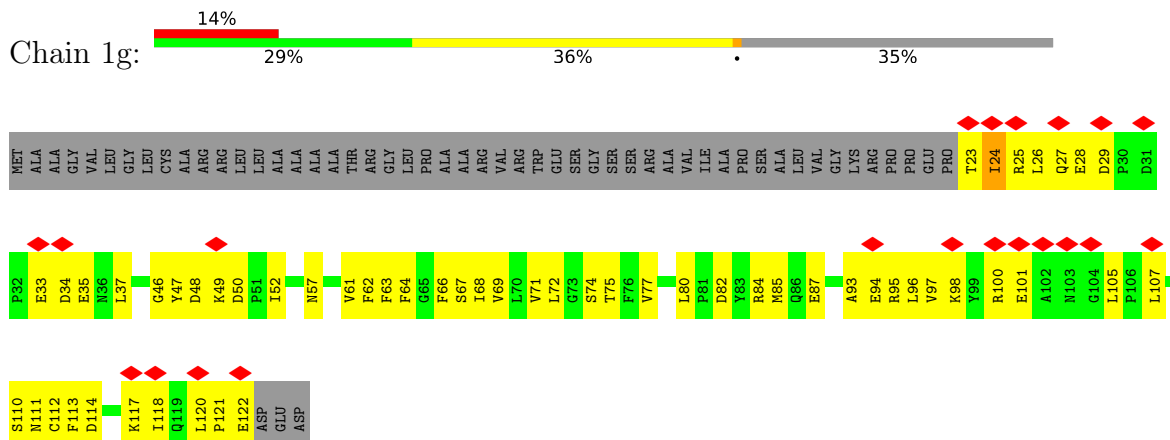
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



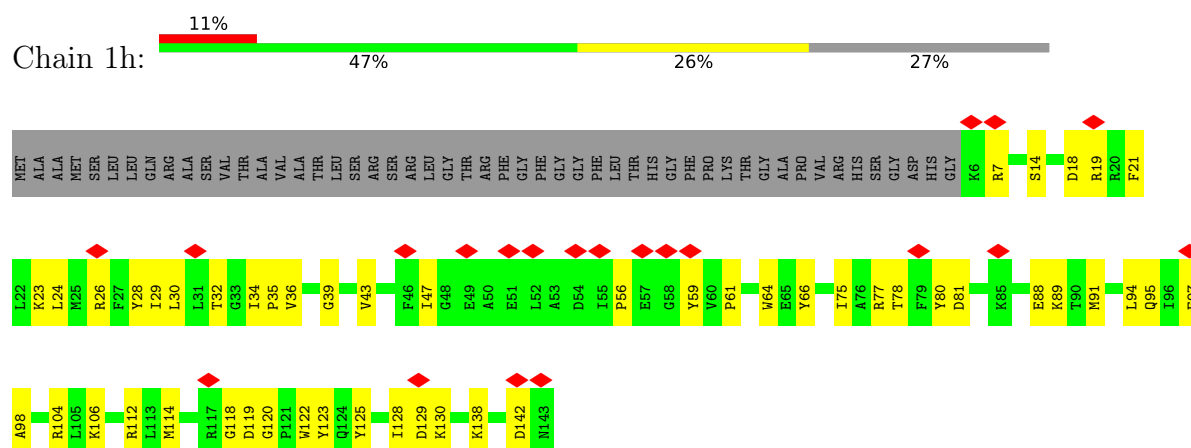
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



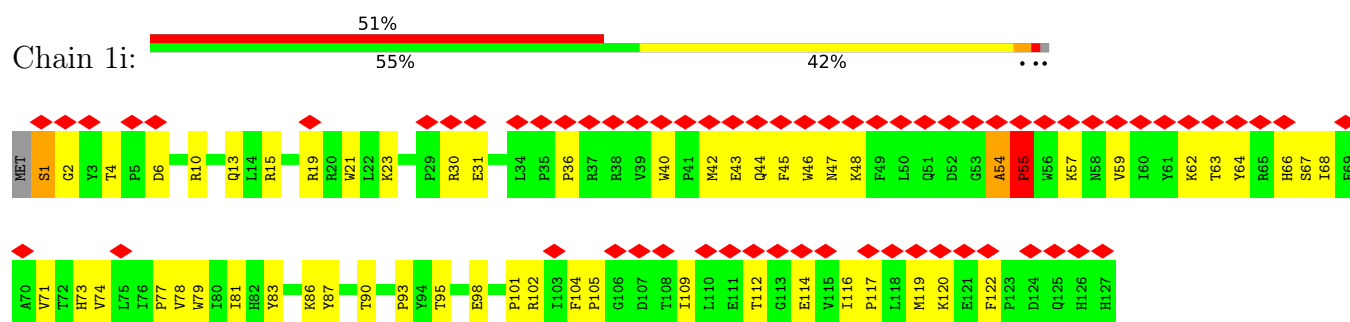
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



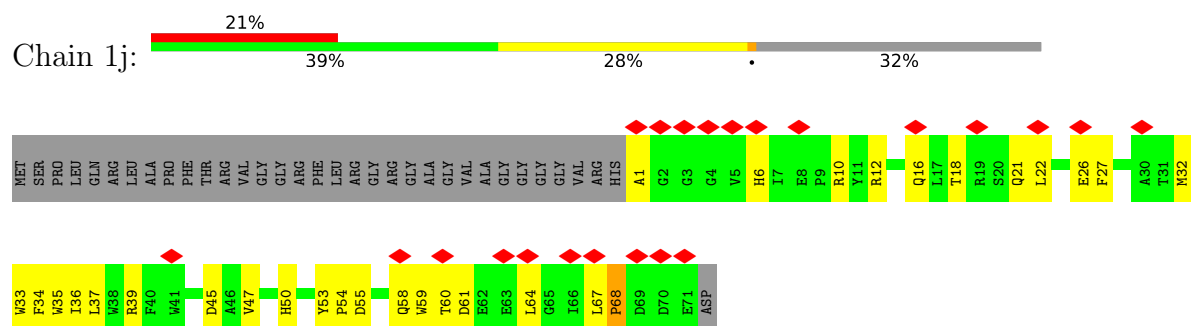
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



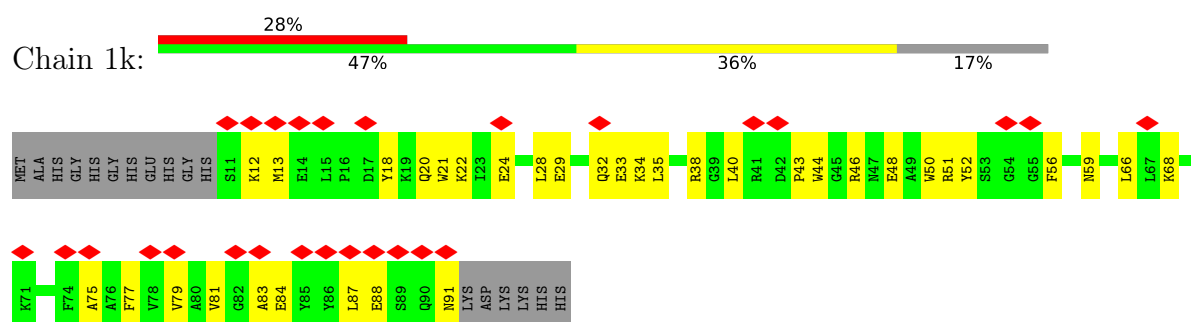
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



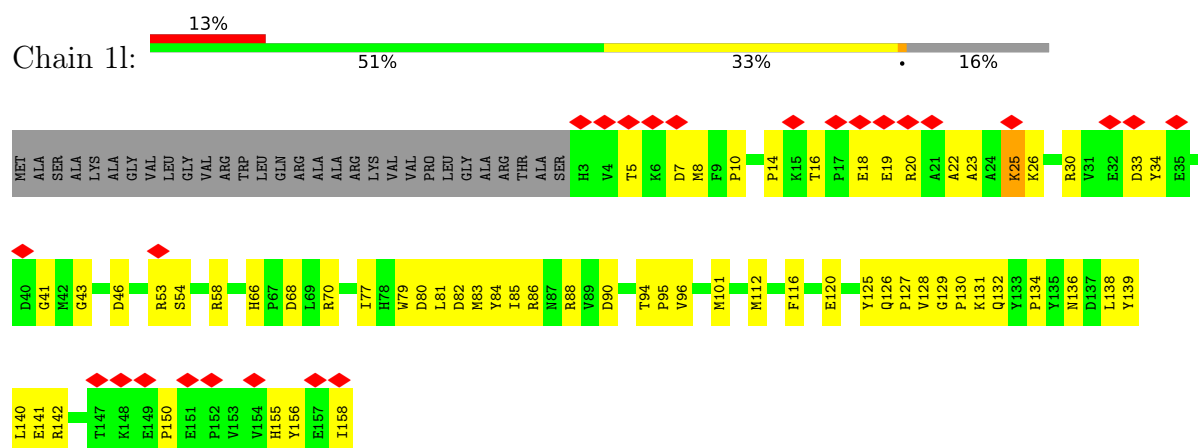
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



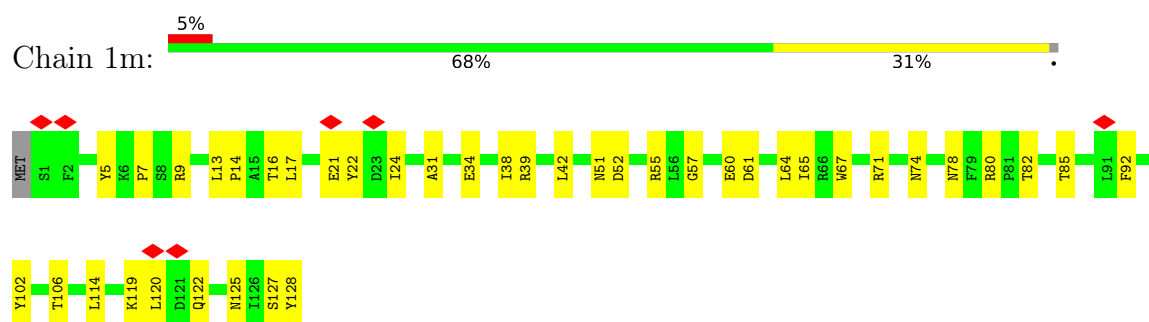
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



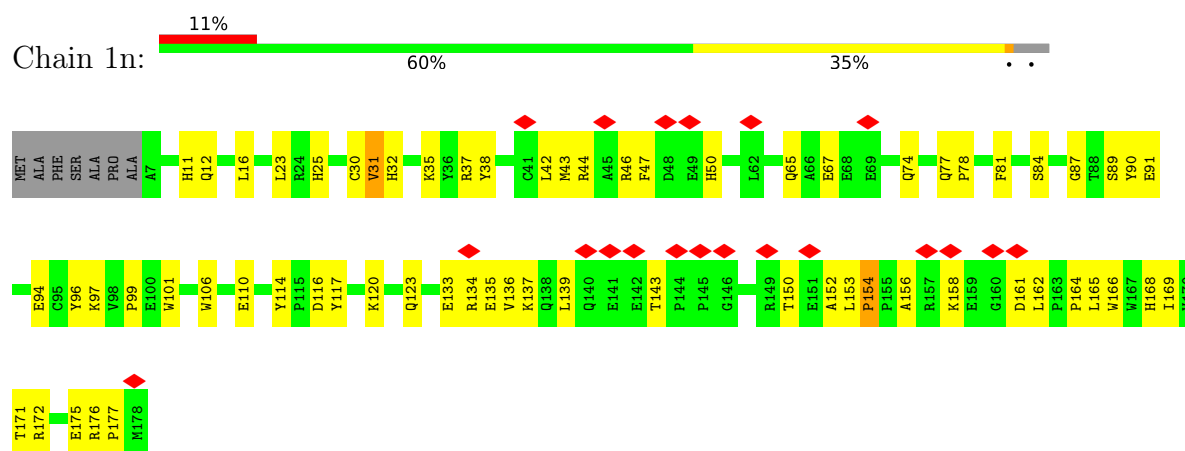
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



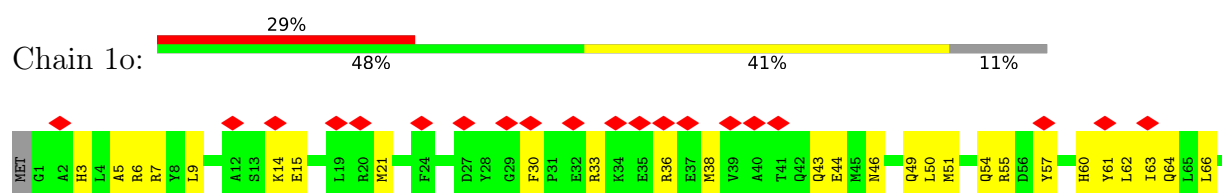
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

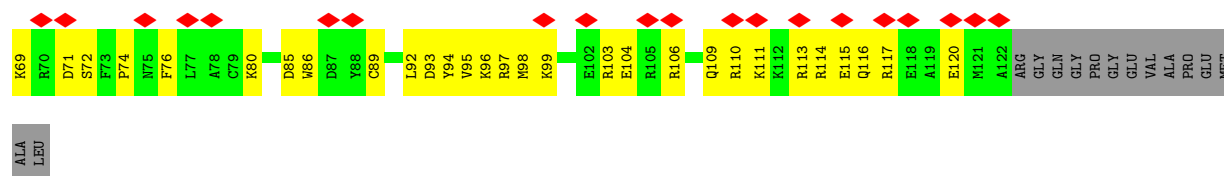


- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

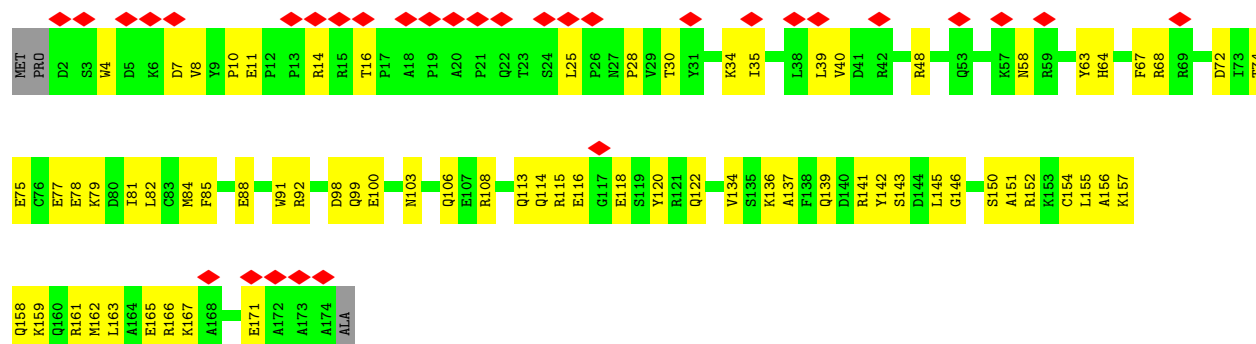


- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

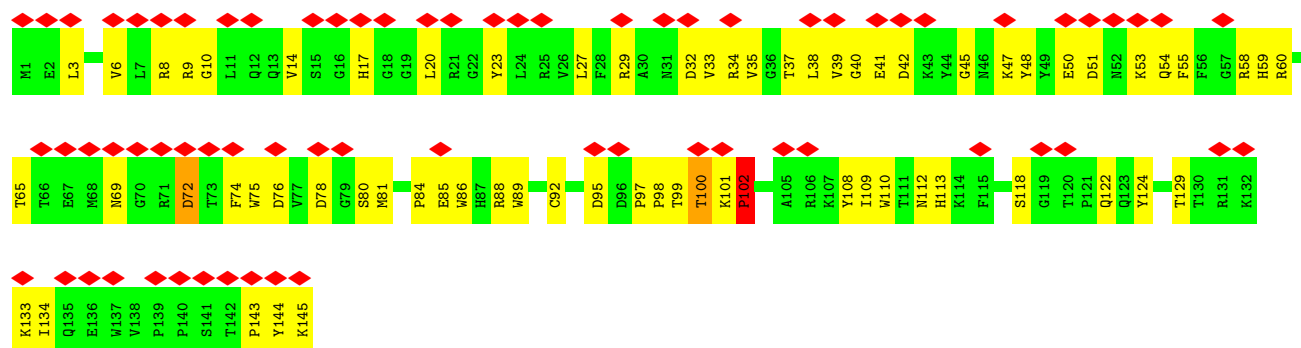




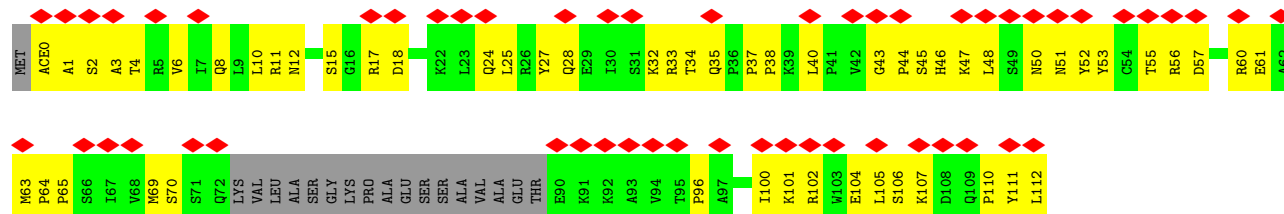
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



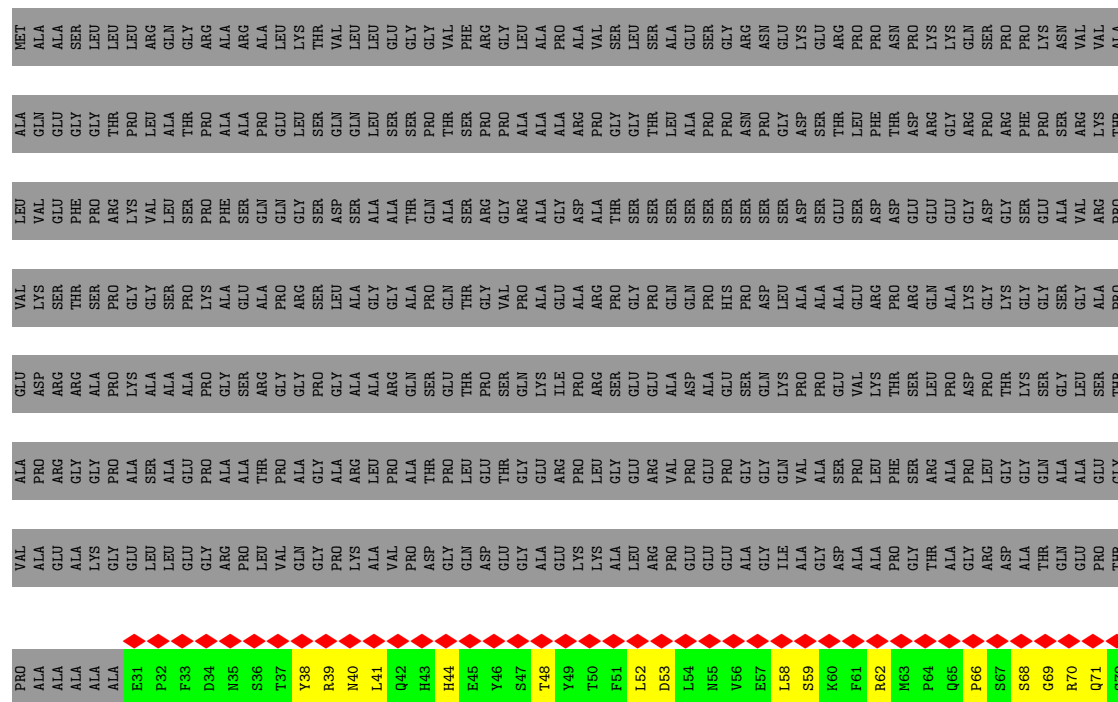
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- 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	37000	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	0.909	Depositor
Minimum map value	-0.399	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.18	0/713	0.42	0/975
2	1B	0.27	0/1273	0.50	1/1722 (0.1%)
3	1C	0.17	0/1791	0.40	0/2439
4	1D	0.18	0/3545	0.37	0/4806
5	1E	0.35	1/1698 (0.1%)	0.62	3/2311 (0.1%)
6	1F	0.24	1/3401 (0.0%)	0.45	1/4595 (0.0%)
7	1G	0.37	6/5451 (0.1%)	0.54	11/7387 (0.1%)
8	1H	0.17	0/2401	0.36	0/3282
9	1I	0.19	0/1443	0.50	1/1952 (0.1%)
10	1J	0.19	0/1364	0.38	0/1850
11	1K	0.24	0/751	0.48	0/1018
12	1L	0.16	0/4939	0.40	0/6718
13	1M	0.16	0/3713	0.33	0/5063
14	1N	0.24	0/2765	0.43	0/3758
15	1O	0.25	1/2650 (0.0%)	0.37	0/3588
16	1P	0.21	0/2828	0.40	0/3834
17	1Q	0.20	0/1070	0.49	1/1446 (0.1%)
18	1R	0.16	0/755	0.37	0/1018
19	1S	0.23	0/711	0.49	0/956
20	1T	0.49	2/701 (0.3%)	0.75	2/946 (0.2%)
20	1U	0.19	0/706	0.43	0/954
21	1V	0.16	0/946	0.36	0/1281
22	1W	1.24	7/995 (0.7%)	1.43	9/1340 (0.7%)
23	1X	0.15	0/1436	0.32	0/1938
24	1Y	0.10	0/1037	0.26	0/1404
25	1Z	0.15	0/1199	0.36	0/1617
26	1a	0.36	0/577	0.78	2/777 (0.3%)
27	1b	0.16	0/664	0.36	0/912
28	1c	0.25	0/430	0.44	0/581
29	1d	0.22	0/1024	0.35	0/1383
30	1e	0.13	0/836	0.32	0/1118
31	1f	0.17	0/499	0.43	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.22	0/858	0.51	0/1165
33	1h	0.19	0/1184	0.40	0/1603
34	1i	1.11	7/1131 (0.6%)	1.34	9/1541 (0.6%)
35	1j	0.19	0/627	0.47	1/858 (0.1%)
36	1k	0.14	0/668	0.39	0/903
37	1l	0.13	0/1365	0.33	0/1867
38	1m	0.12	0/1092	0.29	0/1481
39	1n	0.30	2/1549 (0.1%)	0.57	2/2098 (0.1%)
40	1o	0.14	0/1069	0.35	0/1430
41	1p	0.14	0/1481	0.35	0/1997
42	1q	0.23	0/1253	0.53	1/1704 (0.1%)
43	1r	0.27	0/782	0.45	0/1057
44	1s	0.18	0/394	0.41	0/533
All	All	0.30	27/67765 (0.0%)	0.49	44/91879 (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
5	1E	0	1
13	1M	0	1
34	1i	0	1
42	1q	0	1
All	All	0	4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	1W	76	PRO	CG-CD	-24.05	0.69	1.50
34	1i	54	ALA	C-N	19.53	1.79	1.33
34	1i	55	PRO	CG-CD	-19.12	0.85	1.50
22	1W	75	ASP	C-N	16.36	1.72	1.33
34	1i	55	PRO	CA-CB	-14.61	1.33	1.53
22	1W	76	PRO	N-CD	14.01	1.67	1.47
34	1i	55	PRO	CB-CG	13.68	2.18	1.49
22	1W	76	PRO	CB-CG	12.96	2.14	1.49
7	1G	518	PRO	CG-CD	-12.29	1.08	1.50
7	1G	518	PRO	N-CD	11.56	1.64	1.47
22	1W	76	PRO	CA-CB	-10.04	1.39	1.53
34	1i	55	PRO	CA-C	8.59	1.64	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	1G	518	PRO	N-CA	-8.54	1.29	1.46
34	1i	55	PRO	N-CD	7.94	1.58	1.47
7	1G	412	PRO	CG-CD	-6.84	1.27	1.50
15	1O	208	LYS	CD-CE	-6.50	1.32	1.52
22	1W	76	PRO	N-CA	-6.48	1.39	1.47
20	1T	26	ASP	C-N	5.92	1.41	1.34
39	1n	154	PRO	N-CD	5.87	1.55	1.47
39	1n	154	PRO	N-CA	-5.81	1.35	1.46
20	1T	27	PRO	CG-CD	-5.77	1.31	1.50
5	1E	153	MET	CG-SD	-5.54	1.67	1.80
22	1W	76	PRO	CA-C	5.32	1.59	1.52
7	1G	450	MET	SD-CE	-5.27	1.66	1.79
34	1i	54	ALA	C-O	5.25	1.30	1.23
6	1F	153	ILE	CG1-CD1	-5.18	1.31	1.51
7	1G	517	ASN	N-CA	5.07	1.53	1.45

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	55	PRO	CB-CG-CD	-33.14	0.05	106.10
22	1W	76	PRO	CB-CG-CD	-31.23	6.17	106.10
34	1i	55	PRO	CA-N-CD	-27.91	72.92	112.00
22	1W	76	PRO	CA-N-CD	-21.80	81.47	112.00
7	1G	518	PRO	CA-N-CD	-20.32	83.55	112.00
39	1n	154	PRO	CA-N-CD	-18.71	85.80	112.00
26	1a	1	MET	CG-SD-CE	-17.06	63.36	100.90
20	1T	27	PRO	CA-N-CD	-14.54	91.64	112.00
34	1i	55	PRO	N-CA-CB	-14.51	88.02	103.25
22	1W	113	PRO	CA-N-CD	-13.80	92.68	112.00
5	1E	94	PRO	CA-N-CD	-11.71	95.61	112.00
22	1W	75	ASP	CA-C-O	-11.53	109.96	119.99
42	1q	102	PRO	CA-N-CD	-11.47	95.94	112.00
5	1E	184	PRO	CA-N-CD	-10.77	96.92	112.00
22	1W	75	ASP	C-N-CD	10.46	167.89	125.00
34	1i	54	ALA	C-N-CD	9.56	164.20	125.00
22	1W	76	PRO	N-CD-CG	-9.46	89.01	103.20
34	1i	55	PRO	CA-CB-CG	-9.32	86.80	104.50
7	1G	412	PRO	N-CD-CG	-9.14	89.49	103.20
35	1j	68	PRO	CA-N-CD	-8.89	99.55	112.00
22	1W	76	PRO	CA-CB-CG	-8.77	87.84	104.50
17	1Q	40	PRO	CA-N-CD	-8.67	99.86	112.00
7	1G	450	MET	CG-SD-CE	-8.67	81.83	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1E	103	CYS	CA-CB-SG	7.86	132.47	114.40
26	1a	1	MET	CA-CB-CG	7.73	129.56	114.10
34	1i	54	ALA	CA-C-N	-7.72	110.19	119.84
34	1i	54	ALA	C-N-CA	-7.72	110.19	119.84
22	1W	75	ASP	CA-C-N	-7.39	110.60	119.84
22	1W	75	ASP	C-N-CA	-7.39	110.60	119.84
34	1i	54	ALA	CA-C-O	-7.39	112.65	120.70
7	1G	518	PRO	CA-CB-CG	-7.19	90.84	104.50
7	1G	517	ASN	C-N-CD	6.52	151.74	125.00
9	1I	78	ILE	N-CA-C	-6.46	107.00	113.20
7	1G	412	PRO	CA-N-CD	-6.30	103.17	112.00
7	1G	517	ASN	CA-C-O	-6.12	114.07	120.87
7	1G	412	PRO	CA-CB-CG	-6.05	93.01	104.50
7	1G	518	PRO	N-CD-CG	-6.00	94.20	103.20
34	1i	36	PRO	CA-N-CD	-5.67	104.06	112.00
7	1G	234	VAL	N-CA-C	-5.65	108.34	113.71
39	1n	153	LEU	C-N-CD	5.39	147.09	125.00
6	1F	219	PRO	CA-N-CD	-5.32	104.56	112.00
2	1B	125	TYR	CD1-CE1-CZ	5.11	128.81	119.60
20	1T	27	PRO	N-CD-CG	-5.11	95.54	103.20
7	1G	518	PRO	CB-CG-CD	-5.05	89.95	106.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	1E	152	PRO	Peptide
13	1M	251	ASN	Peptide
34	1i	55	PRO	Mainchain
42	1q	143	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	707	0	757	57	0
2	1B	1242	0	1249	127	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	1C	1740	0	1691	137	0
4	1D	3452	0	3389	244	0
5	1E	1658	0	1662	165	0
6	1F	3325	0	3288	300	0
7	1G	5362	0	5388	427	0
8	1H	2344	0	2460	182	0
9	1I	1412	0	1365	121	0
10	1J	1339	0	1337	107	0
11	1K	750	0	795	84	0
12	1L	4818	0	4956	276	0
13	1M	3632	0	3835	186	0
14	1N	2712	0	2872	223	0
15	1O	2590	0	2556	154	0
16	1P	2751	0	2776	186	0
17	1Q	1047	0	1042	97	0
18	1R	741	0	704	42	0
19	1S	700	0	719	65	0
20	1T	689	0	687	82	0
20	1U	694	0	691	52	0
21	1V	927	0	972	72	0
22	1W	971	0	975	127	0
23	1X	1398	0	1378	82	0
24	1Y	1016	0	1019	26	0
25	1Z	1168	0	1161	68	0
26	1a	562	0	557	63	0
27	1b	643	0	645	22	0
28	1c	417	0	425	29	0
29	1d	996	0	990	72	0
30	1e	816	0	821	42	0
31	1f	487	0	496	31	0
32	1g	835	0	795	85	0
33	1h	1151	0	1164	74	0
34	1i	1100	0	1106	70	0
35	1j	601	0	546	31	0
36	1k	649	0	626	39	0
37	1l	1310	0	1204	74	0
38	1m	1062	0	1075	39	0
39	1n	1495	0	1434	67	0
40	1o	1045	0	1018	68	0
41	1p	1449	0	1416	88	0
42	1q	1212	0	1174	77	0
43	1r	767	0	791	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	1s	382	0	351	29	0
45	1A	47	0	71	3	0
45	1L	88	0	127	10	0
45	1N	51	0	82	2	0
45	1Y	82	0	118	6	0
46	1B	8	0	0	1	0
46	1F	8	0	0	4	0
46	1G	16	0	0	1	0
46	1I	16	0	0	0	0
47	1E	4	0	0	4	0
47	1G	4	0	0	1	0
48	1F	31	0	19	2	0
49	1G	1	0	0	0	0
50	1I	98	0	147	10	0
50	1J	35	0	44	4	0
50	1L	44	0	65	2	0
50	1f	46	0	69	3	0
51	1L	15	0	26	5	0
52	1M	51	0	78	9	0
53	1N	77	0	97	6	0
53	1r	61	0	66	6	0
54	1O	32	0	12	2	0
55	1O	1	0	0	0	0
56	1P	48	0	26	3	0
57	1R	1	0	0	0	0
58	1W	37	0	0	5	0
58	1n	37	0	0	1	0
All	All	67103	0	67405	4013	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 (4013) 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)
22:1W:75:ASP:C	22:1W:76:PRO:N	1.72	1.47
22:1W:76:PRO:N	22:1W:76:PRO:CG	1.79	1.41
34:1i:54:ALA:C	34:1i:55:PRO:N	1.79	1.39
34:1i:55:PRO:N	34:1i:55:PRO:CG	1.88	1.35
5:1E:60:TRP:CZ3	5:1E:94:PRO:HD3	1.65	1.31
22:1W:76:PRO:CG	22:1W:76:PRO:CB	2.14	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:150:GLN:HA	6:1F:153:ILE:HD12	1.22	1.20
34:1i:55:PRO:CG	34:1i:55:PRO:CB	2.18	1.20
15:1O:204:ASN:HB2	15:1O:208:LYS:HE3	1.26	1.18
4:1D:221:ARG:HG3	43:1r:24:GLN:NE2	1.61	1.15
7:1G:518:PRO:O	7:1G:518:PRO:HD2	1.48	1.12
43:1r:45:SER:HA	43:1r:47:LYS:HZ1	1.01	1.12
13:1M:450:ASN:HD21	13:1M:453:MET:HE2	1.05	1.12
42:1q:59:HIS:ND1	42:1q:60:ARG:HG3	1.65	1.11
5:1E:153:MET:HE3	5:1E:154:VAL:H	1.03	1.11
14:1N:251:MET:HG3	14:1N:293:TYR:CZ	1.88	1.09
22:1W:113:PRO:O	22:1W:113:PRO:HD2	1.50	1.09
34:1i:55:PRO:CD	34:1i:55:PRO:HG2	1.63	1.09
5:1E:153:MET:HE3	5:1E:154:VAL:N	1.67	1.08
22:1W:65:GLU:HB2	22:1W:69:LYS:HZ1	0.97	1.08
32:1g:93:ALA:O	32:1g:97:VAL:HG23	1.51	1.08
21:1V:39:LYS:HA	21:1V:44:ARG:HD3	1.31	1.07
42:1q:59:HIS:HE1	42:1q:60:ARG:CD	1.67	1.07
6:1F:101:GLU:OE2	6:1F:104:THR:HG23	1.55	1.07
34:1i:55:PRO:CD	34:1i:55:PRO:HG3	1.63	1.07
20:1T:18:VAL:HA	20:1T:21:LEU:HG	1.36	1.07
7:1G:672:TYR:HB3	7:1G:684:MET:HE3	1.36	1.06
43:1r:63:MET:HE3	43:1r:64:PRO:HD3	1.37	1.06
6:1F:105:CYS:SG	6:1F:257:ASN:ND2	2.28	1.05
14:1N:325:LEU:HD23	53:1N:402:CDL:H732	1.39	1.05
34:1i:109:ILE:HD13	34:1i:114:GLU:OE2	1.55	1.04
20:1T:20:LYS:NZ	20:1T:27:PRO:HA	1.70	1.04
34:1i:55:PRO:CG	34:1i:55:PRO:HD3	1.52	1.03
13:1M:450:ASN:ND2	13:1M:453:MET:HE2	1.73	1.03
7:1G:366:THR:CB	7:1G:450:MET:HE1	1.87	1.03
15:1O:204:ASN:O	15:1O:208:LYS:HG2	1.58	1.02
33:1h:114:MET:HE2	33:1h:122:TRP:CD1	1.93	1.02
42:1q:59:HIS:HE1	42:1q:60:ARG:HD2	1.20	1.02
34:1i:55:PRO:CG	34:1i:55:PRO:HD2	1.53	1.01
24:1Y:80:ARG:HB3	24:1Y:82:LYS:HZ3	1.25	1.01
7:1G:283:MET:HE2	7:1G:283:MET:HA	1.42	1.01
43:1r:63:MET:HE3	43:1r:64:PRO:CD	1.91	1.00
22:1W:76:PRO:CD	22:1W:76:PRO:HG2	1.48	1.00
10:1J:68:PHE:CZ	11:1K:75:LEU:HD21	1.97	0.99
19:1S:63:LYS:HZ1	19:1S:75:ASN:CG	1.71	0.99
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.45	0.99
22:1W:76:PRO:CD	22:1W:76:PRO:HG3	1.48	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:125:TYR:HE1	4:1D:102:TYR:CZ	1.80	0.98
22:1W:65:GLU:HB2	22:1W:69:LYS:NZ	1.79	0.98
28:1c:38:ASP:OD1	29:1d:23:PRO:HG3	1.63	0.97
7:1G:211:LYS:HE3	7:1G:699:GLU:OE2	1.65	0.97
10:1J:68:PHE:CE1	11:1K:75:LEU:HD21	1.98	0.97
14:1N:341:PRO:HB2	29:1d:79:GLN:NE2	1.79	0.97
5:1E:60:TRP:CE3	5:1E:94:PRO:HD3	2.00	0.97
19:1S:37:GLU:HB3	19:1S:38:LYS:HZ3	1.31	0.96
20:1T:27:PRO:HD2	20:1T:28:GLU:N	1.78	0.96
19:1S:17:GLU:HB2	19:1S:67:ARG:HD2	1.45	0.95
42:1q:59:HIS:CE1	42:1q:60:ARG:CD	2.50	0.95
8:1H:86:TRP:CH2	8:1H:233:MET:HA	2.01	0.95
18:1R:28:PHE:HE1	18:1R:33:LYS:HG3	1.32	0.95
7:1G:579:ARG:NH1	7:1G:634:ASP:OD1	1.99	0.94
33:1h:114:MET:HE2	33:1h:122:TRP:HD1	1.27	0.94
12:1L:175:ASN:HD21	12:1L:223:LYS:NZ	1.64	0.94
16:1P:201:VAL:HG12	16:1P:235:ARG:HE	1.29	0.93
43:1r:45:SER:HA	43:1r:47:LYS:NZ	1.83	0.93
32:1g:87:GLU:OE1	32:1g:87:GLU:N	2.00	0.93
16:1P:203:GLN:OE1	16:1P:234:ASN:N	2.01	0.93
16:1P:258:LEU:HD13	16:1P:262:ALA:HB3	1.51	0.93
14:1N:341:PRO:HB2	29:1d:79:GLN:HE21	1.32	0.92
5:1E:60:TRP:CZ3	5:1E:94:PRO:CD	2.52	0.92
42:1q:59:HIS:CE1	42:1q:60:ARG:HG3	2.05	0.92
4:1D:106:LEU:HD11	4:1D:391:ILE:HD12	1.51	0.92
6:1F:149:LEU:O	6:1F:153:ILE:HG13	1.68	0.92
21:1V:54:LYS:HA	21:1V:57:MET:HG3	1.50	0.92
26:1a:64:LYS:HE2	26:1a:68:ASN:ND2	1.86	0.91
2:1B:125:TYR:CE1	4:1D:102:TYR:CZ	2.58	0.91
22:1W:65:GLU:CB	22:1W:69:LYS:HZ1	1.83	0.91
34:1i:119:MET:HE3	34:1i:120:LYS:N	1.85	0.91
22:1W:76:PRO:CG	22:1W:76:PRO:HD3	1.41	0.91
22:1W:76:PRO:CG	22:1W:76:PRO:HD2	1.41	0.91
14:1N:209:ILE:O	14:1N:213:LEU:HD22	1.70	0.90
34:1i:120:LYS:HA	34:1i:120:LYS:HE3	1.54	0.90
5:1E:132:THR:O	5:1E:135:LYS:NZ	2.05	0.90
19:1S:37:GLU:HB3	19:1S:38:LYS:NZ	1.87	0.90
34:1i:55:PRO:CG	34:1i:55:PRO:CA	2.48	0.90
39:1n:154:PRO:HD2	39:1n:154:PRO:O	1.63	0.90
7:1G:366:THR:OG1	7:1G:450:MET:HE1	1.71	0.90
6:1F:150:GLN:HA	6:1F:153:ILE:CD1	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:33:GLU:OE1	32:1g:34:ASP:N	2.05	0.89
2:1B:41:ARG:N	8:1H:54:LYS:HE2	1.87	0.89
15:1O:204:ASN:HB2	15:1O:208:LYS:CE	2.02	0.89
5:1E:108:CYS:HB3	47:1E:301:FES:S2	2.12	0.89
5:1E:153:MET:HE1	5:1E:160:TYR:CE1	2.08	0.89
6:1F:52:GLY:HA2	6:1F:127:ARG:HH22	1.36	0.88
5:1E:60:TRP:HZ3	5:1E:94:PRO:HD3	1.32	0.88
22:1W:76:PRO:CG	22:1W:76:PRO:CA	2.51	0.88
35:1j:67:LEU:HD13	35:1j:68:PRO:HD2	1.55	0.88
5:1E:153:MET:CE	5:1E:160:TYR:HE1	1.87	0.88
42:1q:98:PRO:O	42:1q:102:PRO:HD3	1.73	0.88
19:1S:63:LYS:NZ	19:1S:75:ASN:CG	2.30	0.88
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	1.54	0.88
11:1K:62:ILE:HD11	14:1N:27:LEU:HD21	1.56	0.88
12:1L:401:MET:HE3	12:1L:482:MET:SD	2.12	0.88
22:1W:69:LYS:HD3	22:1W:69:LYS:N	1.89	0.87
43:1r:45:SER:CA	43:1r:47:LYS:HZ1	1.85	0.87
43:1r:47:LYS:HE2	43:1r:51:ASN:HD21	1.38	0.87
2:1B:161:LEU:HD12	2:1B:164:GLN:HE22	1.39	0.87
12:1L:571:MET:HE2	12:1L:571:MET:HA	1.57	0.87
20:1U:35:HIS:CE1	20:1U:38:LYS:HG2	2.10	0.87
20:1T:20:LYS:HZ2	20:1T:27:PRO:HA	1.36	0.87
8:1H:3:MET:O	8:1H:3:MET:HE3	1.74	0.87
3:1C:196:LYS:NZ	17:1Q:81:ASN:HA	1.90	0.87
7:1G:140:LYS:HD3	7:1G:150:MET:CE	2.04	0.87
7:1G:54:MET:HE1	7:1G:94:MET:HB2	1.58	0.86
15:1O:204:ASN:C	15:1O:208:LYS:HZ1	1.83	0.86
2:1B:125:TYR:HE1	4:1D:102:TYR:CE2	1.93	0.86
12:1L:175:ASN:HD21	12:1L:223:LYS:HZ3	1.20	0.86
15:1O:214:MET:HA	15:1O:217:LYS:HZ3	1.41	0.86
42:1q:59:HIS:CE1	42:1q:60:ARG:CG	2.59	0.86
5:1E:153:MET:CE	5:1E:154:VAL:N	2.39	0.85
14:1N:218:LEU:HD12	14:1N:244:MET:HE2	1.56	0.85
15:1O:23:LYS:NZ	15:1O:243:CYS:SG	2.48	0.85
4:1D:151:ILE:HG23	4:1D:170:MET:HB3	1.58	0.85
33:1h:114:MET:CE	33:1h:122:TRP:CD1	2.60	0.85
20:1U:9:GLU:OE1	20:1U:9:GLU:N	2.09	0.85
7:1G:254:MET:HE1	17:1Q:109:LYS:HB3	1.58	0.85
34:1i:55:PRO:CG	34:1i:55:PRO:CD	0.85	0.85
20:1T:69:LYS:HZ2	20:1T:70:LEU:HD23	1.41	0.85
2:1B:125:TYR:HD2	9:1I:117:ILE:HG13	1.40	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:363:THR:HG21	7:1G:97:LEU:HD23	1.59	0.84
34:1i:13:GLN:HE22	39:1n:156:ALA:H	1.25	0.84
7:1G:140:LYS:HD3	7:1G:150:MET:HE3	1.58	0.84
15:1O:214:MET:HA	15:1O:217:LYS:NZ	1.91	0.84
2:1B:161:LEU:HD12	2:1B:164:GLN:NE2	1.92	0.84
16:1P:215:ILE:HA	16:1P:218:ILE:CD1	2.07	0.84
13:1M:257:MET:HE2	13:1M:257:MET:HA	1.58	0.84
14:1N:251:MET:HG3	14:1N:293:TYR:OH	1.78	0.84
14:1N:214:ALA:O	14:1N:218:LEU:HG	1.78	0.84
37:1l:134:PRO:HB3	40:1o:38:MET:HE2	1.58	0.84
5:1E:111:ARG:NH2	5:1E:150:ASN:O	2.11	0.83
12:1L:51:LEU:HD21	12:1L:88:MET:HE1	1.61	0.83
15:1O:81:LYS:HE2	15:1O:92:ASN:HB3	1.57	0.83
5:1E:109:MET:HA	5:1E:113:SER:HB2	1.61	0.83
23:1X:23:VAL:HG13	23:1X:81:PHE:HZ	1.43	0.83
33:1h:98:ALA:HB2	41:1p:81:ILE:HD11	1.61	0.83
13:1M:42:LEU:HD21	13:1M:453:MET:HB3	1.61	0.83
9:1I:8:ARG:NH1	9:1I:8:ARG:HA	1.93	0.82
26:1a:55:SER:HA	26:1a:64:LYS:NZ	1.94	0.82
7:1G:255:HIS:HE1	7:1G:257:ASP:HB3	1.40	0.82
4:1D:221:ARG:CG	43:1r:24:GLN:NE2	2.43	0.82
2:1B:77:ARG:HD3	2:1B:79:SER:HB3	1.59	0.82
5:1E:108:CYS:CB	47:1E:301:FES:S2	2.67	0.82
12:1L:331:MET:HE1	12:1L:468:ILE:HD12	1.60	0.82
4:1D:301:VAL:HA	4:1D:304:MET:HE2	1.60	0.82
5:1E:153:MET:CE	5:1E:154:VAL:H	1.90	0.82
43:1r:1:ALA:H	43:1r:2:SER:HB3	1.44	0.82
43:1r:44:PRO:O	43:1r:47:LYS:NZ	2.12	0.82
33:1h:95:GLN:HB2	41:1p:82:LEU:HD21	1.61	0.81
4:1D:221:ARG:HH21	43:1r:24:GLN:HA	1.45	0.81
2:1B:40:ALA:HB3	8:1H:54:LYS:HZ3	1.42	0.80
7:1G:518:PRO:O	7:1G:518:PRO:CD	2.27	0.80
15:1O:104:ARG:NH2	54:1O:401:GTP:N7	2.27	0.80
39:1n:135:GLU:HG2	39:1n:164:PRO:HA	1.63	0.80
14:1N:134:GLN:OE1	14:1N:135:LYS:HD2	1.81	0.80
15:1O:171:TYR:HE2	15:1O:206:TYR:CD1	1.99	0.80
10:1J:64:MET:HE2	10:1J:68:PHE:CE2	2.15	0.80
7:1G:255:HIS:ND1	7:1G:258:ILE:HG12	1.97	0.80
13:1M:207:MET:HE2	13:1M:298:ILE:HD13	1.64	0.80
14:1N:261:MET:HE1	14:1N:340:THR:HA	1.63	0.80
20:1T:69:LYS:HZ2	20:1T:70:LEU:CD2	1.94	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:40:LEU:HD22	14:1N:71:MET:HG3	1.63	0.80
20:1T:27:PRO:CD	20:1T:28:GLU:H	1.93	0.80
20:1T:70:LEU:HD22	20:1T:76:ILE:HD13	1.63	0.80
6:1F:253:THR:OG1	6:1F:270:GLU:O	2.00	0.80
20:1T:27:PRO:CD	20:1T:28:GLU:N	2.44	0.80
13:1M:342:MET:HE1	13:1M:410:MET:HA	1.64	0.80
22:1W:111:GLU:OE2	22:1W:111:GLU:N	2.15	0.80
16:1P:59:LEU:HD12	16:1P:70:PHE:HE2	1.48	0.79
7:1G:36:GLN:HE22	17:1Q:49:VAL:H	1.27	0.79
34:1i:112:THR:OG1	34:1i:114:GLU:OE1	2.00	0.79
2:1B:49:THR:HG21	2:1B:59:MET:HE3	1.65	0.79
2:1B:83:SER:OG	2:1B:107:MET:HE1	1.82	0.79
14:1N:342:ALA:HA	29:1d:79:GLN:OE1	1.83	0.79
9:1I:145:GLU:N	9:1I:145:GLU:OE1	2.16	0.78
22:1W:75:ASP:C	22:1W:76:PRO:CA	2.56	0.78
42:1q:38:LEU:HD21	42:1q:47:LYS:NZ	1.99	0.78
26:1a:22:ALA:O	26:1a:26:ILE:HG12	1.83	0.78
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.66	0.78
29:1d:2:MET:CE	33:1h:122:TRP:HB3	2.14	0.78
7:1G:571:ALA:H	7:1G:583:THR:HG22	1.49	0.78
12:1L:387:THR:HG22	12:1L:465:GLY:H	1.49	0.78
2:1B:125:TYR:CD2	9:1I:117:ILE:HG13	2.19	0.78
16:1P:203:GLN:CD	16:1P:234:ASN:N	2.41	0.78
6:1F:126:GLY:HA2	6:1F:129:MET:HE1	1.64	0.77
20:1T:27:PRO:HD2	20:1T:28:GLU:H	1.46	0.77
34:1i:40:TRP:HB3	34:1i:42:MET:HE3	1.66	0.77
10:1J:111:GLU:OE1	30:1e:80:ARG:NH2	2.17	0.77
24:1Y:80:ARG:HB3	24:1Y:82:LYS:NZ	1.98	0.77
29:1d:104:LYS:HD3	29:1d:104:LYS:N	1.99	0.77
4:1D:72:MET:HE3	4:1D:73:VAL:O	1.83	0.77
16:1P:214:ILE:O	16:1P:218:ILE:HD12	1.85	0.77
14:1N:95:MET:HE3	14:1N:149:ILE:HA	1.66	0.77
1:1A:87:MET:HE1	8:1H:305:ILE:HD11	1.65	0.77
1:1A:70:ALA:HB2	10:1J:59:ILE:HG21	1.67	0.77
5:1E:34:ILE:HD12	5:1E:49:PRO:HB2	1.66	0.77
15:1O:49:ARG:HE	15:1O:51:PHE:HE1	1.31	0.77
2:1B:62:MET:HE3	2:1B:69:MET:HB3	1.67	0.77
4:1D:216:LYS:HA	25:1Z:19:ILE:HG23	1.66	0.77
12:1L:361:GLY:HA3	12:1L:435:PRO:HG3	1.66	0.77
7:1G:341:ASP:HB3	19:1S:67:ARG:HH22	1.49	0.77
22:1W:69:LYS:HD3	22:1W:69:LYS:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:10:ASN:HD22	8:1H:83:LEU:HB3	1.49	0.77
7:1G:142:ILE:HG22	7:1G:191:PHE:HB2	1.67	0.77
32:1g:25:ARG:HE	32:1g:25:ARG:C	1.93	0.77
2:1B:161:LEU:HA	2:1B:164:GLN:HE21	1.50	0.76
7:1G:248:MET:N	7:1G:248:MET:SD	2.57	0.76
10:1J:33:LEU:HD11	10:1J:65:LEU:HD11	1.67	0.76
14:1N:72:MET:HA	14:1N:75:ILE:HG12	1.67	0.76
14:1N:149:ILE:HG21	14:1N:154:MET:SD	2.25	0.76
42:1q:59:HIS:CE1	42:1q:60:ARG:HD2	2.13	0.76
12:1L:103:PHE:CD1	12:1L:341:MET:HE1	2.20	0.76
21:1V:93:MET:HA	21:1V:96:TRP:HB2	1.66	0.76
22:1W:52:LEU:HD12	22:1W:104:MET:HE3	1.65	0.76
4:1D:20:TYR:CD2	12:1L:571:MET:HE1	2.21	0.76
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.66	0.76
16:1P:325:ARG:O	16:1P:326:TRP:CE3	2.39	0.76
21:1V:39:LYS:CA	21:1V:44:ARG:HD3	2.13	0.76
4:1D:413:ASP:OD2	8:1H:281:ARG:NH1	2.18	0.76
16:1P:215:ILE:HA	16:1P:218:ILE:HD13	1.66	0.76
20:1U:35:HIS:HE1	20:1U:37:MET:HB2	1.51	0.76
22:1W:19:PRO:HA	22:1W:77:ARG:HH12	1.51	0.76
15:1O:45:LYS:HZ2	15:1O:235:VAL:HG21	1.50	0.76
18:1R:49:VAL:HG13	18:1R:90:GLN:HB3	1.67	0.76
16:1P:325:ARG:NE	16:1P:326:TRP:CH2	2.50	0.76
5:1E:172:ILE:HG23	5:1E:182:PRO:HG2	1.67	0.76
15:1O:165:PRO:HG3	15:1O:217:LYS:HD2	1.68	0.76
23:1X:75:ARG:O	23:1X:75:ARG:HD3	1.86	0.75
14:1N:217:MET:HE3	14:1N:323:MET:HA	1.69	0.75
7:1G:399:TRP:HE1	17:1Q:127:ARG:HH11	1.32	0.75
20:1U:37:MET:HE1	20:1U:43:ASP:C	2.12	0.75
7:1G:255:HIS:CE1	7:1G:257:ASP:HB3	2.22	0.75
12:1L:396:ILE:HD11	12:1L:416:THR:HG21	1.69	0.75
3:1C:74:SER:HB2	3:1C:97:LEU:HB3	1.67	0.75
14:1N:66:ALA:HB2	14:1N:104:MET:HG2	1.68	0.75
2:1B:58:GLU:N	2:1B:58:GLU:OE2	2.19	0.75
10:1J:127:ILE:HD13	11:1K:2:PRO:HG3	1.69	0.75
14:1N:211:MET:HG2	14:1N:251:MET:HE1	1.68	0.75
7:1G:549:HIS:HE1	7:1G:677:ILE:HG13	1.52	0.74
14:1N:325:LEU:CD2	53:1N:402:CDL:H732	2.16	0.74
21:1V:92:LYS:HA	21:1V:95:ARG:NH2	2.02	0.74
5:1E:124:LEU:HD21	5:1E:132:THR:HG23	1.67	0.74
16:1P:203:GLN:OE1	16:1P:232:GLY:C	2.31	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:67:LEU:HD13	35:1j:68:PRO:CD	2.17	0.74
7:1G:349:PHE:HB3	7:1G:509:PRO:HB2	1.68	0.74
7:1G:564:ALA:O	7:1G:569:LYS:NZ	2.15	0.74
10:1J:60:TYR:O	10:1J:65:LEU:HD23	1.87	0.74
22:1W:52:LEU:HD11	22:1W:103:ILE:HD11	1.69	0.74
22:1W:84:ILE:HA	22:1W:87:LYS:HG2	1.68	0.74
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.21	0.74
5:1E:103:CYS:HB2	5:1E:153:MET:CG	2.16	0.74
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.69	0.74
16:1P:90:VAL:HG23	16:1P:128:LYS:HB3	1.68	0.74
22:1W:19:PRO:HA	22:1W:77:ARG:NH1	2.02	0.74
39:1n:154:PRO:O	39:1n:154:PRO:CD	2.32	0.74
3:1C:196:LYS:HZ1	17:1Q:81:ASN:HA	1.52	0.74
7:1G:211:LYS:CE	7:1G:699:GLU:OE2	2.36	0.74
14:1N:159:MET:O	14:1N:159:MET:HE3	1.87	0.74
14:1N:279:PRO:HA	14:1N:282:MET:SD	2.28	0.74
17:1Q:130:VAL:HG22	17:1Q:132:THR:H	1.53	0.74
22:1W:50:PHE:HE1	22:1W:96:VAL:HG12	1.53	0.74
20:1T:18:VAL:HG23	20:1T:54:MET:HE1	1.69	0.74
7:1G:70:ALA:O	7:1G:71:MET:HE2	1.88	0.74
9:1I:12:MET:O	27:1b:9:LYS:NZ	2.20	0.74
12:1L:338:MET:HA	12:1L:341:MET:HB2	1.69	0.74
5:1E:103:CYS:HB2	5:1E:153:MET:HG2	1.69	0.74
15:1O:204:ASN:CB	15:1O:208:LYS:HZ1	2.01	0.74
7:1G:366:THR:HG21	7:1G:450:MET:SD	2.28	0.74
28:1c:41:GLU:OE1	28:1c:44:ARG:NH2	2.20	0.74
45:1A:201:3PE:H232	27:1b:18:LEU:HD21	1.70	0.73
33:1h:114:MET:SD	33:1h:122:TRP:NE1	2.61	0.73
5:1E:149:VAL:HB	6:1F:105:CYS:SG	2.28	0.73
17:1Q:59:PHE:HD2	17:1Q:79:LEU:HB3	1.52	0.73
3:1C:141:PHE:CD2	22:1W:84:ILE:HD12	2.23	0.73
6:1F:68:ARG:HE	6:1F:254:LYS:HB2	1.54	0.73
22:1W:65:GLU:C	22:1W:69:LYS:HE2	2.13	0.73
41:1p:81:ILE:HA	41:1p:84:MET:HB2	1.70	0.73
7:1G:24:THR:HG23	7:1G:28:GLN:HB3	1.68	0.73
10:1J:171:ILE:HD11	11:1K:76:SER:HB3	1.70	0.73
11:1K:12:PHE:CD1	14:1N:72:MET:HE1	2.24	0.73
6:1F:365:CYS:HB2	46:1F:502:SF4:S2	2.28	0.73
29:1d:86:ARG:HD2	29:1d:86:ARG:C	2.14	0.73
8:1H:90:PRO:HG3	8:1H:162:LEU:HB3	1.69	0.73
16:1P:325:ARG:O	16:1P:326:TRP:HE3	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:117:ASP:OD2	22:1W:119:LEU:HG	1.89	0.73
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.70	0.73
3:1C:137:MET:HE1	3:1C:153:THR:HG23	1.71	0.73
3:1C:183:VAL:O	22:1W:101:THR:OG1	2.07	0.73
5:1E:60:TRP:HZ3	5:1E:94:PRO:CD	1.92	0.73
7:1G:228:ILE:HD13	7:1G:581:GLN:O	1.89	0.73
14:1N:341:PRO:C	29:1d:79:GLN:NE2	2.47	0.73
20:1T:20:LYS:HZ2	20:1T:27:PRO:CA	2.01	0.73
3:1C:162:PHE:HE2	4:1D:88:GLU:HB2	1.53	0.73
6:1F:82:MET:HE1	6:1F:211:ALA:O	1.89	0.73
6:1F:139:ARG:HD3	6:1F:141:GLU:HG2	1.71	0.73
15:1O:204:ASN:CG	15:1O:208:LYS:NZ	2.47	0.73
2:1B:125:TYR:CE1	4:1D:102:TYR:CE2	2.77	0.73
9:1I:69:ARG:NH2	9:1I:155:LEU:HD12	2.04	0.73
34:1i:31:GLU:HG2	39:1n:114:TYR:HA	1.70	0.72
29:1d:86:ARG:HD2	29:1d:87:ASP:N	2.04	0.72
2:1B:40:ALA:H	8:1H:54:LYS:NZ	1.88	0.72
5:1E:153:MET:CE	5:1E:160:TYR:CE1	2.68	0.72
6:1F:53:PRO:N	6:1F:127:ARG:HH12	1.86	0.72
26:1a:64:LYS:HE2	26:1a:68:ASN:HD21	1.52	0.72
12:1L:375:ILE:HD12	12:1L:462:ILE:HD11	1.70	0.72
13:1M:359:TRP:HE1	13:1M:410:MET:HE2	1.53	0.72
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.55	0.72
16:1P:258:LEU:CD1	16:1P:262:ALA:HB3	2.20	0.72
5:1E:153:MET:SD	5:1E:160:TYR:OH	2.47	0.72
8:1H:86:TRP:CH2	8:1H:233:MET:CA	2.72	0.72
11:1K:93:LEU:HD13	14:1N:54:GLU:OE2	1.89	0.72
23:1X:171:MET:HB3	29:1d:30:ARG:HE	1.54	0.72
28:1c:38:ASP:OD1	29:1d:23:PRO:CG	2.38	0.72
3:1C:193:GLU:OE2	17:1Q:75:THR:HG21	1.89	0.72
6:1F:420:ARG:HG3	6:1F:421:HIS:HD2	1.54	0.72
16:1P:234:ASN:C	16:1P:234:ASN:HD22	1.96	0.72
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.71	0.72
7:1G:275:LYS:HA	42:1q:134:ILE:HG22	1.72	0.72
26:1a:55:SER:HA	26:1a:64:LYS:HZ1	1.54	0.72
34:1i:116:ILE:HD12	34:1i:117:PRO:HD2	1.71	0.72
34:1i:119:MET:HE3	34:1i:120:LYS:H	1.54	0.72
43:1r:47:LYS:HE2	43:1r:47:LYS:H	1.54	0.72
6:1F:386:PRO:HD3	6:1F:430:MET:HE1	1.72	0.72
9:1I:67:LEU:HB3	9:1I:155:LEU:HD22	1.71	0.72
9:1I:97:GLU:HB2	9:1I:98:PRO:HD2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:101:GLU:OE1	6:1F:102:PRO:O	2.07	0.71
29:1d:2:MET:HA	29:1d:2:MET:HE3	1.71	0.71
5:1E:50:VAL:HA	5:1E:53:LEU:HD23	1.72	0.71
7:1G:255:HIS:CE1	7:1G:258:ILE:HG12	2.25	0.71
11:1K:47:ILE:HG12	14:1N:79:LEU:HD13	1.71	0.71
22:1W:113:PRO:O	22:1W:113:PRO:CD	2.36	0.71
5:1E:184:PRO:HD2	44:1s:44:HIS:ND1	2.05	0.71
7:1G:241:SER:C	7:1G:248:MET:HE1	2.15	0.71
19:1S:64:LEU:HD22	19:1S:65:TRP:H	1.54	0.71
15:1O:90:ASP:O	32:1g:27:GLN:NE2	2.23	0.71
16:1P:218:ILE:HD12	16:1P:218:ILE:H	1.55	0.71
19:1S:78:LEU:HD11	19:1S:89:THR:HG21	1.72	0.71
20:1T:69:LYS:NZ	20:1T:70:LEU:CD2	2.53	0.71
26:1a:1:MET:HE1	43:1r:0:ACE:CH3	2.21	0.71
5:1E:202:LEU:H	6:1F:20:ARG:HH22	1.36	0.71
7:1G:582:GLN:NE2	7:1G:583:THR:O	2.23	0.71
16:1P:13:ARG:NH2	16:1P:61:PRO:O	2.22	0.71
5:1E:48:LEU:HD21	5:1E:87:TYR:CZ	2.25	0.71
16:1P:335:LYS:HD2	16:1P:336:PRO:HD2	1.72	0.71
17:1Q:42:ARG:HH21	17:1Q:44:ASN:HA	1.56	0.71
37:1l:14:PRO:HB2	37:1l:20:ARG:HD3	1.72	0.71
16:1P:46:ILE:HD13	18:1R:26:VAL:HG21	1.73	0.71
37:1l:136:ASN:HD22	37:1l:139:TYR:HB3	1.56	0.71
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.24	0.71
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.71	0.71
42:1q:122:GLN:OE1	42:1q:122:GLN:N	2.21	0.71
6:1F:49:LEU:HG	6:1F:127:ARG:HG2	1.73	0.71
15:1O:204:ASN:CG	15:1O:208:LYS:HZ1	1.98	0.71
7:1G:195:LEU:HD12	7:1G:198:ASN:HD21	1.55	0.71
7:1G:264:SER:O	7:1G:267:THR:OG1	2.09	0.71
15:1O:77:CYS:HB2	15:1O:96:LEU:HD23	1.71	0.71
7:1G:122:MET:HA	7:1G:122:MET:HE3	1.73	0.70
16:1P:200:THR:HB	16:1P:238:LEU:HG	1.71	0.70
29:1d:26:LEU:HD12	29:1d:27:THR:HG23	1.72	0.70
9:1I:36:MET:HE2	9:1I:36:MET:HA	1.73	0.70
14:1N:270:MET:HE1	14:1N:282:MET:SD	2.31	0.70
16:1P:325:ARG:C	16:1P:326:TRP:CE3	2.68	0.70
12:1L:88:MET:HE3	12:1L:88:MET:HA	1.71	0.70
12:1L:209:PRO:HB2	12:1L:213:LEU:HG	1.73	0.70
14:1N:45:MET:HE2	14:1N:45:MET:HA	1.72	0.70
5:1E:145:LEU:HD11	5:1E:160:TYR:OH	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:22:TYR:OH	14:1N:61:LEU:HD23	1.91	0.70
41:1p:162:MET:HA	41:1p:165:GLU:HB3	1.73	0.70
6:1F:82:MET:HB3	6:1F:129:MET:HB3	1.73	0.70
6:1F:55:TRP:O	6:1F:55:TRP:CE3	2.45	0.70
6:1F:90:PRO:HG3	44:1s:66:PRO:HG3	1.73	0.70
7:1G:283:MET:HE1	7:1G:292:THR:C	2.17	0.70
8:1H:86:TRP:CZ3	8:1H:233:MET:HA	2.26	0.70
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.74	0.70
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.25	0.70
5:1E:45:ALA:HA	6:1F:198:GLY:HA3	1.73	0.70
37:1l:70:ARG:HE	37:1l:86:ARG:HH11	1.40	0.70
2:1B:94:ASN:HB3	3:1C:174:LEU:CD1	2.22	0.70
4:1D:221:ARG:HE	43:1r:24:GLN:HG2	1.57	0.70
12:1L:253:VAL:HG23	12:1L:310:LEU:HD21	1.72	0.70
22:1W:65:GLU:O	22:1W:69:LYS:CE	2.39	0.70
6:1F:276:LEU:HA	6:1F:317:MET:HE3	1.74	0.69
22:1W:51:GLN:O	22:1W:100:ARG:NH1	2.25	0.69
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.73	0.69
4:1D:326:ASP:OD1	7:1G:127:ARG:NH2	2.25	0.69
13:1M:450:ASN:HD21	13:1M:453:MET:CE	1.96	0.69
14:1N:109:SER:HB3	14:1N:110:PRO:HD2	1.73	0.69
15:1O:78:SER:H	15:1O:92:ASN:HD21	1.40	0.69
18:1R:28:PHE:CE1	18:1R:33:LYS:HG3	2.22	0.69
18:1R:81:THR:OG1	18:1R:90:GLN:OE1	2.09	0.69
20:1T:20:LYS:NZ	20:1T:27:PRO:CA	2.51	0.69
20:1U:21:LEU:HA	36:1k:18:TYR:CE1	2.28	0.69
16:1P:37:HIS:HB3	16:1P:215:ILE:HD13	1.74	0.69
31:1f:49:ARG:HB2	31:1f:52:GLU:HB3	1.75	0.69
13:1M:257:MET:HE2	13:1M:257:MET:CA	2.23	0.69
43:1r:63:MET:HE3	43:1r:64:PRO:HD2	1.74	0.69
6:1F:9:LYS:HE2	6:1F:12:PHE:HA	1.74	0.69
6:1F:321:ALA:HA	6:1F:324:GLN:HE22	1.57	0.69
7:1G:157:THR:OG1	7:1G:161:ARG:NH1	2.24	0.69
7:1G:190:MET:O	7:1G:192:MET:HE3	1.92	0.69
15:1O:171:TYR:CE2	15:1O:206:TYR:CD1	2.80	0.69
21:1V:92:LYS:HA	21:1V:95:ARG:HH21	1.57	0.69
32:1g:111:ASN:HB3	41:1p:161:ARG:HH22	1.58	0.69
6:1F:106:LYS:O	6:1F:110:ILE:HG22	1.92	0.69
6:1F:391:SER:HB3	43:1r:48:LEU:HG	1.74	0.69
9:1I:14:MET:HE2	9:1I:14:MET:HA	1.74	0.69
12:1L:452:ASN:HB3	12:1L:456:ARG:HH12	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:85:GLN:OE1	19:1S:85:GLN:N	2.26	0.69
22:1W:81:LEU:HD13	22:1W:84:ILE:HD11	1.75	0.69
8:1H:55:LEU:HD11	8:1H:220:PHE:HD2	1.56	0.69
14:1N:25:HIS:NE2	30:1e:17:MET:SD	2.66	0.69
14:1N:28:LEU:HA	14:1N:31:ILE:HD12	1.74	0.69
16:1P:234:ASN:C	16:1P:234:ASN:ND2	2.50	0.69
25:1Z:7:LYS:HD2	43:1r:37:PRO:O	1.92	0.69
31:1f:22:PHE:CE1	31:1f:26:LEU:HD21	2.27	0.69
32:1g:75:THR:HG21	33:1h:36:VAL:HG11	1.75	0.69
6:1F:101:GLU:OE2	6:1F:104:THR:CG2	2.38	0.69
20:1U:22:TYR:HE1	36:1k:43:PRO:HB2	1.56	0.69
30:1e:44:HIS:CE1	33:1h:130:LYS:H	2.10	0.69
12:1L:470:ASN:O	40:1o:69:LYS:NZ	2.25	0.69
15:1O:204:ASN:C	15:1O:208:LYS:NZ	2.51	0.69
15:1O:204:ASN:ND2	15:1O:208:LYS:NZ	2.41	0.69
22:1W:76:PRO:CG	22:1W:76:PRO:CD	0.69	0.69
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.25	0.69
20:1T:14:ARG:HG3	20:1T:58:PHE:HE2	1.57	0.68
32:1g:96:LEU:HD11	32:1g:100:ARG:HH21	1.58	0.68
7:1G:336:ASN:HD21	19:1S:67:ARG:HH21	1.40	0.68
15:1O:279:LEU:HD12	15:1O:280:PRO:HD2	1.75	0.68
20:1U:65:ILE:HD12	20:1U:65:ILE:H	1.58	0.68
29:1d:103:GLU:OE1	29:1d:103:GLU:N	2.24	0.68
8:1H:30:TYR:HD2	26:1a:5:ILE:HD11	1.56	0.68
52:1M:501:PGT:H242	14:1N:284:MET:HG3	1.75	0.68
16:1P:268:ARG:NH1	16:1P:271:GLU:OE2	2.26	0.68
22:1W:48:HIS:O	22:1W:51:GLN:NE2	2.26	0.68
30:1e:49:ILE:HD11	33:1h:118:GLY:HA3	1.73	0.68
4:1D:281:VAL:HG21	4:1D:310:ILE:HG23	1.74	0.68
6:1F:202:LYS:CE	6:1F:361:GLN:HG3	2.23	0.68
7:1G:449:PRO:O	7:1G:487:TRP:NE1	2.20	0.68
20:1U:87:TYR:HA	34:1i:19:ARG:HD2	1.75	0.68
2:1B:125:TYR:CE1	4:1D:102:TYR:CE1	2.81	0.68
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.24	0.68
6:1F:202:LYS:NZ	6:1F:361:GLN:HG3	2.09	0.68
8:1H:79:LEU:HB2	8:1H:222:MET:SD	2.33	0.68
18:1R:20:ASP:OD1	18:1R:21:GLY:N	2.27	0.68
23:1X:142:HIS:ND1	25:1Z:114:THR:OG1	2.26	0.68
7:1G:594:ARG:HD2	22:1W:126:HIS:HB3	1.76	0.68
18:1R:34:GLU:HG3	42:1q:124:TYR:HD1	1.58	0.68
1:1A:84:LEU:HD12	8:1H:309:ILE:HD12	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:95:MET:HE3	14:1N:148:SER:C	2.18	0.68
17:1Q:59:PHE:CD2	17:1Q:79:LEU:HB3	2.28	0.68
39:1n:134:ARG:NH1	39:1n:162:LEU:O	2.26	0.68
3:1C:86:ARG:NH2	21:1V:112:LYS:O	2.27	0.68
6:1F:127:ARG:HH11	6:1F:127:ARG:HG3	1.59	0.68
6:1F:150:GLN:OE1	6:1F:153:ILE:CD1	2.42	0.68
8:1H:26:LYS:HG3	8:1H:36:GLY:HA3	1.75	0.68
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.27	0.68
37:1l:22:ALA:O	37:1l:25:LYS:HE3	1.94	0.68
41:1p:11:GLU:HG3	41:1p:14:ARG:NH2	2.09	0.68
4:1D:415:VAL:HA	4:1D:418:ILE:HD12	1.76	0.68
5:1E:37:ASN:OD1	5:1E:38:TYR:CD1	2.46	0.68
17:1Q:11:ILE:HG12	22:1W:77:ARG:NH2	2.08	0.68
20:1U:15:VAL:HG21	20:1U:77:VAL:HG22	1.76	0.68
4:1D:20:TYR:CG	12:1L:571:MET:HE1	2.29	0.68
3:1C:78:LEU:HD21	3:1C:92:ILE:HG23	1.77	0.67
29:1d:2:MET:HE1	33:1h:122:TRP:HB3	1.76	0.67
8:1H:106:LEU:HD12	8:1H:150:LEU:HD12	1.74	0.67
12:1L:142:ILE:HD13	13:1M:370:PRO:HB2	1.75	0.67
14:1N:51:ARG:HG2	14:1N:121:GLY:HA2	1.76	0.67
15:1O:44:GLU:OE2	15:1O:44:GLU:N	2.24	0.67
17:1Q:58:GLU:OE1	17:1Q:58:GLU:N	2.27	0.67
20:1T:8:LEU:HD12	20:1T:88:GLU:HB3	1.74	0.67
20:1U:21:LEU:HG	36:1k:18:TYR:HE1	1.59	0.67
32:1g:120:LEU:HD23	41:1p:166:ARG:HE	1.59	0.67
7:1G:672:TYR:CB	7:1G:684:MET:HE3	2.21	0.67
20:1U:20:LYS:HE3	20:1U:27:PRO:HB3	1.76	0.67
20:1U:35:HIS:CE1	20:1U:37:MET:HB2	2.29	0.67
26:1a:2:TRP:HZ2	53:1r:201:CDL:H521	1.59	0.67
32:1g:94:GLU:HG3	41:1p:8:VAL:HG11	1.76	0.67
2:1B:82:GLN:O	2:1B:82:GLN:NE2	2.26	0.67
2:1B:125:TYR:HE1	4:1D:102:TYR:CE1	2.13	0.67
6:1F:274:VAL:O	6:1F:317:MET:HG3	1.94	0.67
10:1J:64:MET:SD	10:1J:65:LEU:HD22	2.34	0.67
11:1K:26:LEU:HD11	11:1K:78:LEU:HD13	1.77	0.67
12:1L:230:HIS:H	12:1L:231:PRO:HD2	1.59	0.67
13:1M:216:LEU:HD12	13:1M:291:VAL:HG22	1.76	0.67
21:1V:91:ARG:C	21:1V:95:ARG:HH21	2.02	0.67
4:1D:242:ILE:HA	4:1D:409:HIS:CE1	2.30	0.67
6:1F:51:LYS:HD3	6:1F:55:TRP:HD1	1.60	0.67
7:1G:311:GLN:NE2	7:1G:338:VAL:O	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:704:CYS:O	9:1I:104:ARG:N	2.26	0.67
10:1J:31:LEU:HA	10:1J:34:ILE:HG12	1.76	0.67
15:1O:194:ILE:HD13	15:1O:199:LEU:HD11	1.76	0.67
29:1d:112:ILE:O	41:1p:159:LYS:NZ	2.26	0.67
2:1B:40:ALA:CB	8:1H:54:LYS:HZ3	2.07	0.67
5:1E:36:LYS:HE2	44:1s:59:SER:HA	1.75	0.67
12:1L:525:MET:HE1	37:1l:95:PRO:HG2	1.77	0.67
28:1c:13:ASP:OD2	28:1c:16:LYS:HB2	1.94	0.67
2:1B:161:LEU:HA	2:1B:164:GLN:NE2	2.09	0.67
3:1C:210:ARG:NH2	7:1G:35:MET:SD	2.68	0.67
5:1E:135:LYS:HD2	5:1E:135:LYS:N	2.10	0.67
15:1O:37:ARG:NH2	15:1O:41:GLU:OE2	2.28	0.67
16:1P:134:HIS:H	16:1P:149:LYS:HE3	1.60	0.67
16:1P:139:ILE:HA	16:1P:147:ARG:HA	1.76	0.67
16:1P:258:LEU:HD12	16:1P:259:PRO:O	1.93	0.67
15:1O:233:LYS:HZ2	21:1V:91:ARG:HH11	1.42	0.67
20:1U:6:LEU:HD12	20:1U:11:ILE:HD11	1.76	0.67
20:1U:35:HIS:ND1	20:1U:38:LYS:HG2	2.09	0.67
29:1d:99:GLU:OE1	29:1d:99:GLU:N	2.27	0.67
12:1L:283:ILE:HD13	37:1l:112:MET:HG3	1.77	0.67
32:1g:100:ARG:HG2	32:1g:107:LEU:HA	1.75	0.67
4:1D:158:ALA:HB1	4:1D:163:ALA:HB3	1.76	0.67
7:1G:229:ASP:OD1	7:1G:231:MET:N	2.25	0.67
8:1H:5:ASN:ND2	26:1a:26:ILE:HD11	2.10	0.67
12:1L:132:VAL:O	12:1L:262:ARG:NH2	2.25	0.67
14:1N:265:MET:HE3	14:1N:343:LEU:HD21	1.76	0.67
15:1O:72:GLN:OE1	15:1O:76:ASN:ND2	2.28	0.67
43:1r:32:LYS:O	43:1r:35:GLN:NE2	2.28	0.67
4:1D:58:ALA:HB1	4:1D:62:LEU:HB3	1.77	0.66
5:1E:39:PRO:HG2	5:1E:42:HIS:HB2	1.78	0.66
7:1G:284:ILE:HA	7:1G:559:VAL:HG12	1.76	0.66
9:1I:36:MET:HE1	43:1r:15:SER:HB2	1.76	0.66
9:1I:98:PRO:HA	9:1I:104:ARG:HA	1.75	0.66
4:1D:166:PRO:HD3	4:1D:228:MET:HE1	1.76	0.66
6:1F:202:LYS:HD2	6:1F:359:CYS:HB2	1.77	0.66
12:1L:175:ASN:ND2	12:1L:223:LYS:NZ	2.42	0.66
13:1M:30:HIS:HD2	31:1f:16:VAL:HB	1.60	0.66
26:1a:1:MET:HE1	43:1r:0:ACE:H1	1.76	0.66
32:1g:100:ARG:HD2	32:1g:105:LEU:HD22	1.77	0.66
5:1E:37:ASN:OD1	5:1E:38:TYR:HD1	1.77	0.66
6:1F:55:TRP:CH2	6:1F:59:GLU:HB2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:104:TYR:HE2	10:1J:166:VAL:HB	1.60	0.66
3:1C:199:LEU:HD12	4:1D:354:GLU:HA	1.76	0.66
7:1G:278:ARG:NH1	7:1G:548:HIS:O	2.28	0.66
15:1O:171:TYR:CE2	15:1O:207:LYS:NZ	2.63	0.66
42:1q:50:GLU:OE1	42:1q:50:GLU:N	2.28	0.66
15:1O:25:ILE:HG23	15:1O:168:VAL:HB	1.77	0.66
15:1O:65:ASP:HB3	15:1O:67:LYS:HG2	1.76	0.66
12:1L:502:LEU:O	12:1L:506:ASN:ND2	2.29	0.66
16:1P:177:ARG:HA	16:1P:180:ASN:HD21	1.59	0.66
25:1Z:95:ALA:HA	25:1Z:106:VAL:HG11	1.78	0.66
25:1Z:121:MET:HE1	25:1Z:137:THR:HA	1.78	0.66
13:1M:72:LEU:HD23	13:1M:75:LEU:HD12	1.77	0.66
2:1B:102:LYS:O	2:1B:106:GLN:HG3	1.96	0.66
4:1D:152:MET:HE1	4:1D:156:THR:HG21	1.77	0.66
17:1Q:40:PRO:HG3	17:1Q:56:LYS:HD3	1.77	0.66
22:1W:24:ASP:OD1	22:1W:25:MET:N	2.29	0.66
43:1r:101:LYS:NZ	43:1r:102:ARG:O	2.29	0.66
13:1M:22:MET:O	13:1M:26:ASN:ND2	2.29	0.66
20:1T:18:VAL:HA	20:1T:21:LEU:CG	2.21	0.66
22:1W:68:MET:HA	22:1W:68:MET:HE3	1.78	0.66
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.29	0.66
33:1h:64:TRP:CD1	33:1h:77:ARG:HG3	2.31	0.66
34:1i:54:ALA:C	34:1i:55:PRO:CA	2.69	0.66
34:1i:59:VAL:HA	34:1i:62:LYS:HE3	1.76	0.66
2:1B:100:LEU:HD22	2:1B:140:VAL:HG21	1.78	0.65
6:1F:147:SER:HA	6:1F:150:GLN:HG2	1.76	0.65
12:1L:582:GLY:O	14:1N:58:LYS:NZ	2.29	0.65
3:1C:189:GLU:CD	16:1P:14:SER:H	2.04	0.65
6:1F:202:LYS:HE3	6:1F:361:GLN:HG3	1.78	0.65
7:1G:447:LYS:O	7:1G:448:LYS:HD2	1.96	0.65
13:1M:201:MET:HG2	52:1M:501:PGT:H441	1.77	0.65
28:1c:41:GLU:CD	28:1c:44:ARG:NH2	2.53	0.65
32:1g:25:ARG:HE	32:1g:26:LEU:HB3	1.61	0.65
5:1E:7:PHE:HA	5:1E:92:ARG:HH12	1.61	0.65
6:1F:109:GLU:HG3	6:1F:267:THR:HG21	1.78	0.65
7:1G:673:MET:HE1	7:1G:688:VAL:HG11	1.78	0.65
10:1J:125:TRP:HB2	25:1Z:137:THR:HG21	1.77	0.65
13:1M:307:TRP:NE1	38:1m:127:SER:OG	2.29	0.65
17:1Q:106:GLU:OE2	17:1Q:106:GLU:HA	1.95	0.65
20:1T:16:LEU:HD12	20:1T:30:LEU:HD11	1.78	0.65
23:1X:81:PHE:HE1	23:1X:85:TRP:HB3	1.62	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:106:THR:HA	5:1E:109:MET:HG3	1.78	0.65
7:1G:366:THR:CG2	7:1G:450:MET:HE1	2.26	0.65
26:1a:66:LEU:HD13	26:1a:69:ILE:HD11	1.78	0.65
7:1G:336:ASN:ND2	19:1S:67:ARG:HH21	1.93	0.65
7:1G:589:PRO:HD2	22:1W:126:HIS:HD2	1.61	0.65
14:1N:29:ILE:HG13	14:1N:86:ILE:HD11	1.78	0.65
17:1Q:127:ARG:HG2	44:1s:70:ARG:NH1	2.11	0.65
28:1c:17:VAL:O	28:1c:21:LEU:HD12	1.96	0.65
34:1i:54:ALA:HB3	34:1i:57:LYS:HG2	1.78	0.65
4:1D:183:ARG:NH1	4:1D:210:ASP:OD2	2.29	0.65
7:1G:624:GLU:HB2	7:1G:631:VAL:HG21	1.79	0.65
10:1J:3:MET:HE3	25:1Z:130:ASN:OD1	1.97	0.65
15:1O:28:ASP:OD1	15:1O:206:TYR:OH	2.15	0.65
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	1.77	0.65
35:1j:68:PRO:HD2	35:1j:68:PRO:O	1.97	0.65
37:1l:77:ILE:HD11	38:1m:67:TRP:CD2	2.32	0.65
2:1B:69:MET:HE1	2:1B:76:PHE:H	1.61	0.65
3:1C:22:LEU:HD23	3:1C:48:LEU:HD22	1.78	0.65
4:1D:266:GLN:HE22	43:1r:102:ARG:HE	1.44	0.65
6:1F:127:ARG:HD3	6:1F:171:TYR:CE1	2.32	0.65
6:1F:307:ILE:HD12	6:1F:308:PRO:HD2	1.78	0.65
16:1P:8:HIS:H	16:1P:16:VAL:HG23	1.62	0.65
2:1B:41:ARG:H	8:1H:54:LYS:HE2	1.58	0.65
2:1B:41:ARG:HE	2:1B:110:PRO:HG3	1.60	0.65
7:1G:70:ALA:C	7:1G:71:MET:HE2	2.22	0.65
15:1O:183:ILE:HA	15:1O:186:LYS:HD3	1.77	0.65
3:1C:192:GLN:HE21	17:1Q:72:TRP:CB	2.10	0.65
6:1F:30:ASP:HB3	6:1F:35:GLY:HA3	1.79	0.65
7:1G:359:ARG:NH2	7:1G:629:ASN:OD1	2.30	0.65
12:1L:359:MET:N	12:1L:359:MET:SD	2.70	0.65
13:1M:13:PRO:HB3	45:1N:401:3PE:H2C2	1.78	0.65
13:1M:266:MET:HA	13:1M:269:MET:CE	2.26	0.65
14:1N:83:GLN:NE2	30:1e:36:GLU:OE2	2.27	0.65
32:1g:25:ARG:NE	32:1g:26:LEU:HB3	2.12	0.65
6:1F:45:THR:HA	6:1F:48:ILE:HD12	1.78	0.65
8:1H:65:THR:HA	16:1P:324:TYR:HB2	1.79	0.65
10:1J:68:PHE:CZ	11:1K:75:LEU:CD2	2.78	0.65
12:1L:71:LEU:HD11	13:1M:310:MET:SD	2.37	0.65
5:1E:89:MET:HE3	6:1F:181:ALA:O	1.97	0.64
7:1G:140:LYS:CD	7:1G:150:MET:CE	2.75	0.64
7:1G:548:HIS:HE1	7:1G:676:SER:OG	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:265:MET:HE1	23:1X:166:LEU:HD21	1.79	0.64
24:1Y:65:ILE:HD11	24:1Y:100:LEU:HD23	1.79	0.64
31:1f:53:GLU:OE2	31:1f:54:VAL:HG22	1.97	0.64
40:1o:50:LEU:O	40:1o:55:ARG:NH1	2.30	0.64
43:1r:28:GLN:N	43:1r:28:GLN:OE1	2.27	0.64
4:1D:171:PHE:HA	4:1D:174:ARG:HG3	1.79	0.64
12:1L:237:MET:HE1	12:1L:244:SER:OG	1.97	0.64
37:1l:30:ARG:NH2	38:1m:31:ALA:O	2.30	0.64
6:1F:224:ASN:ND2	48:1F:501:FMN:O2	2.31	0.64
32:1g:23:THR:OG1	32:1g:24:ILE:N	2.31	0.64
37:1l:140:LEU:O	41:1p:122:GLN:NE2	2.30	0.64
2:1B:122:GLY:HA3	9:1I:114:THR:HB	1.80	0.64
6:1F:51:LYS:HD3	6:1F:55:TRP:CD1	2.32	0.64
14:1N:154:MET:HE1	14:1N:194:LEU:HB3	1.79	0.64
37:1l:58:ARG:NH1	37:1l:70:ARG:O	2.30	0.64
7:1G:238:ILE:O	7:1G:253:ARG:NH1	2.30	0.64
11:1K:8:ILE:HB	11:1K:43:MET:CE	2.27	0.64
3:1C:175:ARG:NH2	3:1C:186:GLU:OE1	2.30	0.64
6:1F:25:LEU:HD23	6:1F:269:GLU:HB3	1.79	0.64
8:1H:3:MET:HE1	8:1H:7:LEU:HD23	1.79	0.64
12:1L:514:LYS:NZ	45:1L:704:3PE:O12	2.30	0.64
13:1M:168:GLN:HE22	33:1h:104:ARG:HD2	1.63	0.64
2:1B:144:ILE:HA	9:1I:142:GLU:HA	1.80	0.64
5:1E:153:MET:HE2	5:1E:160:TYR:HE1	1.63	0.64
7:1G:56:LEU:HD11	7:1G:65:VAL:HB	1.79	0.64
19:1S:63:LYS:HE3	19:1S:75:ASN:ND2	2.13	0.64
34:1i:74:VAL:O	34:1i:78:VAL:HG12	1.97	0.64
40:1o:96:LYS:HD3	40:1o:96:LYS:H	1.63	0.64
2:1B:62:MET:SD	2:1B:157:LEU:HD13	2.38	0.64
7:1G:9:ILE:HD11	7:1G:75:LYS:HB3	1.80	0.64
12:1L:371:THR:HG22	36:1k:68:LYS:HD3	1.78	0.64
22:1W:76:PRO:N	22:1W:76:PRO:HG2	1.82	0.64
23:1X:23:VAL:HG13	23:1X:81:PHE:CZ	2.29	0.64
40:1o:114:ARG:HD2	40:1o:117:ARG:HH12	1.63	0.64
3:1C:82:ASP:O	4:1D:387:TYR:OH	2.17	0.64
12:1L:310:LEU:HA	12:1L:313:MET:HB2	1.77	0.64
42:1q:59:HIS:ND1	42:1q:60:ARG:CG	2.53	0.64
4:1D:124:LYS:HG2	4:1D:363:THR:HG21	1.80	0.63
4:1D:391:ILE:O	4:1D:430:ARG:NH1	2.31	0.63
29:1d:2:MET:HE3	33:1h:122:TRP:HB3	1.79	0.63
37:1l:80:ASP:HB3	37:1l:83:MET:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:179:GLU:HG3	16:1P:33:TYR:HD2	1.62	0.63
4:1D:301:VAL:HA	4:1D:304:MET:CE	2.27	0.63
7:1G:549:HIS:CE1	7:1G:677:ILE:HG13	2.33	0.63
8:1H:103:LEU:HD13	8:1H:160:TYR:CD2	2.33	0.63
9:1I:97:GLU:OE1	9:1I:97:GLU:N	2.31	0.63
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.62	0.63
15:1O:97:GLN:NE2	15:1O:131:ASP:O	2.31	0.63
16:1P:201:VAL:HG23	16:1P:237:LEU:HD23	1.80	0.63
21:1V:35:GLY:HA2	21:1V:44:ARG:HH12	1.62	0.63
22:1W:98:LYS:HZ2	22:1W:102:HIS:HB3	1.64	0.63
29:1d:108:THR:HG23	29:1d:110:GLY:H	1.63	0.63
2:1B:40:ALA:HB3	8:1H:54:LYS:HD3	1.80	0.63
6:1F:91:LYS:HB3	6:1F:131:ALA:HA	1.79	0.63
6:1F:96:ASN:ND2	6:1F:189:GLU:OE1	2.30	0.63
8:1H:169:GLN:NE2	8:1H:241:LEU:O	2.31	0.63
9:1I:44:GLU:N	26:1a:1:MET:SD	2.71	0.63
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.79	0.63
6:1F:52:GLY:CA	6:1F:127:ARG:HH22	2.09	0.63
7:1G:27:LEU:HD22	7:1G:37:ILE:HG21	1.81	0.63
12:1L:130:ILE:C	12:1L:130:ILE:HD12	2.22	0.63
15:1O:47:GLY:O	15:1O:120:GLN:NE2	2.30	0.63
17:1Q:20:THR:OG1	17:1Q:21:THR:N	2.31	0.63
17:1Q:27:GLU:H	17:1Q:27:GLU:CD	2.06	0.63
17:1Q:66:GLU:HG2	17:1Q:71:GLY:HA2	1.78	0.63
38:1m:39:ARG:NH1	38:1m:39:ARG:O	2.31	0.63
2:1B:101:ARG:NH2	2:1B:105:ASP:OD1	2.30	0.63
22:1W:65:GLU:O	22:1W:69:LYS:NZ	2.31	0.63
2:1B:71:ARG:HG3	2:1B:72:PHE:CD1	2.33	0.63
3:1C:176:TYR:HA	3:1C:183:VAL:HA	1.81	0.63
8:1H:60:PRO:HB3	8:1H:219:PRO:HD3	1.79	0.63
12:1L:542:LEU:HB3	37:1l:83:MET:SD	2.39	0.63
34:1i:40:TRP:HB2	34:1i:43:GLU:HG2	1.79	0.63
5:1E:105:THR:OG1	5:1E:144:CYS:SG	2.52	0.63
6:1F:272:MET:SD	6:1F:273:SER:OG	2.56	0.63
7:1G:244:THR:HG22	42:1q:133:LYS:HZ1	1.64	0.63
8:1H:3:MET:HE3	8:1H:3:MET:C	2.24	0.63
13:1M:286:ILE:HD13	13:1M:326:LEU:HB3	1.79	0.63
14:1N:44:LEU:HD13	14:1N:122:ILE:HG21	1.79	0.63
41:1p:35:ILE:HG22	41:1p:39:LEU:HD12	1.81	0.63
41:1p:118:GLU:OE1	41:1p:118:GLU:N	2.23	0.63
4:1D:221:ARG:HG3	43:1r:24:GLN:HE22	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:342:MET:HE3	4:1D:346:ILE:HG13	1.78	0.63
6:1F:280:ILE:HD13	6:1F:291:TRP:HZ3	1.63	0.63
8:1H:195:ARG:HG3	8:1H:231:ILE:HD11	1.79	0.63
17:1Q:66:GLU:OE1	17:1Q:67:ASN:O	2.17	0.63
20:1T:69:LYS:HD2	20:1T:70:LEU:N	2.14	0.63
23:1X:89:ASP:OD1	23:1X:89:ASP:N	2.32	0.63
1:1A:54:LYS:HD3	1:1A:114:ALA:HB3	1.80	0.63
7:1G:129:ARG:HB3	43:1r:48:LEU:HB2	1.79	0.63
10:1J:44:VAL:HG12	10:1J:49:GLY:HA3	1.78	0.63
31:1f:55:THR:HG1	31:1f:56:TRP:CD1	2.17	0.63
3:1C:193:GLU:HG3	17:1Q:75:THR:OG1	1.99	0.62
6:1F:21:ILE:HG21	6:1F:230:VAL:HG12	1.81	0.62
11:1K:34:GLU:HA	11:1K:37:MET:HG3	1.79	0.62
13:1M:364:LEU:HG	13:1M:369:LEU:HD11	1.79	0.62
53:1r:201:CDL:H741	53:1r:201:CDL:H552	1.80	0.62
1:1A:109:LYS:HE2	1:1A:109:LYS:HA	1.81	0.62
3:1C:64:LEU:HB3	3:1C:72:PHE:HB2	1.81	0.62
7:1G:283:MET:HB3	7:1G:560:ILE:H	1.64	0.62
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.32	0.62
15:1O:204:ASN:ND2	15:1O:208:LYS:HZ3	1.95	0.62
20:1T:29:LYS:NZ	20:1T:40:LEU:O	2.31	0.62
20:1U:54:MET:HA	20:1U:54:MET:HE3	1.81	0.62
27:1b:10:ASN:HA	27:1b:14:LYS:NZ	2.15	0.62
1:1A:55:PHE:HB2	10:1J:70:TYR:OH	2.00	0.62
1:1A:88:LEU:HD21	8:1H:309:ILE:HG13	1.80	0.62
7:1G:601:ARG:NH1	7:1G:612:PRO:O	2.32	0.62
12:1L:306:THR:HG22	12:1L:336:LYS:HG2	1.82	0.62
45:1L:702:3PE:H231	37:1l:88:ARG:HG2	1.80	0.62
16:1P:203:GLN:OE1	16:1P:233:PRO:N	2.32	0.62
16:1P:258:LEU:HD13	16:1P:262:ALA:CB	2.28	0.62
31:1f:33:LYS:HG2	31:1f:34:LEU:HD12	1.80	0.62
36:1k:34:LYS:O	36:1k:38:ARG:NH1	2.32	0.62
43:1r:47:LYS:H	43:1r:47:LYS:CE	2.12	0.62
6:1F:306:LEU:HD22	6:1F:418:LEU:HD22	1.79	0.62
7:1G:257:ASP:O	7:1G:394:ARG:NH2	2.32	0.62
16:1P:202:LYS:HG2	16:1P:291:ASP:HB2	1.82	0.62
18:1R:32:GLN:HG2	42:1q:122:GLN:HA	1.81	0.62
37:1l:53:ARG:NH2	38:1m:13:LEU:O	2.33	0.62
41:1p:141:ARG:O	41:1p:157:LYS:NZ	2.31	0.62
42:1q:38:LEU:HD21	42:1q:47:LYS:HZ1	1.61	0.62
5:1E:135:LYS:HA	5:1E:135:LYS:HE3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:161:TYR:HB3	5:1E:184:PRO:HA	1.81	0.62
6:1F:364:PRO:HB3	6:1F:399:ILE:HG22	1.82	0.62
15:1O:207:LYS:HA	15:1O:207:LYS:HE3	1.79	0.62
5:1E:72:ILE:C	5:1E:74:GLN:HE22	2.08	0.62
6:1F:207:PRO:HG2	7:1G:72:PRO:HD2	1.82	0.62
9:1I:92:ILE:HG12	9:1I:111:ILE:HG12	1.81	0.62
10:1J:20:PHE:HE1	11:1K:32:CYS:HA	1.64	0.62
11:1K:30:LEU:HD21	11:1K:75:LEU:HD22	1.82	0.62
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.34	0.62
4:1D:221:ARG:HD2	43:1r:24:GLN:HE21	1.64	0.62
7:1G:230:VAL:HG23	7:1G:497:ALA:CB	2.29	0.62
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.80	0.62
12:1L:362:LEU:HB2	12:1L:431:PHE:HD1	1.65	0.62
13:1M:373:ILE:HD11	13:1M:447:LEU:HB2	1.80	0.62
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.65	0.62
25:1Z:24:ASN:O	25:1Z:24:ASN:ND2	2.26	0.62
6:1F:150:GLN:OE1	6:1F:153:ILE:HD12	2.00	0.62
8:1H:91:MET:HE2	8:1H:259:PHE:HE2	1.63	0.62
12:1L:545:SER:OG	13:1M:274:SER:O	2.17	0.62
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	1.80	0.62
20:1T:54:MET:N	20:1T:54:MET:HE2	2.15	0.62
22:1W:65:GLU:C	22:1W:69:LYS:CE	2.73	0.62
22:1W:65:GLU:OE1	22:1W:69:LYS:HE2	1.99	0.62
3:1C:83:VAL:HG21	3:1C:86:ARG:HD2	1.82	0.62
4:1D:135:GLN:OE1	4:1D:138:ARG:NH2	2.33	0.62
5:1E:10:ARG:HH22	18:1R:77:LYS:HG2	1.65	0.62
6:1F:137:TYR:CE2	6:1F:186:CYS:HB3	2.35	0.62
12:1L:294:THR:O	12:1L:524:ASN:ND2	2.32	0.62
14:1N:209:ILE:O	14:1N:213:LEU:CD2	2.48	0.62
19:1S:39:ARG:CZ	19:1S:90:LEU:HD21	2.29	0.62
7:1G:391:PHE:CE1	7:1G:395:ILE:HD11	2.35	0.62
7:1G:494:HIS:ND1	7:1G:499:GLN:HB3	2.15	0.62
9:1I:99:ARG:N	9:1I:103:SER:O	2.28	0.62
13:1M:1:FME:HG2	13:1M:111:THR:HG21	1.82	0.62
15:1O:92:ASN:OD1	15:1O:95:ARG:NH1	2.33	0.62
20:1U:49:GLU:OE1	36:1k:44:TRP:NE1	2.32	0.62
25:1Z:24:ASN:C	25:1Z:24:ASN:HD22	2.06	0.62
34:1i:79:TRP:HD1	41:1p:40:VAL:HG13	1.65	0.62
40:1o:96:LYS:HD3	40:1o:96:LYS:N	2.14	0.62
3:1C:204:GLU:HA	17:1Q:50:ASN:HD22	1.64	0.61
6:1F:190:THR:HB	6:1F:204:ARG:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:28:LEU:O	36:1k:32:GLN:NE2	2.33	0.61
3:1C:61:LEU:HB3	3:1C:123:VAL:HG11	1.82	0.61
21:1V:21:GLU:O	21:1V:25:ILE:HG22	1.99	0.61
38:1m:52:ASP:HB3	38:1m:55:ARG:HB2	1.82	0.61
39:1n:117:TYR:HA	39:1n:120:LYS:HD2	1.81	0.61
6:1F:178:VAL:HG21	6:1F:196:ILE:HG12	1.83	0.61
7:1G:672:TYR:O	7:1G:684:MET:HE1	2.00	0.61
8:1H:40:VAL:HB	8:1H:47:GLN:HG2	1.81	0.61
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.00	0.61
43:1r:45:SER:CA	43:1r:47:LYS:NZ	2.54	0.61
7:1G:632:ARG:NH1	19:1S:59:ASP:OD1	2.31	0.61
12:1L:69:MET:HE1	12:1L:71:LEU:HD13	1.82	0.61
14:1N:95:MET:HE3	14:1N:149:ILE:CA	2.30	0.61
26:1a:54:ILE:C	26:1a:64:LYS:HZ1	2.08	0.61
5:1E:24:THR:OG1	5:1E:27:ASN:OD1	2.16	0.61
7:1G:229:ASP:OD1	7:1G:230:VAL:N	2.33	0.61
12:1L:161:ARG:HG2	12:1L:164:ALA:H	1.66	0.61
12:1L:175:ASN:HD21	12:1L:223:LYS:HZ2	1.49	0.61
40:1o:92:LEU:O	40:1o:95:VAL:HG12	2.00	0.61
42:1q:29:ARG:HH12	42:1q:74:PHE:HA	1.66	0.61
7:1G:368:ILE:HA	7:1G:371:VAL:HG23	1.82	0.61
12:1L:76:LEU:HD11	12:1L:196:TRP:HZ3	1.66	0.61
15:1O:270:LEU:O	15:1O:273:THR:OG1	2.18	0.61
22:1W:44:PRO:HD3	22:1W:60:ARG:HH12	1.65	0.61
32:1g:26:LEU:HD11	32:1g:28:GLU:HB2	1.82	0.61
6:1F:91:LYS:O	6:1F:132:ARG:N	2.33	0.61
6:1F:389:ILE:HG23	6:1F:419:ILE:HD13	1.82	0.61
3:1C:68:THR:HA	21:1V:82:GLN:NE2	2.15	0.61
5:1E:153:MET:HE2	5:1E:154:VAL:C	2.26	0.61
7:1G:399:TRP:HA	7:1G:404:LEU:H	1.65	0.61
9:1I:49:ASN:O	9:1I:53:GLU:N	2.31	0.61
17:1Q:82:LEU:N	17:1Q:82:LEU:HD23	2.15	0.61
20:1U:35:HIS:ND1	20:1U:38:LYS:CG	2.63	0.61
21:1V:35:GLY:HA2	21:1V:44:ARG:NH1	2.16	0.61
28:1c:41:GLU:HA	28:1c:41:GLU:OE2	1.98	0.61
35:1j:18:THR:O	35:1j:22:LEU:HD13	2.00	0.61
4:1D:221:ARG:HG3	43:1r:24:GLN:CD	2.23	0.61
6:1F:150:GLN:HE22	6:1F:177:VAL:HG11	1.65	0.61
16:1P:57:MET:O	16:1P:60:ARG:HG2	2.00	0.61
36:1k:48:GLU:OE1	39:1n:37:ARG:NH1	2.30	0.61
2:1B:139:ILE:HG22	2:1B:140:VAL:HG23	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:214:GLN:H	5:1E:217:LEU:HD21	1.64	0.61
6:1F:82:MET:CE	6:1F:211:ALA:O	2.48	0.61
6:1F:101:GLU:OE2	6:1F:101:GLU:C	2.44	0.61
13:1M:70:THR:HA	13:1M:103:GLN:HE21	1.66	0.61
15:1O:219:GLU:OE2	15:1O:243:CYS:HA	1.99	0.61
16:1P:71:MET:HE1	18:1R:29:SER:HB2	1.82	0.61
17:1Q:28:GLU:OE1	17:1Q:28:GLU:N	2.26	0.61
23:1X:136:LEU:HD22	23:1X:137:PRO:HD2	1.83	0.61
31:1f:50:PRO:HD2	31:1f:51:ASN:H	1.66	0.61
7:1G:462:ASP:O	7:1G:466:ILE:HG13	2.01	0.60
14:1N:274:GLU:OE1	24:1Y:139:LYS:HD3	2.01	0.60
7:1G:94:MET:HE3	7:1G:120:SER:HA	1.82	0.60
7:1G:380:VAL:HG12	7:1G:409:ILE:HD11	1.82	0.60
7:1G:399:TRP:NE1	17:1Q:127:ARG:HH11	1.98	0.60
8:1H:30:TYR:CD2	26:1a:5:ILE:HD11	2.35	0.60
10:1J:175:ASN:HB2	14:1N:48:PHE:HD2	1.64	0.60
12:1L:594:THR:HG1	24:1Y:38:TYR:HH	1.47	0.60
13:1M:278:ARG:O	38:1m:71:ARG:NH2	2.34	0.60
16:1P:283:LYS:HA	16:1P:286:ARG:HG3	1.84	0.60
27:1b:30:ILE:O	27:1b:33:SER:OG	2.18	0.60
38:1m:5:TYR:HE2	38:1m:14:PRO:HD3	1.66	0.60
44:1s:70:ARG:HB3	44:1s:75:HIS:HB2	1.82	0.60
3:1C:149:ARG:HD2	4:1D:79:HIS:HE1	1.66	0.60
7:1G:237:ASN:O	7:1G:259:ASN:ND2	2.28	0.60
13:1M:381:ILE:O	13:1M:385:SER:OG	2.18	0.60
14:1N:230:LEU:O	14:1N:233:THR:OG1	2.19	0.60
4:1D:55:HIS:HE2	8:1H:127:TYR:HH	1.48	0.60
7:1G:237:ASN:OD1	7:1G:253:ARG:NH2	2.34	0.60
8:1H:26:LYS:HZ2	26:1a:5:ILE:HD13	1.67	0.60
12:1L:279:CYS:HA	37:1l:116:PHE:CE2	2.37	0.60
12:1L:298:ILE:HG12	12:1L:343:SER:OG	2.01	0.60
35:1j:37:LEU:CB	36:1k:77:PHE:HE1	2.15	0.60
38:1m:122:GLN:HB2	38:1m:125:ASN:HB3	1.82	0.60
6:1F:65:LEU:O	6:1F:75:THR:OG1	2.18	0.60
15:1O:97:GLN:HE22	15:1O:134:PHE:HB2	1.67	0.60
16:1P:251:ARG:HD3	16:1P:252:PRO:HD2	1.83	0.60
18:1R:37:GLU:OE1	18:1R:37:GLU:N	2.24	0.60
41:1p:100:GLU:HA	41:1p:103:ASN:HD22	1.65	0.60
2:1B:94:ASN:HD22	3:1C:174:LEU:HG	1.67	0.60
2:1B:171:LYS:HB3	2:1B:174:ARG:HB3	1.83	0.60
5:1E:132:THR:HB	5:1E:136:LEU:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:43:TYR:HB3	6:1F:236:ARG:HD2	1.82	0.60
6:1F:298:ILE:HB	6:1F:335:ILE:HG23	1.83	0.60
16:1P:145:TYR:HB2	16:1P:282:ASP:OD1	2.00	0.60
21:1V:54:LYS:HB2	21:1V:71:LEU:HD11	1.82	0.60
39:1n:154:PRO:CD	39:1n:164:PRO:HG2	2.32	0.60
2:1B:42:ARG:HD2	2:1B:168:LYS:HG2	1.83	0.60
6:1F:227:THR:O	6:1F:231:SER:OG	2.20	0.60
7:1G:374:ALA:HA	7:1G:448:LYS:HB2	1.83	0.60
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.34	0.60
14:1N:142:LEU:HB3	14:1N:194:LEU:HD21	1.84	0.60
14:1N:154:MET:HE3	14:1N:191:THR:HG22	1.84	0.60
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.35	0.60
20:1U:35:HIS:CE1	20:1U:38:LYS:H	2.19	0.60
22:1W:19:PRO:HA	22:1W:77:ARG:NH2	2.16	0.60
34:1i:109:ILE:HD12	34:1i:109:ILE:N	2.16	0.60
2:1B:67:TYR:CE2	2:1B:154:GLU:HB3	2.37	0.60
7:1G:302:ARG:HG3	7:1G:542:PHE:HZ	1.66	0.60
7:1G:514:ILE:HD12	7:1G:519:PRO:HG3	1.84	0.60
7:1G:614:ASP:OD1	7:1G:618:GLN:NE2	2.34	0.60
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.82	0.60
12:1L:570:GLN:HG3	14:1N:288:LEU:HD11	1.84	0.60
19:1S:23:CYS:SG	19:1S:24:GLN:N	2.74	0.60
36:1k:33:GLU:N	36:1k:33:GLU:OE2	2.34	0.60
7:1G:160:ILE:HD11	7:1G:183:VAL:HG13	1.84	0.60
13:1M:249:ILE:HD12	13:1M:250:LEU:HG	1.82	0.60
16:1P:113:ILE:H	16:1P:113:ILE:HD12	1.66	0.60
27:1b:59:ASP:OD1	27:1b:62:MET:HE1	2.02	0.60
2:1B:39:TRP:HA	2:1B:42:ARG:HE	1.67	0.60
2:1B:117:GLY:O	2:1B:121:ASN:ND2	2.35	0.60
5:1E:69:VAL:HA	5:1E:72:ILE:HG22	1.83	0.60
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	1.82	0.60
7:1G:239:VAL:HB	7:1G:251:LEU:HB2	1.82	0.60
11:1K:73:LEU:O	11:1K:77:LEU:HD22	2.02	0.60
14:1N:95:MET:HE2	14:1N:148:SER:OG	2.02	0.60
14:1N:278:MET:O	14:1N:282:MET:SD	2.60	0.60
3:1C:114:LEU:HG	22:1W:77:ARG:HG3	1.83	0.59
12:1L:306:THR:O	12:1L:310:LEU:HD12	2.02	0.59
13:1M:60:SER:HB3	13:1M:457:PRO:HA	1.83	0.59
14:1N:274:GLU:OE2	14:1N:274:GLU:N	2.36	0.59
23:1X:12:LEU:HD13	25:1Z:85:GLN:HB2	1.83	0.59
38:1m:16:THR:HG23	38:1m:17:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:106:SER:HB3	43:1r:110:PRO:HA	1.83	0.59
1:1A:105:GLU:HG2	1:1A:111:LEU:HD23	1.83	0.59
2:1B:65:PRO:HG3	8:1H:34:ARG:HH21	1.67	0.59
14:1N:134:GLN:HE22	14:1N:138:PRO:HG2	1.67	0.59
15:1O:223:TYR:HB3	15:1O:227:GLU:HG2	1.83	0.59
18:1R:34:GLU:HG3	42:1q:124:TYR:CD1	2.38	0.59
22:1W:23:ARG:C	22:1W:23:ARG:HE	2.10	0.59
23:1X:146:ARG:NH2	30:1e:41:GLU:OE1	2.35	0.59
7:1G:609:MET:SD	7:1G:609:MET:N	2.64	0.59
12:1L:183:VAL:HA	12:1L:186:MET:HB2	1.84	0.59
14:1N:265:MET:HE3	14:1N:343:LEU:CD2	2.32	0.59
15:1O:73:LEU:HD13	15:1O:299:LEU:HD11	1.83	0.59
32:1g:25:ARG:CZ	32:1g:26:LEU:HD23	2.31	0.59
12:1L:135:ASN:ND2	12:1L:199:GLN:OE1	2.36	0.59
20:1T:31:SER:H	20:1T:34:SER:HB2	1.67	0.59
2:1B:154:GLU:OE1	2:1B:154:GLU:N	2.35	0.59
7:1G:38:PRO:HB3	7:1G:123:PHE:CZ	2.37	0.59
7:1G:566:TYR:HA	7:1G:569:LYS:HE2	1.83	0.59
8:1H:97:ASN:HD22	26:1a:38:VAL:HG12	1.66	0.59
12:1L:383:MET:HE2	12:1L:383:MET:HA	1.85	0.59
13:1M:266:MET:HA	13:1M:269:MET:HE2	1.84	0.59
14:1N:87:THR:HG22	14:1N:88:LYS:H	1.68	0.59
14:1N:120:GLN:HE21	14:1N:177:LYS:HE2	1.66	0.59
19:1S:63:LYS:NZ	19:1S:75:ASN:ND2	2.49	0.59
26:1a:2:TRP:O	26:1a:5:ILE:HG12	2.01	0.59
33:1h:114:MET:SD	33:1h:122:TRP:CD1	2.96	0.59
4:1D:107:ASP:OD1	4:1D:371:LYS:NZ	2.36	0.59
6:1F:103:GLY:O	6:1F:257:ASN:ND2	2.25	0.59
6:1F:127:ARG:HG3	6:1F:127:ARG:NH1	2.16	0.59
7:1G:67:ALA:O	7:1G:71:MET:HG2	2.03	0.59
7:1G:377:ILE:HG22	7:1G:406:VAL:HA	1.84	0.59
12:1L:254:VAL:HG23	12:1L:329:ILE:HD12	1.84	0.59
13:1M:237:LYS:HD2	13:1M:316:MET:HB3	1.84	0.59
17:1Q:95:PHE:O	17:1Q:99:ASN:ND2	2.35	0.59
21:1V:47:THR:O	21:1V:51:THR:OG1	2.11	0.59
29:1d:114:GLU:OE1	29:1d:114:GLU:N	2.35	0.59
33:1h:7:ARG:H	33:1h:7:ARG:HD2	1.67	0.59
6:1F:257:ASN:HA	6:1F:267:THR:HA	1.83	0.59
7:1G:632:ARG:HH21	19:1S:57:CYS:HB3	1.66	0.59
12:1L:331:MET:HE2	12:1L:465:GLY:HA2	1.84	0.59
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:84:GLU:OE1	36:1k:88:GLU:HG2	2.03	0.59
6:1F:150:GLN:CA	6:1F:153:ILE:HD12	2.14	0.59
12:1L:53:MET:O	12:1L:57:THR:OG1	2.20	0.59
12:1L:425:ARG:NH2	45:1L:704:3PE:O13	2.36	0.59
15:1O:315:LYS:O	15:1O:320:LYS:NZ	2.34	0.59
16:1P:181:TYR:O	16:1P:184:SER:OG	2.20	0.59
19:1S:39:ARG:NH1	19:1S:87:THR:HG22	2.17	0.59
24:1Y:86:PRO:HA	24:1Y:125:LYS:HD3	1.85	0.59
2:1B:160:ILE:O	2:1B:164:GLN:HG3	2.03	0.59
4:1D:393:ALA:HB1	4:1D:427:GLU:HB3	1.83	0.59
6:1F:409:ASP:HB3	6:1F:413:TRP:HE1	1.67	0.59
7:1G:26:VAL:HB	7:1G:68:ALA:HB1	1.85	0.59
7:1G:500:VAL:HG21	7:1G:576:THR:HA	1.85	0.59
8:1H:32:GLN:HG3	8:1H:34:ARG:NH2	2.18	0.59
9:1I:108:ARG:HD2	9:1I:110:ASP:OD2	2.02	0.59
15:1O:204:ASN:CB	15:1O:208:LYS:CE	2.79	0.59
23:1X:122:GLY:HA3	27:1b:77:LEU:HD21	1.85	0.59
25:1Z:88:ARG:NH1	25:1Z:92:GLU:OE2	2.35	0.59
37:1l:125:TYR:OH	40:1o:7:ARG:NE	2.36	0.59
39:1n:136:VAL:HG23	39:1n:137:LYS:HE3	1.84	0.59
1:1A:105:GLU:HG2	1:1A:111:LEU:CD2	2.32	0.59
3:1C:68:THR:HA	21:1V:82:GLN:HE22	1.67	0.59
14:1N:338:PRO:O	23:1X:169:TRP:NE1	2.32	0.59
21:1V:45:LYS:O	21:1V:45:LYS:HD3	2.02	0.59
23:1X:122:GLY:N	25:1Z:66:GLU:OE2	2.35	0.59
32:1g:107:LEU:HD21	41:1p:134:VAL:HG22	1.85	0.59
33:1h:114:MET:HE3	33:1h:120:GLY:HA3	1.84	0.59
37:1l:156:TYR:HB2	40:1o:33:ARG:HH21	1.67	0.59
2:1B:125:TYR:CD1	4:1D:102:TYR:CE1	2.90	0.58
5:1E:48:LEU:HB3	5:1E:49:PRO:HD3	1.84	0.58
5:1E:148:CYS:HA	47:1E:301:FES:S2	2.42	0.58
6:1F:20:ARG:HB2	6:1F:269:GLU:HG3	1.85	0.58
6:1F:55:TRP:CZ3	6:1F:59:GLU:HB2	2.38	0.58
6:1F:258:ILE:HD13	6:1F:284:ALA:HB2	1.85	0.58
8:1H:149:ILE:HD11	8:1H:184:MET:HG3	1.85	0.58
13:1M:257:MET:HA	13:1M:257:MET:CE	2.32	0.58
14:1N:128:LEU:HD11	14:1N:213:LEU:CD1	2.33	0.58
32:1g:63:PHE:O	32:1g:67:SER:OG	2.21	0.58
5:1E:10:ARG:HH21	18:1R:77:LYS:HA	1.68	0.58
6:1F:55:TRP:CH2	6:1F:59:GLU:OE1	2.56	0.58
6:1F:277:LYS:NZ	6:1F:313:GLU:HA	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:40:PHE:O	7:1G:158:ARG:NH1	2.36	0.58
7:1G:195:LEU:HD12	7:1G:198:ASN:ND2	2.18	0.58
7:1G:306:MET:N	7:1G:306:MET:SD	2.76	0.58
9:1I:69:ARG:HD2	42:1q:108:TYR:CG	2.37	0.58
12:1L:496:MET:O	12:1L:500:LEU:HD12	2.02	0.58
14:1N:109:SER:OG	14:1N:157:MET:HG3	2.03	0.58
15:1O:205:ALA:N	15:1O:208:LYS:HZ1	2.01	0.58
40:1o:93:ASP:HA	40:1o:96:LYS:HG2	1.84	0.58
43:1r:27:TYR:HB3	43:1r:28:GLN:OE1	2.03	0.58
6:1F:212:ASP:OD1	6:1F:212:ASP:N	2.34	0.58
6:1F:277:LYS:HZ1	6:1F:313:GLU:HA	1.68	0.58
6:1F:409:ASP:HB3	6:1F:413:TRP:NE1	2.17	0.58
14:1N:268:GLN:HG3	23:1X:167:PHE:HZ	1.67	0.58
15:1O:171:TYR:HE1	15:1O:173:ASP:HA	1.68	0.58
2:1B:60:MET:HE3	4:1D:167:PHE:CZ	2.38	0.58
7:1G:341:ASP:N	7:1G:341:ASP:OD1	2.35	0.58
7:1G:673:MET:HE3	7:1G:684:MET:CE	2.33	0.58
8:1H:85:MET:HE1	8:1H:108:MET:CB	2.34	0.58
12:1L:161:ARG:HH21	39:1n:90:TYR:H	1.51	0.58
12:1L:238:GLU:N	12:1L:238:GLU:OE2	2.30	0.58
23:1X:81:PHE:CE1	23:1X:85:TRP:CD1	2.91	0.58
5:1E:124:LEU:HD22	5:1E:126:ILE:HG12	1.84	0.58
8:1H:85:MET:HE1	8:1H:108:MET:HB2	1.85	0.58
28:1c:41:GLU:OE2	28:1c:44:ARG:NH2	2.36	0.58
30:1e:48:GLY:HA3	33:1h:125:TYR:HB2	1.85	0.58
2:1B:40:ALA:HB3	8:1H:54:LYS:NZ	2.17	0.58
4:1D:115:GLU:HB3	4:1D:194:ILE:HB	1.84	0.58
12:1L:10:THR:HA	12:1L:13:ILE:HG22	1.86	0.58
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	1.86	0.58
14:1N:134:GLN:HE22	14:1N:138:PRO:CG	2.17	0.58
18:1R:9:GLU:HG3	18:1R:33:LYS:HD2	1.85	0.58
20:1T:18:VAL:HG11	20:1T:57:GLU:HB2	1.85	0.58
34:1i:43:GLU:O	34:1i:47:ASN:ND2	2.37	0.58
36:1k:21:TRP:HE1	36:1k:50:TRP:HB3	1.69	0.58
40:1o:7:ARG:HA	40:1o:15:GLU:HG3	1.86	0.58
6:1F:115:PRO:HB2	6:1F:149:LEU:HG	1.84	0.58
7:1G:592:LEU:HD11	16:1P:7:PRO:HD2	1.86	0.58
11:1K:93:LEU:HD12	12:1L:584:ILE:HD11	1.85	0.58
22:1W:119:LEU:HD12	22:1W:120:SER:N	2.18	0.58
40:1o:92:LEU:HB3	40:1o:96:LYS:HZ1	1.67	0.58
42:1q:38:LEU:HD21	42:1q:47:LYS:HZ3	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:1s:41:LEU:HD22	44:1s:44:HIS:HD2	1.69	0.58
2:1B:161:LEU:HB3	2:1B:165:ARG:HH12	1.69	0.58
4:1D:8:VAL:HG13	32:1g:25:ARG:HH12	1.68	0.58
12:1L:296:ASN:H	39:1n:77:GLN:HE22	1.52	0.58
20:1T:18:VAL:CA	20:1T:21:LEU:HG	2.24	0.58
2:1B:116:MET:HA	2:1B:146:VAL:HG13	1.85	0.58
3:1C:196:LYS:HZ1	17:1Q:81:ASN:HD22	1.52	0.58
4:1D:140:LEU:HG	4:1D:314:CYS:SG	2.44	0.58
5:1E:30:ARG:NH1	44:1s:53:ASP:OD1	2.37	0.58
6:1F:91:LYS:NZ	6:1F:129:MET:O	2.30	0.58
6:1F:218:CYS:HB3	17:1Q:124:TRP:CD1	2.39	0.58
7:1G:41:CYS:HB3	7:1G:52:CYS:HB3	1.85	0.58
9:1I:64:GLU:OE1	9:1I:157:ASN:ND2	2.37	0.58
16:1P:212:LYS:O	16:1P:216:ASN:OD1	2.21	0.58
36:1k:35:LEU:HB3	36:1k:40:LEU:HB2	1.86	0.58
6:1F:14:SER:O	6:1F:16:LYS:NZ	2.36	0.58
7:1G:376:VAL:HG22	7:1G:405:LYS:HB2	1.84	0.58
7:1G:386:PHE:HE1	7:1G:668:ILE:HA	1.69	0.58
16:1P:110:PHE:HA	16:1P:114:PRO:HG2	1.86	0.58
25:1Z:55:ARG:NH1	27:1b:83:LEU:O	2.37	0.58
31:1f:57:LYS:O	31:1f:57:LYS:NZ	2.37	0.58
39:1n:81:PHE:O	39:1n:84:SER:OG	2.16	0.58
6:1F:55:TRP:CZ3	6:1F:59:GLU:CA	2.87	0.57
6:1F:126:GLY:HA2	6:1F:129:MET:CE	2.32	0.57
7:1G:354:ALA:HB3	7:1G:361:ASN:HD21	1.68	0.57
7:1G:367:THR:O	7:1G:370:GLY:N	2.29	0.57
7:1G:522:LEU:HB3	7:1G:543:ILE:HD13	1.86	0.57
8:1H:157:ASN:ND2	8:1H:159:SER:O	2.37	0.57
15:1O:204:ASN:CB	15:1O:208:LYS:NZ	2.67	0.57
21:1V:22:ARG:NH1	21:1V:22:ARG:O	2.37	0.57
22:1W:65:GLU:C	22:1W:69:LYS:NZ	2.62	0.57
23:1X:14:VAL:HG11	23:1X:60:LYS:HB2	1.85	0.57
23:1X:43:MET:HG2	27:1b:52:TYR:CE1	2.39	0.57
25:1Z:25:LEU:HD12	25:1Z:26:PRO:HD2	1.86	0.57
33:1h:26:ARG:O	33:1h:30:LEU:HD23	2.04	0.57
34:1i:4:THR:OG1	34:1i:6:ASP:OD1	2.15	0.57
12:1L:49:VAL:HA	12:1L:52:LEU:HD23	1.86	0.57
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.85	0.57
13:1M:450:ASN:C	13:1M:450:ASN:OD1	2.47	0.57
27:1b:27:LEU:O	27:1b:31:LEU:HD22	2.04	0.57
32:1g:35:GLU:N	32:1g:35:GLU:OE1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:10:ARG:HH22	35:1j:16:GLN:HB3	1.68	0.57
39:1n:50:HIS:ND1	39:1n:50:HIS:O	2.37	0.57
6:1F:60:VAL:HA	6:1F:63:SER:HB3	1.86	0.57
6:1F:420:ARG:HG3	6:1F:421:HIS:CD2	2.39	0.57
7:1G:39:ARG:HD3	7:1G:42:TYR:HD2	1.68	0.57
7:1G:386:PHE:HB3	7:1G:665:GLN:HB3	1.86	0.57
13:1M:243:MET:HG3	13:1M:301:ILE:HG21	1.85	0.57
16:1P:162:GLU:HB3	16:1P:224:LYS:HB2	1.85	0.57
18:1R:57:ILE:HG12	18:1R:75:LEU:HD21	1.86	0.57
30:1e:98:LEU:HD23	30:1e:98:LEU:H	1.70	0.57
39:1n:133:GLU:O	39:1n:137:LYS:HG2	2.04	0.57
4:1D:139:VAL:HG11	4:1D:277:VAL:HG12	1.86	0.57
8:1H:286:MET:HG3	8:1H:290:TRP:CD1	2.40	0.57
12:1L:162:THR:OG1	37:1l:86:ARG:NH2	2.32	0.57
13:1M:130:LEU:HG	13:1M:150:LEU:HD12	1.86	0.57
22:1W:50:PHE:HD2	22:1W:103:ILE:HG12	1.70	0.57
7:1G:418:ARG:HH12	44:1s:75:HIS:CD2	2.22	0.57
22:1W:19:PRO:HA	22:1W:77:ARG:HH22	1.70	0.57
22:1W:47:VAL:HA	22:1W:52:LEU:HD23	1.87	0.57
43:1r:110:PRO:C	43:1r:111:TYR:HD2	2.12	0.57
2:1B:65:PRO:HG2	4:1D:172:GLU:HB2	1.86	0.57
4:1D:141:PHE:HZ	4:1D:184:VAL:HG11	1.70	0.57
4:1D:391:ILE:HB	4:1D:430:ARG:HD3	1.87	0.57
7:1G:324:ASP:OD2	7:1G:569:LYS:HE3	2.04	0.57
9:1I:114:THR:HG21	9:1I:144:HIS:CD2	2.40	0.57
10:1J:34:ILE:HB	10:1J:61:LEU:HD21	1.86	0.57
12:1L:175:ASN:ND2	12:1L:223:LYS:HZ2	2.02	0.57
15:1O:134:PHE:O	15:1O:138:MET:HG3	2.05	0.57
38:1m:125:ASN:O	41:1p:139:GLN:NE2	2.38	0.57
3:1C:6:ASP:OD2	4:1D:129:GLN:NE2	2.38	0.57
5:1E:99:HIS:HB3	5:1E:101:GLN:HE22	1.69	0.57
6:1F:41:ASP:HA	6:1F:236:ARG:NH1	2.20	0.57
6:1F:276:LEU:HA	6:1F:317:MET:CE	2.35	0.57
7:1G:165:GLU:HA	7:1G:396:ARG:HH21	1.69	0.57
12:1L:213:LEU:HB3	12:1L:273:VAL:HG21	1.86	0.57
13:1M:346:ARG:NH1	37:1l:68:ASP:OD2	2.37	0.57
14:1N:237:MET:HB3	14:1N:240:ILE:HD13	1.87	0.57
20:1U:15:VAL:HG12	20:1U:19:LEU:CD2	2.35	0.57
23:1X:81:PHE:HD1	23:1X:81:PHE:O	1.88	0.57
29:1d:108:THR:HA	41:1p:77:GLU:HA	1.85	0.57
2:1B:60:MET:HE1	4:1D:171:PHE:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:82:GLN:NE2	2:1B:82:GLN:C	2.63	0.57
4:1D:154:VAL:HG11	4:1D:225:LEU:HD11	1.87	0.57
5:1E:50:VAL:HG11	5:1E:73:LEU:HD21	1.87	0.57
15:1O:76:ASN:O	15:1O:95:ARG:NH1	2.30	0.57
16:1P:294:LEU:HD12	16:1P:296:HIS:HE1	1.69	0.57
20:1U:48:VAL:O	20:1U:52:MET:HG3	2.05	0.57
29:1d:87:ASP:HB3	29:1d:91:PHE:CE1	2.39	0.57
32:1g:95:ARG:HH12	41:1p:64:HIS:CD2	2.22	0.57
42:1q:59:HIS:CE1	42:1q:60:ARG:NE	2.73	0.57
2:1B:42:ARG:HB2	2:1B:164:GLN:HB3	1.87	0.57
7:1G:317:ALA:O	7:1G:344:CYS:N	2.32	0.57
9:1I:99:ARG:HH21	9:1I:105:ARG:HE	1.51	0.57
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.05	0.57
16:1P:170:ASP:HB3	16:1P:204:PRO:HB3	1.87	0.57
18:1R:20:ASP:HA	18:1R:25:ARG:HH21	1.70	0.57
19:1S:78:LEU:HA	19:1S:81:PHE:CE1	2.40	0.57
25:1Z:108:GLU:HB2	30:1e:74:ARG:HH12	1.70	0.57
29:1d:44:ILE:H	29:1d:44:ILE:HD12	1.69	0.57
4:1D:402:LEU:HA	4:1D:405:MET:HB2	1.87	0.57
6:1F:400:GLU:OE1	6:1F:416:GLN:NE2	2.38	0.57
7:1G:58:GLU:HB2	7:1G:65:VAL:HG12	1.86	0.57
7:1G:258:ILE:O	7:1G:260:GLU:N	2.37	0.57
8:1H:269:THR:O	8:1H:273:ILE:HG13	2.05	0.57
11:1K:55:LEU:HG	30:1e:25:PRO:HD3	1.86	0.57
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.23	0.57
52:1M:501:PGT:H131	52:1M:501:PGT:H361	1.85	0.57
14:1N:341:PRO:CB	29:1d:79:GLN:NE2	2.60	0.57
15:1O:176:VAL:HA	15:1O:179:ILE:HD12	1.87	0.57
25:1Z:4:SER:OG	25:1Z:5:LYS:N	2.37	0.57
26:1a:6:LEU:HD21	53:1r:201:CDL:H732	1.87	0.57
2:1B:100:LEU:CD2	2:1B:140:VAL:HG21	2.34	0.56
7:1G:119:GLN:OE1	7:1G:123:PHE:HZ	1.88	0.56
9:1I:62:ARG:HA	9:1I:133:GLU:HB3	1.87	0.56
12:1L:486:MET:O	12:1L:489:THR:HG22	2.05	0.56
15:1O:285:GLY:H	32:1g:26:LEU:HD13	1.68	0.56
23:1X:81:PHE:CD1	23:1X:81:PHE:C	2.82	0.56
34:1i:43:GLU:HA	34:1i:46:TRP:CD1	2.39	0.56
39:1n:134:ARG:HD2	39:1n:161:ASP:HB2	1.87	0.56
3:1C:198:ASP:OD2	7:1G:224:LYS:NZ	2.32	0.56
5:1E:40:GLU:OE2	44:1s:69:GLY:N	2.31	0.56
5:1E:60:TRP:HA	5:1E:91:ASN:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:76:PRO:HG2	5:1E:79:ARG:HG2	1.88	0.56
8:1H:31:MET:HE1	8:1H:275:ALA:HB3	1.86	0.56
16:1P:1:LEU:HD12	16:1P:5:LEU:HB3	1.87	0.56
16:1P:155:GLU:OE1	16:1P:155:GLU:N	2.38	0.56
17:1Q:123:SER:H	17:1Q:129:ARG:HG2	1.69	0.56
19:1S:39:ARG:NH2	19:1S:90:LEU:HD21	2.20	0.56
25:1Z:121:MET:HE1	25:1Z:137:THR:HG22	1.86	0.56
35:1j:37:LEU:HB2	36:1k:77:PHE:CE1	2.40	0.56
4:1D:20:TYR:OH	14:1N:295:ARG:NH2	2.38	0.56
4:1D:218:PHE:HA	4:1D:221:ARG:HH11	1.70	0.56
4:1D:403:ASP:OD1	4:1D:404:LYS:N	2.35	0.56
5:1E:100:ILE:HB	5:1E:139:LEU:HA	1.87	0.56
7:1G:358:LEU:HD23	7:1G:645:ALA:HB2	1.87	0.56
7:1G:627:SER:HB3	7:1G:630:LEU:HD23	1.87	0.56
8:1H:3:MET:CE	8:1H:7:LEU:HD23	2.34	0.56
8:1H:87:VAL:HG22	8:1H:95:LEU:HD23	1.87	0.56
9:1I:8:ARG:HA	9:1I:8:ARG:HH11	1.66	0.56
9:1I:42:PHE:O	43:1r:11:ARG:NH1	2.38	0.56
10:1J:50:SER:N	10:1J:139:GLU:OE1	2.38	0.56
12:1L:203:MET:HE1	41:1p:120:TYR:HD2	1.70	0.56
12:1L:248:HIS:CE1	12:1L:252:MET:HE3	2.40	0.56
12:1L:370:THR:O	12:1L:374:ILE:HG12	2.06	0.56
13:1M:130:LEU:O	13:1M:134:THR:OG1	2.20	0.56
14:1N:95:MET:CE	14:1N:149:ILE:HA	2.36	0.56
15:1O:61:SER:HA	15:1O:66:GLY:HA2	1.87	0.56
17:1Q:27:GLU:OE2	17:1Q:27:GLU:N	2.26	0.56
32:1g:23:THR:O	32:1g:25:ARG:N	2.37	0.56
33:1h:7:ARG:H	33:1h:7:ARG:CD	2.18	0.56
33:1h:88:GLU:HA	33:1h:91:MET:HE3	1.88	0.56
39:1n:46:ARG:HH22	39:1n:47:PHE:HD1	1.53	0.56
7:1G:228:ILE:HG21	7:1G:581:GLN:HB3	1.87	0.56
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.70	0.56
13:1M:252:PRO:HB3	29:1d:117:HIS:CD2	2.41	0.56
14:1N:207:ILE:HG21	14:1N:262:PRO:HD3	1.86	0.56
19:1S:20:ILE:HD12	19:1S:64:LEU:HA	1.88	0.56
21:1V:49:GLN:OE1	21:1V:49:GLN:C	2.48	0.56
23:1X:126:LYS:HD2	27:1b:74:GLY:HA3	1.87	0.56
27:1b:77:LEU:H	27:1b:77:LEU:HD23	1.70	0.56
42:1q:81:MET:N	42:1q:81:MET:SD	2.79	0.56
4:1D:142:GLY:O	4:1D:145:THR:OG1	2.21	0.56
6:1F:154:ARG:HG3	44:1s:58:LEU:HD21	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:273:SER:HB3	6:1F:316:LEU:HD21	1.88	0.56
14:1N:100:MET:CE	14:1N:111:PHE:CE2	2.89	0.56
22:1W:23:ARG:O	22:1W:23:ARG:NE	2.32	0.56
29:1d:119:VAL:HG21	41:1p:146:GLY:HA2	1.87	0.56
37:1l:141:GLU:HA	41:1p:122:GLN:HB2	1.87	0.56
3:1C:59:PRO:HA	21:1V:96:TRP:CZ3	2.41	0.56
4:1D:50:ASN:ND2	4:1D:52:GLY:O	2.37	0.56
4:1D:242:ILE:HD13	4:1D:413:ASP:OD1	2.06	0.56
4:1D:350:LYS:HB2	7:1G:121:MET:SD	2.45	0.56
5:1E:149:VAL:HG23	6:1F:259:SER:HB2	1.86	0.56
7:1G:38:PRO:HG3	7:1G:123:PHE:CE2	2.41	0.56
11:1K:89:TYR:O	11:1K:92:ASN:ND2	2.37	0.56
12:1L:89:PHE:HE2	12:1L:128:MET:HE3	1.70	0.56
20:1T:35:HIS:CE1	20:1T:71:MET:HB2	2.40	0.56
21:1V:92:LYS:CA	21:1V:95:ARG:HH21	2.19	0.56
22:1W:61:ASP:HA	22:1W:64:ARG:HB3	1.87	0.56
36:1k:46:ARG:H	36:1k:46:ARG:HD3	1.71	0.56
3:1C:65:ARG:O	3:1C:73:LYS:NZ	2.37	0.56
4:1D:146:ARG:HD3	4:1D:370:PRO:HB3	1.87	0.56
4:1D:261:ARG:HG3	4:1D:287:ILE:HG13	1.88	0.56
7:1G:244:THR:HG22	7:1G:244:THR:O	2.06	0.56
8:1H:234:MET:HA	8:1H:234:MET:HE3	1.87	0.56
12:1L:83:ASP:N	12:1L:86:SER:OG	2.39	0.56
13:1M:250:LEU:O	13:1M:254:THR:OG1	2.20	0.56
19:1S:12:LYS:HG3	19:1S:14:GLY:H	1.71	0.56
29:1d:102:PRO:O	29:1d:104:LYS:HD3	2.05	0.56
30:1e:44:HIS:CE1	33:1h:129:ASP:HA	2.41	0.56
42:1q:34:ARG:HD3	42:1q:54:GLN:HE21	1.71	0.56
1:1A:72:LEU:HD23	8:1H:151:LEU:HG	1.86	0.56
4:1D:246:THR:HA	21:1V:11:VAL:HG13	1.87	0.56
6:1F:376:MET:C	6:1F:376:MET:HE2	2.30	0.56
13:1M:442:LEU:O	13:1M:446:LEU:HD23	2.05	0.56
15:1O:204:ASN:C	15:1O:208:LYS:HG2	2.28	0.56
17:1Q:11:ILE:HD11	22:1W:23:ARG:HA	1.87	0.56
28:1c:44:ARG:HE	28:1c:45:ARG:N	2.03	0.56
33:1h:75:ILE:HA	33:1h:78:THR:HG22	1.88	0.56
3:1C:77:ASP:OD1	4:1D:364:TYR:CE1	2.58	0.56
12:1L:237:MET:HE2	12:1L:299:LYS:HE2	1.88	0.56
13:1M:26:ASN:OD1	31:1f:13:HIS:NE2	2.39	0.56
20:1U:35:HIS:CG	20:1U:38:LYS:HE2	2.41	0.56
29:1d:5:ARG:HG2	29:1d:8:ARG:HD3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:78:VAL:HG22	41:1p:40:VAL:HG11	1.88	0.56
37:1l:129:GLY:O	40:1o:97:ARG:NH2	2.30	0.56
1:1A:67:LEU:HD22	11:1K:65:VAL:HA	1.88	0.56
3:1C:59:PRO:HA	21:1V:96:TRP:CH2	2.40	0.56
4:1D:306:GLN:NE2	25:1Z:21:TYR:OH	2.33	0.56
6:1F:101:GLU:CD	6:1F:102:PRO:O	2.48	0.56
6:1F:361:GLN:NE2	46:1F:502:SF4:S4	2.79	0.56
7:1G:379:LEU:HD12	7:1G:452:VAL:HG12	1.87	0.56
7:1G:381:GLY:O	7:1G:456:SER:OG	2.22	0.56
9:1I:65:HIS:CD2	9:1I:113:MET:HE1	2.41	0.56
22:1W:91:GLU:OE1	22:1W:91:GLU:N	2.37	0.56
25:1Z:84:LEU:HA	25:1Z:87:LEU:HB2	1.87	0.56
37:1l:77:ILE:HD11	38:1m:67:TRP:CG	2.41	0.56
1:1A:22:PHE:HD1	8:1H:60:PRO:HG2	1.70	0.55
4:1D:155:THR:O	4:1D:159:LEU:N	2.34	0.55
6:1F:295:LEU:HD12	6:1F:339:ARG:HH11	1.69	0.55
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.87	0.55
11:1K:21:MET:HG2	11:1K:21:MET:O	2.05	0.55
14:1N:248:LEU:HD11	14:1N:296:LEU:HD23	1.88	0.55
15:1O:171:TYR:CD2	15:1O:207:LYS:NZ	2.74	0.55
16:1P:236:TYR:HB3	16:1P:241:LEU:HG	1.89	0.55
16:1P:290:SER:OG	16:1P:291:ASP:N	2.40	0.55
17:1Q:11:ILE:CB	22:1W:77:ARG:HH21	2.19	0.55
29:1d:2:MET:HE1	33:1h:122:TRP:CE3	2.41	0.55
42:1q:39:VAL:HB	42:1q:50:GLU:OE2	2.06	0.55
4:1D:150:HIS:CD2	4:1D:300:ARG:HA	2.42	0.55
6:1F:245:PHE:O	6:1F:252:GLY:N	2.37	0.55
7:1G:164:SER:O	7:1G:396:ARG:NH2	2.40	0.55
7:1G:357:ASP:OD2	19:1S:44:LYS:NZ	2.38	0.55
7:1G:392:ASN:HA	7:1G:395:ILE:HD12	1.88	0.55
8:1H:5:ASN:CG	26:1a:26:ILE:HD11	2.30	0.55
14:1N:85:THR:HG21	33:1h:128:ILE:HD12	1.88	0.55
15:1O:251:GLN:HB3	15:1O:255:THR:OG1	2.06	0.55
16:1P:335:LYS:HD2	16:1P:336:PRO:CD	2.36	0.55
22:1W:19:PRO:HA	22:1W:77:ARG:CZ	2.35	0.55
29:1d:95:LYS:HA	29:1d:95:LYS:HE2	1.88	0.55
37:1l:156:TYR:HB2	40:1o:33:ARG:HE	1.71	0.55
44:1s:41:LEU:HD22	44:1s:44:HIS:CD2	2.41	0.55
3:1C:88:ASN:ND2	21:1V:110:GLN:OE1	2.30	0.55
4:1D:145:THR:HA	4:1D:148:LEU:HB2	1.88	0.55
6:1F:371:TRP:HH2	7:1G:129:ARG:HG3	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:119:PHE:HD2	11:1K:6:MET:HE3	1.71	0.55
12:1L:233:LEU:HD21	12:1L:248:HIS:HB3	1.88	0.55
12:1L:237:MET:HA	12:1L:237:MET:CE	2.29	0.55
12:1L:384:PRO:HB3	35:1j:47:VAL:HG21	1.87	0.55
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.38	0.55
14:1N:134:GLN:OE1	14:1N:134:GLN:C	2.49	0.55
14:1N:251:MET:HG3	14:1N:293:TYR:CE1	2.40	0.55
14:1N:258:SER:N	14:1N:334:THR:O	2.35	0.55
16:1P:13:ARG:HG2	16:1P:64:ASP:HB2	1.89	0.55
20:1U:35:HIS:CD2	20:1U:71:MET:HG2	2.40	0.55
22:1W:66:MET:HA	22:1W:66:MET:HE3	1.88	0.55
23:1X:81:PHE:HE2	26:1a:66:LEU:HD21	1.72	0.55
4:1D:55:HIS:NE2	8:1H:127:TYR:OH	2.33	0.55
6:1F:42:TRP:HE1	6:1F:116:HIS:HB2	1.72	0.55
7:1G:46:LEU:HD21	7:1G:161:ARG:HE	1.71	0.55
7:1G:349:PHE:HD2	7:1G:350:PRO:HD2	1.71	0.55
17:1Q:19:ILE:O	17:1Q:21:THR:N	2.39	0.55
19:1S:63:LYS:HZ1	19:1S:75:ASN:CB	2.18	0.55
20:1U:27:PRO:HA	20:1U:30:LEU:HD23	1.89	0.55
21:1V:75:GLN:OE1	21:1V:75:GLN:N	2.39	0.55
22:1W:32:VAL:HG11	58:1W:201:EHZ:N1	2.20	0.55
22:1W:65:GLU:C	22:1W:69:LYS:HZ3	2.14	0.55
22:1W:103:ILE:HA	22:1W:106:PHE:HE1	1.71	0.55
32:1g:23:THR:C	32:1g:25:ARG:H	2.13	0.55
41:1p:139:GLN:O	41:1p:157:LYS:NZ	2.39	0.55
3:1C:211:GLN:NE2	21:1V:115:ILE:O	2.39	0.55
4:1D:312:SER:O	4:1D:316:ASN:ND2	2.40	0.55
6:1F:111:ILE:HD13	6:1F:138:ILE:HD12	1.89	0.55
7:1G:386:PHE:CE1	7:1G:668:ILE:HA	2.42	0.55
7:1G:451:VAL:HG22	7:1G:489:VAL:HG12	1.89	0.55
8:1H:273:ILE:HG22	9:1I:34:LEU:HD11	1.89	0.55
8:1H:281:ARG:HE	8:1H:283:ASP:CG	2.14	0.55
9:1I:98:PRO:HD3	9:1I:104:ARG:HH21	1.72	0.55
9:1I:113:MET:HB2	9:1I:147:LEU:HB3	1.88	0.55
14:1N:341:PRO:C	29:1d:79:GLN:HE22	2.14	0.55
16:1P:237:LEU:O	16:1P:241:LEU:N	2.32	0.55
17:1Q:90:GLU:H	17:1Q:90:GLU:CD	2.15	0.55
19:1S:18:ILE:HG23	19:1S:52:ILE:HG23	1.87	0.55
19:1S:43:LEU:HD23	19:1S:43:LEU:H	1.71	0.55
20:1T:69:LYS:NZ	20:1T:70:LEU:HD21	2.22	0.55
22:1W:34:GLU:HA	22:1W:37:ARG:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:88:ASN:HB2	24:1Y:125:LYS:HZ3	1.71	0.55
40:1o:92:LEU:HB3	40:1o:96:LYS:NZ	2.21	0.55
9:1I:7:MET:O	9:1I:8:ARG:HD2	2.07	0.55
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.41	0.55
10:1J:173:ARG:HD3	15:1O:254:ARG:HH21	1.71	0.55
11:1K:40:LEU:HD23	14:1N:75:ILE:HD13	1.88	0.55
12:1L:577:VAL:HA	45:1Y:201:3PE:H331	1.89	0.55
13:1M:435:ALA:O	13:1M:439:LEU:HG	2.06	0.55
16:1P:29:PHE:CE2	16:1P:176:ASP:HA	2.42	0.55
16:1P:216:ASN:O	16:1P:220:ASP:N	2.37	0.55
22:1W:27:GLU:HA	22:1W:30:ARG:HB3	1.88	0.55
26:1a:55:SER:CA	26:1a:64:LYS:HZ1	2.19	0.55
7:1G:496:ILE:HG22	7:1G:499:GLN:H	1.70	0.55
10:1J:57:PHE:HA	10:1J:61:LEU:HB2	1.87	0.55
12:1L:203:MET:CE	41:1p:120:TYR:HD2	2.20	0.55
14:1N:251:MET:HE2	14:1N:251:MET:HA	1.88	0.55
16:1P:90:VAL:HG21	16:1P:218:ILE:HG23	1.89	0.55
20:1T:10:ALA:O	20:1T:14:ARG:HG2	2.07	0.55
32:1g:48:ASP:OD1	32:1g:49:LYS:N	2.40	0.55
33:1h:56:PRO:HG2	33:1h:59:TYR:HB3	1.88	0.55
34:1i:63:THR:O	34:1i:67:SER:OG	2.23	0.55
42:1q:59:HIS:ND1	42:1q:60:ARG:N	2.55	0.55
3:1C:10:THR:HG21	43:1r:56:ARG:HD2	1.89	0.55
5:1E:161:TYR:OH	5:1E:172:ILE:HG21	2.06	0.55
5:1E:162:GLU:O	5:1E:186:PRO:HA	2.07	0.55
7:1G:27:LEU:HD21	7:1G:55:CYS:HB2	1.88	0.55
13:1M:271:MET:HA	13:1M:271:MET:HE3	1.87	0.55
13:1M:399:ASN:O	13:1M:403:THR:OG1	2.20	0.55
15:1O:209:THR:O	15:1O:213:GLU:HG3	2.07	0.55
21:1V:82:GLN:HA	21:1V:85:ASN:HD21	1.72	0.55
39:1n:30:CYS:SG	39:1n:31:VAL:N	2.80	0.55
1:1A:71:LEU:O	10:1J:147:TYR:OH	2.22	0.55
7:1G:241:SER:HB2	7:1G:248:MET:HE2	1.88	0.55
7:1G:327:ALA:HB2	7:1G:596:ASP:HB3	1.89	0.55
7:1G:504:ASP:O	19:1S:55:ARG:NH1	2.40	0.55
11:1K:48:ILE:HD13	11:1K:56:ALA:HB1	1.89	0.55
12:1L:42:TYR:OH	34:1i:66:HIS:ND1	2.31	0.55
32:1g:62:PHE:O	33:1h:28:TYR:OH	2.15	0.55
7:1G:326:GLU:OE2	7:1G:620:ARG:NH2	2.33	0.55
7:1G:366:THR:HB	7:1G:450:MET:HE1	1.82	0.55
16:1P:153:GLU:HB3	16:1P:154:LYS:NZ	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:313:LYS:NZ	16:1P:316:GLU:HG2	2.21	0.55
20:1T:43:ASP:OD1	20:1T:46:ASP:N	2.38	0.55
1:1A:9:THR:HG21	8:1H:6:ILE:HG21	1.88	0.54
1:1A:83:ASN:HD22	50:1J:201:PC1:H122	1.72	0.54
2:1B:37:VAL:O	8:1H:54:LYS:HE3	2.06	0.54
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.40	0.54
7:1G:244:THR:HG22	42:1q:133:LYS:NZ	2.21	0.54
10:1J:170:GLU:OE1	14:1N:1:FME:HG3	2.07	0.54
12:1L:35:TYR:OH	34:1i:73:HIS:NE2	2.35	0.54
12:1L:230:HIS:H	12:1L:231:PRO:CD	2.20	0.54
13:1M:1:FME:O	13:1M:4:ILE:N	2.40	0.54
13:1M:182:TRP:HE1	41:1p:79:LYS:HA	1.71	0.54
13:1M:430:PHE:HB3	32:1g:46:GLY:HA3	1.88	0.54
20:1U:37:MET:HE1	20:1U:43:ASP:CA	2.37	0.54
24:1Y:139:LYS:HG3	33:1h:112:ARG:HG3	1.88	0.54
32:1g:74:SER:HA	32:1g:77:VAL:HG12	1.89	0.54
35:1j:37:LEU:HB3	36:1k:77:PHE:HE1	1.72	0.54
37:1l:136:ASN:ND2	37:1l:139:TYR:HB3	2.20	0.54
4:1D:166:PRO:HD3	4:1D:228:MET:CE	2.36	0.54
7:1G:254:MET:HA	7:1G:260:GLU:O	2.07	0.54
7:1G:283:MET:HA	7:1G:283:MET:CE	2.24	0.54
7:1G:478:ARG:HH21	7:1G:481:SER:HA	1.71	0.54
8:1H:184:MET:HE1	50:1I:203:PC1:H322	1.88	0.54
17:1Q:11:ILE:HA	22:1W:23:ARG:NH1	2.22	0.54
32:1g:82:ASP:OD1	32:1g:87:GLU:OE1	2.26	0.54
32:1g:117:LYS:HD3	41:1p:74:THR:HG21	1.89	0.54
40:1o:110:ARG:HA	40:1o:113:ARG:HE	1.72	0.54
41:1p:78:GLU:HG2	41:1p:79:LYS:HG2	1.88	0.54
44:1s:71:GLN:OE1	44:1s:71:GLN:N	2.39	0.54
2:1B:62:MET:HE3	2:1B:69:MET:CB	2.36	0.54
5:1E:103:CYS:HB2	5:1E:153:MET:HG3	1.90	0.54
5:1E:165:THR:HG23	5:1E:168:ASP:H	1.72	0.54
6:1F:202:LYS:HB3	6:1F:361:GLN:OE1	2.07	0.54
6:1F:372:MET:O	6:1F:376:MET:HG3	2.07	0.54
8:1H:312:ALA:HB3	25:1Z:55:ARG:HH21	1.73	0.54
12:1L:260:LEU:HB3	12:1L:267:MET:HE1	1.89	0.54
16:1P:167:LYS:HB2	16:1P:229:ALA:HA	1.89	0.54
16:1P:322:ARG:NH1	16:1P:329:SER:O	2.41	0.54
16:1P:325:ARG:NE	16:1P:326:TRP:CZ3	2.72	0.54
20:1T:69:LYS:NZ	20:1T:70:LEU:HD23	2.16	0.54
35:1j:59:TRP:CD1	40:1o:99:LYS:HZ2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:92:LEU:HB3	2:1B:133:VAL:HG22	1.88	0.54
5:1E:98:TYR:N	5:1E:136:LEU:O	2.41	0.54
6:1F:65:LEU:HD11	6:1F:227:THR:HG22	1.90	0.54
13:1M:129:THR:O	13:1M:133:ILE:HD12	2.08	0.54
13:1M:373:ILE:HA	13:1M:376:ILE:HG22	1.89	0.54
15:1O:204:ASN:ND2	15:1O:208:LYS:CE	2.69	0.54
16:1P:191:VAL:HG11	16:1P:253:PHE:HE1	1.73	0.54
18:1R:56:VAL:C	18:1R:57:ILE:HD13	2.32	0.54
26:1a:59:ARG:HB3	26:1a:61:HIS:CD2	2.42	0.54
28:1c:13:ASP:OD2	28:1c:13:ASP:O	2.26	0.54
32:1g:63:PHE:O	32:1g:68:ILE:HG12	2.08	0.54
4:1D:281:VAL:HG23	4:1D:313:GLN:HB2	1.90	0.54
14:1N:95:MET:HE1	14:1N:149:ILE:HG12	1.90	0.54
20:1U:11:ILE:O	20:1U:15:VAL:HG23	2.08	0.54
38:1m:5:TYR:CE2	38:1m:14:PRO:HD3	2.42	0.54
6:1F:27:GLY:HA3	44:1s:38:TYR:HE1	1.73	0.54
6:1F:138:ILE:HD11	6:1F:142:PHE:HB2	1.90	0.54
7:1G:254:MET:SD	7:1G:254:MET:C	2.90	0.54
9:1I:164:GLU:HG3	42:1q:88:ARG:HG3	1.90	0.54
45:1L:702:3PE:H2H1	13:1M:398:MET:HE1	1.90	0.54
14:1N:7:THR:HG21	53:1N:402:CDL:H322	1.90	0.54
15:1O:20:GLU:HG2	15:1O:21:THR:HG23	1.89	0.54
15:1O:100:LEU:HD13	54:1O:401:GTP:C2	2.42	0.54
18:1R:57:ILE:HG12	18:1R:75:LEU:CD2	2.38	0.54
19:1S:17:GLU:OE1	19:1S:51:PRO:HG2	2.07	0.54
25:1Z:77:ALA:HB1	25:1Z:81:ARG:HH12	1.72	0.54
31:1f:22:PHE:O	31:1f:22:PHE:HD1	1.90	0.54
31:1f:43:LEU:HD21	41:1p:67:PHE:HB3	1.89	0.54
2:1B:118:SER:N	46:1B:201:SF4:S1	2.81	0.54
4:1D:414:VAL:HA	4:1D:417:ILE:HD12	1.89	0.54
7:1G:231:MET:HB3	7:1G:266:LYS:NZ	2.23	0.54
7:1G:673:MET:HE3	7:1G:684:MET:HE2	1.89	0.54
12:1L:375:ILE:HG13	12:1L:458:LEU:HD21	1.88	0.54
13:1M:243:MET:CG	13:1M:301:ILE:HG21	2.37	0.54
14:1N:154:MET:O	14:1N:158:ALA:N	2.27	0.54
19:1S:63:LYS:CE	19:1S:75:ASN:ND2	2.70	0.54
26:1a:55:SER:HA	26:1a:64:LYS:HZ2	1.72	0.54
41:1p:25:LEU:HD23	41:1p:25:LEU:H	1.73	0.54
6:1F:143:TYR:HB3	6:1F:179:ARG:NH1	2.23	0.54
7:1G:462:ASP:HB3	7:1G:657:LEU:HD13	1.90	0.54
11:1K:75:LEU:HD13	11:1K:78:LEU:HD23	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:22:MET:N	13:1M:22:MET:SD	2.81	0.54
14:1N:273:ASN:C	14:1N:274:GLU:OE2	2.51	0.54
16:1P:132:ILE:HD12	56:1P:501:NDP:H6N	1.90	0.54
22:1W:67:PHE:HA	58:1W:201:EHZ:S1	2.47	0.54
26:1a:39:ALA:HA	26:1a:44:GLN:HB2	1.88	0.54
6:1F:95:VAL:HG22	6:1F:228:VAL:HG21	1.90	0.54
8:1H:195:ARG:HH22	8:1H:270:PHE:HB3	1.72	0.54
10:1J:151:THR:OG1	50:1J:201:PC1:O32	2.26	0.54
12:1L:331:MET:N	12:1L:331:MET:SD	2.80	0.54
12:1L:587:TYR:O	12:1L:590:SER:OG	2.22	0.54
13:1M:300:ALA:O	13:1M:308:SER:OG	2.19	0.54
14:1N:325:LEU:HD23	53:1N:402:CDL:C73	2.24	0.54
16:1P:236:TYR:CE2	16:1P:337:ALA:HB3	2.42	0.54
17:1Q:91:ASP:OD1	17:1Q:91:ASP:N	2.32	0.54
19:1S:63:LYS:HE3	19:1S:75:ASN:HD21	1.72	0.54
23:1X:6:LEU:HD12	23:1X:7:PRO:O	2.08	0.54
40:1o:3:HIS:H	40:1o:3:HIS:CD2	2.25	0.54
1:1A:76:PRO:HG2	8:1H:160:TYR:CE1	2.43	0.54
4:1D:163:ALA:HB2	8:1H:278:PRO:HG3	1.89	0.54
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.48	0.54
9:1I:42:PHE:CD1	43:1r:10:LEU:HD12	2.43	0.54
12:1L:154:LEU:HD23	12:1L:247:LEU:HD11	1.90	0.54
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.33	0.54
13:1M:306:PRO:HA	13:1M:458:LEU:HD13	1.90	0.54
16:1P:72:GLU:OE1	16:1P:72:GLU:N	2.36	0.54
19:1S:62:PRO:O	19:1S:78:LEU:HB2	2.08	0.54
20:1U:70:LEU:HD12	20:1U:75:GLU:HG3	1.89	0.54
25:1Z:111:PHE:HZ	30:1e:68:ARG:HE	1.56	0.54
42:1q:53:LYS:HZ1	43:1r:2:SER:HB2	1.73	0.54
2:1B:77:ARG:NH1	2:1B:82:GLN:HG3	2.23	0.53
3:1C:192:GLN:HE21	17:1Q:72:TRP:HB3	1.73	0.53
7:1G:450:MET:SD	7:1G:487:TRP:CZ2	3.00	0.53
7:1G:548:HIS:CE1	7:1G:676:SER:OG	2.61	0.53
8:1H:3:MET:HE3	8:1H:3:MET:CA	2.38	0.53
8:1H:70:MET:HE2	8:1H:70:MET:HA	1.91	0.53
10:1J:13:PHE:CE1	11:1K:8:ILE:HG23	2.42	0.53
13:1M:441:ILE:HG23	13:1M:442:LEU:HD12	1.89	0.53
14:1N:268:GLN:HG3	23:1X:167:PHE:CZ	2.43	0.53
15:1O:164:LEU:HB2	15:1O:248:TRP:CZ3	2.43	0.53
15:1O:204:ASN:CA	15:1O:208:LYS:HZ1	2.21	0.53
16:1P:202:LYS:HA	16:1P:291:ASP:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:75:ARG:O	23:1X:75:ARG:CD	2.55	0.53
3:1C:77:ASP:HA	3:1C:130:TYR:CE1	2.43	0.53
3:1C:149:ARG:HA	22:1W:88:MET:HE2	1.90	0.53
3:1C:205:ALA:HA	7:1G:122:MET:HE2	1.90	0.53
6:1F:320:ASP:O	6:1F:324:GLN:NE2	2.40	0.53
7:1G:366:THR:HG21	7:1G:450:MET:HE1	1.89	0.53
11:1K:30:LEU:CD2	11:1K:75:LEU:HD22	2.38	0.53
13:1M:105:PHE:O	13:1M:109:THR:OG1	2.18	0.53
15:1O:46:LEU:HB2	15:1O:48:LEU:HD23	1.91	0.53
15:1O:219:GLU:OE1	15:1O:219:GLU:N	2.41	0.53
16:1P:236:TYR:CZ	16:1P:337:ALA:HB3	2.44	0.53
37:1L:130:PRO:HD3	40:1o:21:MET:SD	2.48	0.53
40:1o:38:MET:HE1	40:1o:57:TYR:CD2	2.43	0.53
40:1o:116:GLN:O	40:1o:120:GLU:N	2.40	0.53
4:1D:19:MET:HE2	14:1N:173:THR:HG22	1.90	0.53
4:1D:46:ASN:ND2	4:1D:67:GLU:OE1	2.42	0.53
14:1N:210:THR:HG22	53:1N:402:CDL:H801	1.90	0.53
15:1O:279:LEU:HB3	15:1O:282:ILE:HG22	1.89	0.53
16:1P:74:ASN:HB3	16:1P:77:ASP:HB2	1.90	0.53
16:1P:214:ILE:O	16:1P:218:ILE:CD1	2.54	0.53
22:1W:39:TRP:HB3	22:1W:63:VAL:HG11	1.89	0.53
23:1X:146:ARG:NE	30:1e:41:GLU:OE2	2.40	0.53
25:1Z:91:LEU:HA	25:1Z:94:GLU:HB3	1.89	0.53
32:1g:66:PHE:HB2	33:1h:28:TYR:CE2	2.42	0.53
3:1C:155:TYR:HD2	22:1W:98:LYS:HA	1.73	0.53
4:1D:161:ILE:HD13	4:1D:238:ARG:HH21	1.73	0.53
4:1D:231:ASN:HD21	25:1Z:25:LEU:HD21	1.72	0.53
7:1G:366:THR:HG21	7:1G:450:MET:CE	2.38	0.53
10:1J:31:LEU:C	10:1J:31:LEU:HD12	2.34	0.53
10:1J:117:PHE:HZ	14:1N:76:ILE:HD13	1.73	0.53
13:1M:80:SER:HB2	13:1M:226:ALA:HB2	1.91	0.53
15:1O:204:ASN:O	15:1O:208:LYS:CG	2.45	0.53
16:1P:59:LEU:HD12	16:1P:70:PHE:CE2	2.37	0.53
16:1P:268:ARG:HB2	16:1P:281:ARG:HH21	1.73	0.53
17:1Q:93:VAL:HG12	17:1Q:103:PHE:CZ	2.43	0.53
19:1S:63:LYS:NZ	19:1S:75:ASN:CB	2.71	0.53
20:1U:15:VAL:O	20:1U:19:LEU:HD22	2.09	0.53
26:1a:69:ILE:HD12	26:1a:69:ILE:O	2.08	0.53
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.25	0.53
30:1e:21:SER:OG	30:1e:33:HIS:CD2	2.61	0.53
5:1E:53:LEU:HD11	44:1s:52:LEU:HG	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:59:GLU:HG2	6:1F:235:CYS:HA	1.90	0.53
6:1F:94:VAL:HG12	6:1F:222:VAL:HG13	1.90	0.53
7:1G:123:PHE:O	7:1G:123:PHE:HD1	1.91	0.53
8:1H:195:ARG:NH2	8:1H:270:PHE:HB3	2.24	0.53
11:1K:75:LEU:HD22	11:1K:75:LEU:N	2.23	0.53
13:1M:227:GLY:O	13:1M:231:LEU:HG	2.08	0.53
16:1P:81:ILE:H	16:1P:81:ILE:HD12	1.74	0.53
19:1S:36:ILE:HA	19:1S:40:TYR:HB2	1.90	0.53
20:1T:35:HIS:CD2	20:1T:38:LYS:HE3	2.43	0.53
20:1U:61:GLU:OE2	39:1n:81:PHE:N	2.41	0.53
23:1X:156:ASP:N	23:1X:156:ASP:OD1	2.39	0.53
34:1i:79:TRP:HE1	41:1p:40:VAL:HA	1.73	0.53
3:1C:152:LEU:HD22	4:1D:84:HIS:HD2	1.73	0.53
4:1D:86:GLY:O	4:1D:90:LEU:HD12	2.08	0.53
5:1E:78:MET:CE	7:1G:185:THR:HA	2.38	0.53
6:1F:305:PRO:HB3	6:1F:417:GLY:HA3	1.88	0.53
7:1G:119:GLN:HB3	7:1G:123:PHE:CE1	2.44	0.53
7:1G:283:MET:HE1	7:1G:292:THR:O	2.09	0.53
12:1L:128:MET:HE1	12:1L:251:THR:HA	1.90	0.53
12:1L:405:ASN:O	12:1L:407:TRP:N	2.42	0.53
15:1O:136:GLU:HA	15:1O:139:TYR:HB3	1.90	0.53
15:1O:171:TYR:CZ	15:1O:207:LYS:NZ	2.75	0.53
16:1P:29:PHE:CD1	16:1P:175:GLU:HG2	2.44	0.53
16:1P:311:GLU:H	16:1P:311:GLU:CD	2.16	0.53
20:1T:69:LYS:C	20:1T:69:LYS:CD	2.82	0.53
22:1W:103:ILE:HA	22:1W:106:PHE:CE1	2.43	0.53
34:1i:6:ASP:OD1	34:1i:6:ASP:N	2.41	0.53
43:1r:1:ALA:O	43:1r:2:SER:N	2.42	0.53
4:1D:202:ASP:HB2	4:1D:323:ILE:HD13	1.90	0.53
8:1H:26:LYS:HZ1	26:1a:4:GLU:HB3	1.73	0.53
19:1S:17:GLU:HB2	19:1S:67:ARG:CD	2.30	0.53
23:1X:74:LYS:NZ	26:1a:69:ILE:O	2.41	0.53
23:1X:76:HIS:O	23:1X:78:ALA:N	2.41	0.53
30:1e:44:HIS:HE1	33:1h:129:ASP:HA	1.73	0.53
40:1o:114:ARG:HE	40:1o:117:ARG:HH22	1.55	0.53
3:1C:18:VAL:O	3:1C:22:LEU:HD13	2.08	0.53
7:1G:211:LYS:HZ1	7:1G:699:GLU:CD	2.16	0.53
7:1G:524:LEU:HD23	7:1G:527:ALA:HB3	1.89	0.53
9:1I:150:ASN:OD1	9:1I:152:GLU:N	2.42	0.53
12:1L:173:LEU:HD13	45:1L:702:3PE:H321	1.89	0.53
14:1N:267:ILE:O	14:1N:271:THR:OG1	2.17	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:203:GLN:HE22	16:1P:233:PRO:C	2.17	0.53
21:1V:30:ILE:HD11	21:1V:51:THR:HG23	1.91	0.53
29:1d:46:ASN:ND2	29:1d:56:ALA:O	2.41	0.53
32:1g:112:CYS:SG	32:1g:113:PHE:N	2.81	0.53
37:1l:90:ASP:OD1	37:1l:90:ASP:N	2.42	0.53
37:1l:128:VAL:HG21	40:1o:94:TYR:HE1	1.74	0.53
44:1s:38:TYR:CE1	44:1s:40:ASN:HB3	2.44	0.53
3:1C:35:LYS:HD2	21:1V:98:PRO:HA	1.90	0.53
3:1C:189:GLU:OE2	16:1P:14:SER:N	2.40	0.53
5:1E:145:LEU:HD12	5:1E:146:GLY:N	2.24	0.53
6:1F:99:GLU:OE1	6:1F:108:ARG:N	2.37	0.53
7:1G:258:ILE:HG22	7:1G:259:ASN:H	1.74	0.53
10:1J:115:ILE:O	10:1J:117:PHE:N	2.42	0.53
14:1N:211:MET:HG2	14:1N:251:MET:CE	2.37	0.53
23:1X:81:PHE:CE2	26:1a:66:LEU:CD2	2.92	0.53
36:1k:88:GLU:OE1	36:1k:88:GLU:HA	2.08	0.53
38:1m:39:ARG:HH12	38:1m:42:LEU:HB2	1.74	0.53
5:1E:22:ASP:O	5:1E:57:GLN:NE2	2.38	0.53
5:1E:78:MET:HE3	7:1G:171:ASP:O	2.09	0.53
6:1F:20:ARG:HD3	6:1F:23:THR:HA	1.91	0.53
7:1G:142:ILE:HG22	7:1G:142:ILE:O	2.08	0.53
7:1G:161:ARG:O	7:1G:165:GLU:HB2	2.09	0.53
9:1I:75:GLU:OE2	9:1I:155:LEU:HD21	2.09	0.53
12:1L:363:TYR:N	12:1L:431:PHE:HB3	2.24	0.53
22:1W:66:MET:HA	22:1W:69:LYS:HG2	1.90	0.53
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	1.90	0.53
31:1f:5:GLN:NE2	31:1f:9:ASP:OD2	2.34	0.53
33:1h:14:SER:HB2	39:1n:106:TRP:HA	1.91	0.53
6:1F:53:PRO:CA	6:1F:127:ARG:HH12	2.21	0.52
7:1G:494:HIS:HD1	7:1G:499:GLN:HB3	1.74	0.52
7:1G:620:ARG:NH1	7:1G:633:TYR:OH	2.42	0.52
12:1L:51:LEU:HD11	12:1L:88:MET:CE	2.39	0.52
13:1M:338:HIS:NE2	32:1g:34:ASP:OD2	2.42	0.52
14:1N:100:MET:CE	14:1N:111:PHE:HE2	2.21	0.52
16:1P:192:PRO:O	16:1P:263:TYR:OH	2.20	0.52
21:1V:39:LYS:HA	21:1V:44:ARG:CD	2.20	0.52
3:1C:152:LEU:HB3	4:1D:84:HIS:CD2	2.44	0.52
4:1D:146:ARG:NH1	4:1D:270:ARG:HH12	2.07	0.52
5:1E:78:MET:HE1	7:1G:185:THR:HA	1.92	0.52
6:1F:15:LEU:HD13	6:1F:271:GLU:HG2	1.91	0.52
6:1F:101:GLU:C	6:1F:101:GLU:CD	2.76	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:292:SER:OG	50:1I:203:PC1:O32	2.27	0.52
10:1J:30:GLY:O	10:1J:34:ILE:HG23	2.09	0.52
12:1L:107:TYR:CE2	12:1L:348:HIS:HB2	2.44	0.52
13:1M:317:ILE:HB	13:1M:454:ILE:HD11	1.92	0.52
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD11	1.90	0.52
20:1T:35:HIS:CB	20:1T:38:LYS:HZ2	2.23	0.52
32:1g:67:SER:N	33:1h:28:TYR:OH	2.29	0.52
41:1p:145:LEU:HD11	41:1p:154:CYS:SG	2.50	0.52
3:1C:78:LEU:H	3:1C:130:TYR:HD1	1.57	0.52
4:1D:3:GLN:NE2	4:1D:5:GLN:OE1	2.38	0.52
5:1E:53:LEU:H	5:1E:53:LEU:HD22	1.74	0.52
7:1G:102:PRO:HG3	7:1G:151:THR:HG23	1.91	0.52
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.91	0.52
8:1H:91:MET:HE2	8:1H:259:PHE:CE2	2.44	0.52
8:1H:133:LEU:HD21	10:1J:73:ALA:HB1	1.91	0.52
9:1I:70:TYR:HD1	9:1I:76:ARG:HG2	1.75	0.52
13:1M:158:LEU:HD22	14:1N:283:ALA:HB1	1.91	0.52
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.92	0.52
14:1N:159:MET:HE3	14:1N:159:MET:C	2.34	0.52
17:1Q:22:LEU:HD21	22:1W:82:LEU:HB2	1.91	0.52
20:1T:20:LYS:HZ1	20:1T:27:PRO:HA	1.66	0.52
36:1k:81:VAL:HA	36:1k:84:GLU:HB3	1.89	0.52
38:1m:82:THR:HG23	38:1m:85:THR:H	1.74	0.52
4:1D:161:ILE:HG13	4:1D:235:TRP:CZ3	2.44	0.52
4:1D:166:PRO:CD	4:1D:228:MET:HE1	2.40	0.52
6:1F:215:VAL:HG22	6:1F:216:PHE:CD2	2.45	0.52
7:1G:255:HIS:CE1	7:1G:579:ARG:NH2	2.77	0.52
8:1H:91:MET:O	8:1H:93:TYR:N	2.43	0.52
8:1H:292:SER:HB2	50:1I:203:PC1:H143	1.91	0.52
10:1J:25:SER:HB2	10:1J:81:GLU:C	2.34	0.52
17:1Q:19:ILE:H	17:1Q:19:ILE:HD12	1.75	0.52
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.43	0.52
29:1d:2:MET:SD	33:1h:122:TRP:HE3	2.32	0.52
32:1g:101:GLU:OE1	32:1g:101:GLU:N	2.42	0.52
39:1n:43:MET:HE3	39:1n:44:ARG:N	2.25	0.52
39:1n:139:LEU:O	39:1n:143:THR:OG1	2.22	0.52
42:1q:86:TRP:CE3	42:1q:98:PRO:HD2	2.43	0.52
2:1B:148:GLY:CA	9:1I:118:TYR:HE1	2.23	0.52
4:1D:294:TYR:CZ	4:1D:298:LEU:HD21	2.45	0.52
7:1G:296:TRP:O	7:1G:300:LEU:HG	2.10	0.52
7:1G:336:ASN:CG	19:1S:67:ARG:HH21	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:30:TYR:OH	26:1a:4:GLU:OE1	2.28	0.52
9:1I:75:GLU:O	9:1I:105:ARG:NH1	2.42	0.52
10:1J:58:LEU:HD12	10:1J:59:ILE:HG23	1.92	0.52
10:1J:60:TYR:HE1	11:1K:38:LEU:HG	1.74	0.52
11:1K:27:MET:HE3	11:1K:27:MET:HA	1.92	0.52
15:1O:205:ALA:N	15:1O:208:LYS:NZ	2.56	0.52
2:1B:52:LEU:HB2	2:1B:90:GLY:HA3	1.90	0.52
6:1F:161:LEU:HD23	6:1F:167:CYS:HB3	1.91	0.52
7:1G:575:ASN:OD1	7:1G:578:GLY:N	2.43	0.52
7:1G:675:ASP:OD2	7:1G:678:SER:N	2.35	0.52
9:1I:112:ASP:OD2	9:1I:114:THR:N	2.42	0.52
12:1L:175:ASN:OD1	12:1L:223:LYS:HD3	2.10	0.52
12:1L:485:TYR:CD2	51:1L:701:MYR:H71	2.44	0.52
25:1Z:120:MET:HG3	25:1Z:122:GLY:H	1.75	0.52
38:1m:51:ASN:HD22	39:1n:165:LEU:HD12	1.75	0.52
39:1n:97:LYS:NZ	39:1n:175:GLU:O	2.42	0.52
39:1n:169:ILE:H	39:1n:169:ILE:HD12	1.75	0.52
2:1B:46:TRP:CD1	2:1B:75:VAL:HG12	2.44	0.52
3:1C:99:LEU:H	3:1C:99:LEU:HD12	1.73	0.52
3:1C:196:LYS:HZ2	17:1Q:81:ASN:HA	1.70	0.52
4:1D:246:THR:HG23	4:1D:249:ASP:HB2	1.92	0.52
6:1F:101:GLU:O	6:1F:104:THR:OG1	2.21	0.52
7:1G:56:LEU:HD11	7:1G:65:VAL:CB	2.39	0.52
10:1J:33:LEU:O	10:1J:37:GLY:N	2.37	0.52
12:1L:489:THR:HA	12:1L:492:ILE:HG12	1.91	0.52
20:1T:67:ALA:HA	20:1T:70:LEU:HD12	1.91	0.52
21:1V:3:LEU:HD22	21:1V:4:LEU:H	1.75	0.52
29:1d:110:GLY:HA2	32:1g:118:ILE:HG22	1.91	0.52
36:1k:88:GLU:OE1	36:1k:91:ASN:ND2	2.32	0.52
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.90	0.52
40:1o:60:HIS:HE1	40:1o:89:CYS:SG	2.33	0.52
42:1q:84:PRO:HD3	42:1q:113:HIS:HB2	1.90	0.52
5:1E:191:PHE:HB3	44:1s:38:TYR:HB2	1.89	0.52
6:1F:150:GLN:HA	6:1F:153:ILE:CG1	2.40	0.52
6:1F:202:LYS:HE3	6:1F:361:GLN:CG	2.39	0.52
7:1G:366:THR:OG1	7:1G:450:MET:CE	2.51	0.52
7:1G:493:LEU:HA	7:1G:576:THR:HG21	1.91	0.52
11:1K:12:PHE:CD1	14:1N:72:MET:CE	2.90	0.52
11:1K:71:ALA:O	11:1K:75:LEU:HD23	2.10	0.52
12:1L:121:LEU:HD22	12:1L:246:LEU:HD23	1.92	0.52
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:293:ILE:HD11	45:1L:704:3PE:H242	1.92	0.52
14:1N:42:PRO:HA	14:1N:45:MET:HB2	1.92	0.52
16:1P:50:ARG:HH21	56:1P:501:NDP:C5A	2.23	0.52
20:1T:18:VAL:HG12	20:1T:21:LEU:HD12	1.92	0.52
26:1a:59:ARG:HB3	26:1a:61:HIS:HD2	1.75	0.52
42:1q:50:GLU:HB3	42:1q:89:TRP:HZ2	1.74	0.52
6:1F:247:ARG:HH22	6:1F:316:LEU:HD22	1.75	0.52
7:1G:364:LEU:HB2	7:1G:576:THR:HG22	1.91	0.52
9:1I:32:ARG:HG2	50:1I:204:PC1:H31	1.92	0.52
12:1L:51:LEU:HD11	12:1L:88:MET:SD	2.50	0.52
12:1L:486:MET:HG3	51:1L:701:MYR:H41	1.91	0.52
19:1S:39:ARG:NH2	19:1S:90:LEU:HD11	2.25	0.52
1:1A:6:THR:HG21	8:1H:96:ILE:HD11	1.92	0.52
4:1D:130:PRO:HG2	4:1D:138:ARG:HH22	1.75	0.52
4:1D:233:ARG:HG3	4:1D:234:ILE:HD12	1.91	0.52
6:1F:376:MET:SD	6:1F:377:ALA:N	2.83	0.52
6:1F:409:ASP:O	6:1F:413:TRP:CD1	2.63	0.52
8:1H:149:ILE:O	8:1H:153:VAL:HG22	2.10	0.52
14:1N:100:MET:HE3	14:1N:100:MET:HA	1.92	0.52
16:1P:81:ILE:O	16:1P:85:VAL:HG22	2.10	0.52
21:1V:36:GLN:OE1	21:1V:36:GLN:N	2.42	0.52
21:1V:43:TYR:HD2	21:1V:99:TRP:HH2	1.58	0.52
24:1Y:68:ILE:HG21	24:1Y:99:THR:HG21	1.90	0.52
32:1g:50:ASP:OD1	32:1g:52:ILE:HG22	2.10	0.52
32:1g:93:ALA:C	32:1g:97:VAL:HG23	2.30	0.52
39:1n:94:GLU:HA	39:1n:97:LYS:HE2	1.92	0.52
1:1A:65:PHE:O	1:1A:69:ILE:HG23	2.10	0.51
4:1D:233:ARG:NE	9:1I:29:GLU:OE2	2.41	0.51
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.26	0.51
5:1E:74:GLN:CD	5:1E:74:GLN:N	2.68	0.51
5:1E:89:MET:HE3	6:1F:181:ALA:C	2.35	0.51
10:1J:20:PHE:CD2	10:1J:33:LEU:HB3	2.45	0.51
15:1O:133:VAL:HG21	15:1O:206:TYR:CE2	2.45	0.51
16:1P:134:HIS:O	16:1P:167:LYS:NZ	2.37	0.51
21:1V:98:PRO:HD2	21:1V:99:TRP:CZ2	2.45	0.51
22:1W:65:GLU:OE1	22:1W:69:LYS:CE	2.57	0.51
23:1X:74:LYS:HD2	26:1a:66:LEU:HD12	1.92	0.51
23:1X:78:ALA:O	23:1X:82:THR:OG1	2.26	0.51
25:1Z:127:LEU:HD13	30:1e:97:HIS:CG	2.45	0.51
32:1g:50:ASP:OD1	32:1g:50:ASP:C	2.51	0.51
32:1g:85:MET:N	32:1g:85:MET:SD	2.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:149:VAL:HG11	5:1E:193:CYS:SG	2.50	0.51
6:1F:324:GLN:OE1	6:1F:324:GLN:N	2.30	0.51
7:1G:194:GLU:HG2	7:1G:195:LEU:HD22	1.91	0.51
7:1G:364:LEU:HD23	7:1G:577:GLU:HG2	1.92	0.51
15:1O:301:GLY:HA3	28:1c:2:PHE:HE2	1.75	0.51
19:1S:42:GLU:O	19:1S:45:LYS:HG2	2.10	0.51
21:1V:37:ILE:HG13	21:1V:38:PRO:HD2	1.91	0.51
22:1W:65:GLU:CA	22:1W:69:LYS:NZ	2.73	0.51
23:1X:81:PHE:O	23:1X:81:PHE:CD1	2.62	0.51
37:1l:70:ARG:NE	37:1l:86:ARG:HH11	2.08	0.51
4:1D:174:ARG:HA	4:1D:177:MET:HE1	1.91	0.51
6:1F:193:ILE:HD11	6:1F:214:GLY:C	2.36	0.51
15:1O:174:VAL:HG12	15:1O:179:ILE:HG13	1.92	0.51
16:1P:176:ASP:OD2	16:1P:179:LEU:N	2.26	0.51
16:1P:262:ALA:HA	16:1P:265:TRP:CD1	2.46	0.51
25:1Z:140:PHE:HB2	26:1a:45:TRP:CG	2.45	0.51
30:1e:46:ILE:HG23	30:1e:50:ARG:HH21	1.75	0.51
2:1B:56:ALA:O	2:1B:59:MET:HB3	2.10	0.51
2:1B:71:ARG:HH12	9:1I:49:ASN:HA	1.74	0.51
6:1F:205:LEU:HB2	17:1Q:118:TYR:CZ	2.45	0.51
6:1F:266:CYS:HB3	6:1F:268:VAL:HG23	1.92	0.51
15:1O:204:ASN:O	15:1O:208:LYS:N	2.36	0.51
15:1O:204:ASN:HD22	15:1O:208:LYS:CE	2.24	0.51
18:1R:49:VAL:HG12	18:1R:92:ARG:HG2	1.91	0.51
28:1c:41:GLU:OE2	28:1c:41:GLU:CA	2.58	0.51
29:1d:17:GLU:H	29:1d:17:GLU:CD	2.18	0.51
32:1g:100:ARG:HD2	32:1g:105:LEU:CD2	2.39	0.51
35:1j:21:GLN:HG3	35:1j:22:LEU:HD12	1.92	0.51
2:1B:40:ALA:H	8:1H:54:LYS:HZ3	1.58	0.51
6:1F:334:VAL:HG12	6:1F:334:VAL:O	2.11	0.51
7:1G:42:TYR:HB2	7:1G:69:CYS:SG	2.50	0.51
7:1G:46:LEU:HD23	7:1G:47:SER:O	2.11	0.51
7:1G:495:ARG:HH12	7:1G:664:PRO:HG2	1.76	0.51
9:1I:39:SER:O	9:1I:43:ARG:NH1	2.44	0.51
12:1L:49:VAL:HG13	12:1L:50:PRO:HD3	1.92	0.51
12:1L:159:HIS:HD2	13:1M:416:ARG:HA	1.75	0.51
12:1L:161:ARG:HA	39:1n:91:GLU:HB2	1.93	0.51
13:1M:355:MET:HE1	13:1M:437:MET:HE3	1.93	0.51
14:1N:58:LYS:O	14:1N:62:THR:HG23	2.11	0.51
15:1O:37:ARG:O	15:1O:41:GLU:HG2	2.11	0.51
22:1W:80:ASP:OD1	22:1W:80:ASP:N	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:21:SER:HA	23:1X:24:LEU:HD23	1.91	0.51
31:1f:12:VAL:HG23	31:1f:15:LEU:HD11	1.93	0.51
40:1o:106:ARG:HA	40:1o:109:GLN:NE2	2.26	0.51
1:1A:95:LEU:HD13	8:1H:302:MET:HG3	1.93	0.51
3:1C:204:GLU:HA	17:1Q:50:ASN:ND2	2.26	0.51
4:1D:221:ARG:CD	43:1r:24:GLN:NE2	2.74	0.51
7:1G:282:PRO:HG3	7:1G:296:TRP:CD2	2.45	0.51
7:1G:373:GLU:OE2	7:1G:448:LYS:NZ	2.44	0.51
13:1M:443:PRO:O	13:1M:447:LEU:HG	2.11	0.51
14:1N:100:MET:HE3	14:1N:111:PHE:HE2	1.75	0.51
32:1g:100:ARG:CD	32:1g:105:LEU:HD22	2.41	0.51
36:1k:77:PHE:CE2	36:1k:81:VAL:HG21	2.46	0.51
3:1C:179:GLU:HG3	16:1P:33:TYR:CD2	2.44	0.51
4:1D:221:ARG:NH2	43:1r:24:GLN:HA	2.21	0.51
7:1G:36:GLN:HG3	7:1G:39:ARG:HH22	1.75	0.51
7:1G:584:LYS:HZ3	7:1G:585:VAL:HB	1.76	0.51
8:1H:26:LYS:HZ1	26:1a:4:GLU:C	2.19	0.51
12:1L:482:MET:HB3	12:1L:487:LYS:HB2	1.92	0.51
20:1T:72:CYS:SG	20:1T:74:GLN:HB2	2.50	0.51
22:1W:90:LEU:O	22:1W:93:THR:OG1	2.26	0.51
42:1q:100:THR:OG1	42:1q:101:LYS:N	2.41	0.51
42:1q:101:LYS:HD2	42:1q:101:LYS:O	2.11	0.51
3:1C:66:ASP:HB2	21:1V:89:LEU:HB2	1.93	0.51
4:1D:398:HIS:O	4:1D:421:GLN:NE2	2.38	0.51
6:1F:287:VAL:HG21	6:1F:294:LEU:HD12	1.92	0.51
7:1G:259:ASN:N	7:1G:259:ASN:OD1	2.43	0.51
9:1I:65:HIS:CD2	9:1I:111:ILE:HG21	2.46	0.51
12:1L:129:MET:HA	12:1L:129:MET:HE3	1.92	0.51
52:1M:501:PGT:H472	52:1M:501:PGT:H232	1.92	0.51
14:1N:175:LEU:HD21	14:1N:227:THR:HA	1.93	0.51
16:1P:197:GLY:O	16:1P:238:LEU:HB2	2.10	0.51
20:1T:14:ARG:HG3	20:1T:58:PHE:CE2	2.44	0.51
23:1X:81:PHE:CE2	26:1a:66:LEU:HD21	2.45	0.51
31:1f:53:GLU:HG2	31:1f:54:VAL:HG13	1.93	0.51
34:1i:1:SAC:C	34:1i:2:GLY:HA3	2.41	0.51
34:1i:104:PHE:CZ	40:1o:66:LEU:HB3	2.46	0.51
36:1k:21:TRP:NE1	36:1k:50:TRP:HB3	2.26	0.51
3:1C:125:LYS:NZ	4:1D:252:ASN:HB3	2.25	0.51
6:1F:134:ALA:HB3	6:1F:175:VAL:HA	1.92	0.51
7:1G:123:PHE:O	7:1G:123:PHE:CD1	2.64	0.51
7:1G:256:GLU:O	7:1G:260:GLU:HG3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:283:MET:HE1	7:1G:293:TYR:HA	1.93	0.51
10:1J:151:THR:HG21	50:1J:201:PC1:H32	1.93	0.51
11:1K:96:LEU:HB2	14:1N:54:GLU:HG2	1.93	0.51
12:1L:501:ALA:O	12:1L:505:ASN:ND2	2.44	0.51
13:1M:1:FME:CG	13:1M:111:THR:HG21	2.40	0.51
14:1N:95:MET:HE3	14:1N:148:SER:O	2.09	0.51
15:1O:13:ARG:O	15:1O:17:LYS:NZ	2.30	0.51
16:1P:210:VAL:O	16:1P:214:ILE:HG12	2.11	0.51
17:1Q:57:MET:HG3	17:1Q:84:LEU:HB2	1.92	0.51
18:1R:18:TYR:HB3	18:1R:25:ARG:HD3	1.93	0.51
19:1S:63:LYS:NZ	19:1S:75:ASN:HB2	2.26	0.51
20:1T:43:ASP:HB2	58:1W:201:EHZ:O7	2.11	0.51
3:1C:116:PRO:HG3	22:1W:20:ILE:HG13	1.92	0.51
3:1C:198:ASP:OD1	3:1C:198:ASP:N	2.43	0.51
5:1E:10:ARG:NH2	18:1R:77:LYS:HA	2.25	0.51
5:1E:143:GLU:HG3	6:1F:357:GLU:OE2	2.11	0.51
6:1F:93:LEU:HD22	6:1F:94:VAL:H	1.76	0.51
7:1G:65:VAL:HG13	7:1G:85:LYS:HG2	1.93	0.51
7:1G:379:LEU:HD23	7:1G:384:PRO:HG3	1.91	0.51
9:1I:70:TYR:CD1	9:1I:76:ARG:HG2	2.45	0.51
12:1L:103:PHE:CG	12:1L:341:MET:HE1	2.45	0.51
13:1M:14:MET:O	13:1M:18:SER:OG	2.24	0.51
14:1N:154:MET:CE	14:1N:194:LEU:HB3	2.41	0.51
32:1g:87:GLU:H	32:1g:87:GLU:CD	2.05	0.51
39:1n:31:VAL:HG22	39:1n:32:HIS:H	1.76	0.51
2:1B:94:ASN:HB3	3:1C:174:LEU:HD11	1.91	0.50
5:1E:9:HIS:CD2	7:1G:187:ILE:HG12	2.45	0.50
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.92	0.50
10:1J:119:PHE:CD2	11:1K:6:MET:HG3	2.46	0.50
12:1L:155:ILE:HD11	12:1L:248:HIS:NE2	2.26	0.50
12:1L:246:LEU:C	12:1L:246:LEU:HD12	2.36	0.50
12:1L:350:LEU:O	12:1L:350:LEU:HD23	2.11	0.50
14:1N:190:MET:HE1	14:1N:205:LEU:HA	1.92	0.50
16:1P:248:VAL:HG22	16:1P:334:VAL:HG11	1.92	0.50
16:1P:262:ALA:O	16:1P:266:VAL:HG23	2.12	0.50
18:1R:16:GLN:HE21	18:1R:18:TYR:HD1	1.59	0.50
20:1T:69:LYS:HZ1	20:1T:70:LEU:HD21	1.74	0.50
21:1V:22:ARG:HH11	21:1V:25:ILE:HG23	1.76	0.50
22:1W:82:LEU:HD11	58:1W:201:EHZ:C9	2.41	0.50
23:1X:81:PHE:CD1	23:1X:85:TRP:HD1	2.29	0.50
25:1Z:94:GLU:OE2	25:1Z:104:TRP:NE1	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:42:MET:HA	34:1i:45:PHE:CD2	2.47	0.50
34:1i:109:ILE:HD13	34:1i:114:GLU:CD	2.32	0.50
38:1m:60:GLU:OE2	38:1m:60:GLU:C	2.54	0.50
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.36	0.50
6:1F:55:TRP:HH2	6:1F:59:GLU:OE1	1.94	0.50
7:1G:6:SER:OG	7:1G:7:ASN:N	2.40	0.50
7:1G:365:ASN:N	7:1G:491:ASN:OD1	2.44	0.50
7:1G:375:ASP:OD2	7:1G:448:LYS:N	2.28	0.50
11:1K:8:ILE:HB	11:1K:43:MET:HE1	1.92	0.50
12:1L:373:LEU:HD23	12:1L:431:PHE:CE2	2.46	0.50
12:1L:550:SER:HA	13:1M:275:ILE:HD12	1.93	0.50
13:1M:269:MET:O	13:1M:273:SER:OG	2.28	0.50
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.45	0.50
14:1N:122:ILE:HD11	14:1N:127:GLY:HA2	1.94	0.50
19:1S:75:ASN:C	19:1S:75:ASN:OD1	2.54	0.50
23:1X:8:THR:HG23	23:1X:10:GLU:H	1.77	0.50
26:1a:37:ARG:HB3	26:1a:48:MET:SD	2.50	0.50
29:1d:28:ASP:HB3	29:1d:31:LEU:HB3	1.92	0.50
33:1h:47:ILE:HG13	41:1p:58:ASN:HD22	1.76	0.50
6:1F:46:LYS:HD2	6:1F:47:GLU:HG2	1.94	0.50
6:1F:55:TRP:CZ3	6:1F:59:GLU:HA	2.45	0.50
8:1H:179:TRP:NE1	25:1Z:43:LEU:HG	2.26	0.50
13:1M:44:GLN:HG3	13:1M:60:SER:HA	1.93	0.50
13:1M:313:THR:HG21	13:1M:456:GLY:HA3	1.93	0.50
14:1N:179:MET:HE3	14:1N:179:MET:O	2.12	0.50
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.47	0.50
15:1O:308:TYR:OH	28:1c:9:HIS:ND1	2.41	0.50
17:1Q:12:ALA:H	22:1W:23:ARG:HH12	1.58	0.50
17:1Q:64:ARG:HA	17:1Q:75:THR:HG22	1.93	0.50
20:1T:7:THR:OG1	20:1T:9:GLU:HG3	2.11	0.50
22:1W:59:GLY:O	22:1W:63:VAL:HG23	2.11	0.50
36:1k:44:TRP:O	39:1n:37:ARG:NH1	2.44	0.50
37:1l:10:PRO:HA	37:1l:26:LYS:HZ2	1.76	0.50
37:1l:85:ILE:HD11	37:1l:88:ARG:HG3	1.93	0.50
40:1o:62:LEU:HD23	40:1o:86:TRP:CD2	2.46	0.50
43:1r:51:ASN:HB3	43:1r:56:ARG:HH12	1.77	0.50
1:1A:59:ALA:HB1	10:1J:67:VAL:HG12	1.93	0.50
4:1D:350:LYS:NZ	7:1G:118:ASP:OD1	2.35	0.50
4:1D:411:LEU:H	4:1D:411:LEU:HD22	1.76	0.50
7:1G:363:LEU:HD22	7:1G:577:GLU:O	2.11	0.50
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:151:SER:CB	12:1L:252:MET:HE2	2.41	0.50
14:1N:218:LEU:HD12	14:1N:244:MET:CE	2.36	0.50
19:1S:78:LEU:HA	19:1S:81:PHE:CD1	2.45	0.50
25:1Z:120:MET:CG	25:1Z:122:GLY:H	2.23	0.50
28:1c:3:TYR:HD2	28:1c:7:PRO:HD3	1.77	0.50
32:1g:37:LEU:HD22	32:1g:46:GLY:HA2	1.94	0.50
32:1g:114:ASP:HB3	32:1g:117:LYS:HD2	1.94	0.50
34:1i:13:GLN:HE22	39:1n:156:ALA:N	2.04	0.50
37:1l:82:ASP:O	37:1l:88:ARG:HD2	2.10	0.50
2:1B:92:LEU:HD11	2:1B:100:LEU:HD12	1.93	0.50
4:1D:312:SER:HB2	25:1Z:19:ILE:HD13	1.93	0.50
6:1F:16:LYS:HB2	6:1F:19:ASP:HB2	1.93	0.50
6:1F:254:LYS:HB3	6:1F:256:PHE:HE2	1.76	0.50
7:1G:56:LEU:HD11	7:1G:65:VAL:CG2	2.41	0.50
7:1G:218:ARG:HD2	7:1G:219:PRO:HD2	1.94	0.50
7:1G:460:ARG:NH2	7:1G:662:VAL:O	2.45	0.50
7:1G:478:ARG:HH22	7:1G:483:VAL:HB	1.75	0.50
9:1I:108:ARG:NH2	17:1Q:71:GLY:O	2.33	0.50
10:1J:34:ILE:HG13	10:1J:35:VAL:N	2.25	0.50
12:1L:370:THR:HG23	12:1L:431:PHE:CD2	2.47	0.50
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.47	0.50
15:1O:2:GLN:H	15:1O:2:GLN:CD	2.19	0.50
22:1W:43:VAL:O	22:1W:47:VAL:HG23	2.11	0.50
35:1j:55:ASP:HB3	35:1j:58:GLN:HG2	1.93	0.50
38:1m:60:GLU:OE1	38:1m:65:ILE:HG13	2.11	0.50
3:1C:81:VAL:O	3:1C:81:VAL:HG12	2.11	0.50
5:1E:175:GLU:HB2	5:1E:180:LYS:HB2	1.92	0.50
6:1F:82:MET:O	6:1F:91:LYS:NZ	2.41	0.50
6:1F:351:ILE:HD11	6:1F:376:MET:HG2	1.93	0.50
7:1G:399:TRP:CZ3	7:1G:417:TYR:HB3	2.47	0.50
7:1G:412:PRO:HD3	7:1G:421:HIS:CE1	2.45	0.50
7:1G:545:TYR:HB3	7:1G:560:ILE:HD13	1.92	0.50
7:1G:632:ARG:HB3	7:1G:635:ASP:HB2	1.94	0.50
9:1I:36:MET:HA	9:1I:36:MET:CE	2.42	0.50
10:1J:52:LEU:HD13	11:1K:45:THR:HG22	1.93	0.50
50:1L:703:PC1:H282	13:1M:447:LEU:HD23	1.94	0.50
14:1N:197:ASN:HB3	14:1N:269:GLU:OE1	2.11	0.50
19:1S:23:CYS:HA	19:1S:57:CYS:O	2.11	0.50
34:1i:83:TYR:HE1	41:1p:48:ARG:HD3	1.77	0.50
2:1B:93:THR:O	2:1B:96:MET:HG2	2.12	0.50
3:1C:162:PHE:CE2	4:1D:88:GLU:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:30:ASP:HB2	44:1s:39:ARG:HE	1.77	0.50
7:1G:585:VAL:O	17:1Q:61:THR:OG1	2.29	0.50
8:1H:155:LEU:HD12	8:1H:308:PRO:HG2	1.92	0.50
8:1H:287:HIS:CE1	50:1I:203:PC1:H151	2.47	0.50
12:1L:51:LEU:HG	12:1L:55:MET:HE1	1.93	0.50
12:1L:102:GLU:HA	12:1L:105:MET:HE2	1.93	0.50
12:1L:553:LEU:HD21	38:1m:92:PHE:HB3	1.94	0.50
13:1M:40:SER:O	33:1h:80:TYR:OH	2.25	0.50
14:1N:319:HIS:ND1	15:1O:267:LEU:HD12	2.27	0.50
15:1O:137:ALA:HA	15:1O:201:ASP:OD2	2.12	0.50
17:1Q:38:PHE:CE2	17:1Q:40:PRO:HD3	2.47	0.50
25:1Z:98:MET:HE3	30:1e:78:ILE:HD13	1.94	0.50
29:1d:44:ILE:O	29:1d:48:ILE:HG13	2.12	0.50
34:1i:64:TYR:O	34:1i:68:ILE:HG22	2.11	0.50
1:1A:102:LEU:HD13	8:1H:294:LEU:HD22	1.94	0.50
5:1E:9:HIS:CE1	5:1E:63:ILE:HG12	2.47	0.50
7:1G:366:THR:O	7:1G:366:THR:HG22	2.10	0.50
8:1H:5:ASN:HD21	26:1a:23:THR:HG22	1.77	0.50
9:1I:69:ARG:HH22	9:1I:155:LEU:HD12	1.75	0.50
12:1L:147:VAL:CG2	12:1L:252:MET:HG2	2.42	0.50
13:1M:309:PHE:HB2	13:1M:458:LEU:HD12	1.94	0.50
16:1P:21:ALA:HB3	16:1P:45:VAL:HG22	1.94	0.50
4:1D:167:PHE:O	4:1D:171:PHE:HB2	2.12	0.50
4:1D:293:CYS:SG	4:1D:420:THR:HG21	2.52	0.50
5:1E:161:TYR:CZ	5:1E:172:ILE:HG21	2.47	0.50
5:1E:199:LEU:HD21	6:1F:28:ARG:HH21	1.77	0.50
6:1F:307:ILE:HD11	6:1F:311:VAL:HB	1.94	0.50
6:1F:358:SER:OG	6:1F:365:CYS:SG	2.66	0.50
6:1F:360:GLY:HA2	6:1F:366:ARG:HB2	1.93	0.50
6:1F:401:GLY:HA2	7:1G:64:LYS:HE2	1.94	0.50
7:1G:335:LEU:HD23	7:1G:343:LEU:HG	1.94	0.50
7:1G:347:GLU:OE1	7:1G:495:ARG:NH2	2.44	0.50
8:1H:268:ILE:HA	8:1H:271:LEU:HD12	1.94	0.50
52:1M:501:PGT:C11	14:1N:276:ILE:HD12	2.41	0.50
14:1N:6:TYR:HE2	14:1N:46:LYS:HD2	1.76	0.50
14:1N:85:THR:HG22	30:1e:18:THR:OG1	2.12	0.50
15:1O:135:LEU:HD13	15:1O:152:TYR:CD2	2.47	0.50
16:1P:319:ARG:NH2	16:1P:329:SER:O	2.44	0.50
17:1Q:67:ASN:HB2	17:1Q:72:TRP:HB2	1.94	0.50
23:1X:20:SER:OG	26:1a:64:LYS:N	2.42	0.50
34:1i:10:ARG:HA	34:1i:13:GLN:HE21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:127:PRO:HD3	40:1o:3:HIS:NE2	2.26	0.50
40:1o:61:TYR:HA	40:1o:64:GLN:HE22	1.76	0.50
4:1D:149:ASN:ND2	4:1D:371:LYS:HE3	2.27	0.49
4:1D:270:ARG:HB2	4:1D:278:TYR:CD2	2.47	0.49
5:1E:41:GLY:HA2	44:1s:71:GLN:C	2.37	0.49
5:1E:72:ILE:O	5:1E:74:GLN:NE2	2.34	0.49
5:1E:149:VAL:CB	6:1F:105:CYS:SG	2.99	0.49
6:1F:205:LEU:HG	6:1F:404:ILE:HD12	1.94	0.49
7:1G:377:ILE:HD12	7:1G:450:MET:HB3	1.94	0.49
7:1G:378:LEU:HB2	7:1G:450:MET:O	2.12	0.49
7:1G:640:ASN:ND2	7:1G:641:TYR:CE1	2.80	0.49
8:1H:286:MET:HG3	8:1H:290:TRP:NE1	2.27	0.49
10:1J:173:ARG:HD3	15:1O:254:ARG:NH2	2.27	0.49
13:1M:114:GLU:HA	13:1M:175:ASN:HA	1.93	0.49
13:1M:450:ASN:OD1	13:1M:452:LYS:N	2.44	0.49
14:1N:128:LEU:HD11	14:1N:213:LEU:HD12	1.93	0.49
16:1P:268:ARG:O	16:1P:272:VAL:HG23	2.12	0.49
19:1S:83:ALA:O	19:1S:87:THR:HG23	2.12	0.49
22:1W:69:LYS:N	22:1W:69:LYS:CD	2.67	0.49
23:1X:81:PHE:CE1	23:1X:85:TRP:HB3	2.43	0.49
38:1m:51:ASN:ND2	39:1n:165:LEU:HD12	2.27	0.49
38:1m:114:LEU:HB3	38:1m:119:LYS:HB2	1.94	0.49
42:1q:60:ARG:HD3	42:1q:89:TRP:CE2	2.47	0.49
2:1B:40:ALA:H	8:1H:54:LYS:HZ1	1.57	0.49
2:1B:100:LEU:HD22	2:1B:140:VAL:CG2	2.41	0.49
4:1D:161:ILE:HA	4:1D:238:ARG:NH2	2.26	0.49
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.42	0.49
7:1G:154:ILE:HD11	7:1G:204:PRO:HG2	1.93	0.49
7:1G:286:ASN:OD1	7:1G:289:GLY:N	2.45	0.49
8:1H:281:ARG:NE	8:1H:283:ASP:OD1	2.45	0.49
15:1O:178:GLU:O	15:1O:182:ARG:HG2	2.12	0.49
16:1P:270:PHE:HD2	16:1P:278:TRP:HB2	1.78	0.49
17:1Q:42:ARG:NH2	17:1Q:44:ASN:OD1	2.45	0.49
31:1f:11:TRP:CZ3	31:1f:15:LEU:HD21	2.47	0.49
1:1A:5:LEU:O	1:1A:9:THR:HG23	2.12	0.49
6:1F:176:PHE:HE1	44:1s:62:ARG:HH11	1.60	0.49
7:1G:54:MET:CE	7:1G:94:MET:HB2	2.35	0.49
7:1G:379:LEU:CD2	7:1G:384:PRO:HG3	2.42	0.49
8:1H:154:LEU:HD12	8:1H:157:ASN:HB3	1.94	0.49
13:1M:14:MET:HE1	13:1M:30:HIS:CG	2.47	0.49
13:1M:36:LEU:CD1	32:1g:68:ILE:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:187:SER:O	13:1M:192:ASN:ND2	2.45	0.49
30:1e:60:ASP:HA	30:1e:63:VAL:HG12	1.94	0.49
43:1r:44:PRO:C	43:1r:47:LYS:NZ	2.68	0.49
7:1G:198:ASN:CG	7:1G:262:TRP:HB3	2.37	0.49
9:1I:5:VAL:HA	43:1r:112:LEU:HD12	1.95	0.49
15:1O:265:ASN:HD22	15:1O:268:GLU:H	1.59	0.49
16:1P:248:VAL:HG22	16:1P:334:VAL:HG21	1.94	0.49
23:1X:76:HIS:CD2	23:1X:114:LEU:HD22	2.47	0.49
43:1r:4:THR:HG23	43:1r:6:VAL:HG12	1.93	0.49
1:1A:56:PHE:HA	10:1J:70:TYR:HE2	1.78	0.49
2:1B:60:MET:HE3	4:1D:167:PHE:CE2	2.48	0.49
6:1F:393:TRP:CZ3	6:1F:419:ILE:HB	2.47	0.49
6:1F:395:ILE:O	6:1F:399:ILE:HG13	2.13	0.49
7:1G:215:PHE:HB2	9:1I:104:ARG:HB2	1.95	0.49
7:1G:255:HIS:CG	7:1G:255:HIS:O	2.65	0.49
7:1G:615:THR:OG1	7:1G:617:ASP:OD1	2.29	0.49
11:1K:96:LEU:HD21	14:1N:117:GLU:O	2.12	0.49
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.94	0.49
12:1L:356:ILE:HA	12:1L:359:MET:SD	2.52	0.49
13:1M:329:LEU:HG	13:1M:437:MET:HE1	1.94	0.49
22:1W:36:TYR:O	22:1W:40:TYR:N	2.36	0.49
27:1b:40:TYR:O	27:1b:44:ILE:HG23	2.12	0.49
34:1i:102:ARG:NH2	40:1o:49:GLN:O	2.31	0.49
35:1j:32:MET:O	35:1j:36:ILE:HG23	2.12	0.49
41:1p:98:ASP:OD2	41:1p:141:ARG:NH1	2.45	0.49
42:1q:144:TYR:HB3	42:1q:145:LYS:HG2	1.94	0.49
2:1B:101:ARG:NH1	2:1B:104:TYR:HB3	2.26	0.49
6:1F:68:ARG:HD2	6:1F:254:LYS:HD3	1.94	0.49
7:1G:59:ILE:HD12	7:1G:77:TRP:HD1	1.78	0.49
7:1G:331:LEU:HD12	7:1G:525:LEU:HD22	1.95	0.49
8:1H:12:PRO:HB2	26:1a:15:CYS:O	2.12	0.49
8:1H:80:SER:O	8:1H:84:THR:HG23	2.13	0.49
9:1I:12:MET:HE2	9:1I:12:MET:HA	1.94	0.49
12:1L:55:MET:HG2	12:1L:471:ASN:HB3	1.93	0.49
13:1M:117:LEU:HB2	23:1X:168:PHE:CG	2.47	0.49
14:1N:172:GLN:HB2	14:1N:178:ILE:HG13	1.94	0.49
20:1T:69:LYS:HD2	20:1T:69:LYS:C	2.38	0.49
37:1I:70:ARG:NE	37:1I:86:ARG:HD3	2.28	0.49
38:1m:102:TYR:O	38:1m:106:THR:OG1	2.23	0.49
43:1r:47:LYS:CE	43:1r:51:ASN:HD21	2.19	0.49
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:128:VAL:HG23	5:1E:140:ILE:HA	1.95	0.49
9:1I:49:ASN:HD22	9:1I:52:PHE:HB2	1.76	0.49
9:1I:105:ARG:HG2	9:1I:106:THR:H	1.78	0.49
12:1L:237:MET:HE1	12:1L:244:SER:CB	2.42	0.49
13:1M:451:PRO:HA	13:1M:454:ILE:HG22	1.94	0.49
14:1N:313:MET:HE1	15:1O:103:SER:HA	1.93	0.49
16:1P:73:TRP:HA	16:1P:80:SER:HB2	1.93	0.49
16:1P:185:MET:HA	16:1P:185:MET:HE3	1.95	0.49
25:1Z:110:VAL:HG13	30:1e:70:LYS:HZ2	1.78	0.49
29:1d:90:MET:HE1	33:1h:106:LYS:HD2	1.95	0.49
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.13	0.49
33:1h:91:MET:HB2	41:1p:85:PHE:HD2	1.77	0.49
3:1C:197:PHE:HA	7:1G:220:TRP:O	2.13	0.49
4:1D:116:GLN:O	4:1D:120:LEU:HG	2.12	0.49
5:1E:127:LYS:H	5:1E:130:GLU:HB2	1.78	0.49
6:1F:101:GLU:OE2	6:1F:102:PRO:O	2.31	0.49
6:1F:276:LEU:HD12	6:1F:312:CYS:HB2	1.94	0.49
6:1F:294:LEU:HD21	6:1F:297:VAL:HG13	1.95	0.49
7:1G:276:ARG:HB2	7:1G:680:ALA:HB1	1.94	0.49
10:1J:119:PHE:CD2	11:1K:6:MET:HE3	2.47	0.49
11:1K:75:LEU:O	11:1K:79:VAL:N	2.35	0.49
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.12	0.49
13:1M:42:LEU:HD21	13:1M:453:MET:CB	2.37	0.49
15:1O:188:ASN:O	15:1O:191:GLU:HG2	2.13	0.49
16:1P:325:ARG:HG3	16:1P:326:TRP:CD2	2.47	0.49
20:1U:37:MET:HE1	20:1U:44:SER:N	2.27	0.49
26:1a:6:LEU:HA	26:1a:9:ILE:HG12	1.93	0.49
37:1l:127:PRO:HD3	40:1o:3:HIS:CE1	2.47	0.49
39:1n:154:PRO:HD3	39:1n:164:PRO:HG2	1.94	0.49
3:1C:68:THR:HG21	21:1V:50:ILE:HD12	1.94	0.49
3:1C:150:ARG:NH2	22:1W:92:GLU:OE1	2.46	0.49
4:1D:157:HIS:O	4:1D:161:ILE:HG12	2.12	0.49
6:1F:94:VAL:HB	6:1F:222:VAL:HG22	1.94	0.49
6:1F:101:GLU:OE2	6:1F:101:GLU:O	2.30	0.49
7:1G:174:THR:HG22	7:1G:183:VAL:HG22	1.93	0.49
12:1L:385:TYR:HA	12:1L:390:TYR:CE1	2.48	0.49
14:1N:7:THR:HA	53:1N:402:CDL:H112	1.94	0.49
14:1N:88:LYS:NZ	14:1N:89:MET:O	2.45	0.49
14:1N:216:PHE:O	14:1N:220:ILE:HG12	2.12	0.49
15:1O:303:LYS:H	15:1O:309:ASN:HD21	1.61	0.49
3:1C:39:GLN:HB3	43:1r:70:SER:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:57:VAL:O	3:1C:61:LEU:HB2	2.13	0.49
4:1D:107:ASP:HB3	4:1D:114:ASN:HD21	1.78	0.49
5:1E:72:ILE:C	5:1E:74:GLN:NE2	2.71	0.49
5:1E:143:GLU:HB3	6:1F:353:PHE:CE1	2.48	0.49
5:1E:144:CYS:HB3	5:1E:148:CYS:SG	2.53	0.49
10:1J:56:VAL:O	10:1J:61:LEU:N	2.39	0.49
11:1K:33:LEU:HA	11:1K:36:MET:HE3	1.95	0.49
16:1P:49:TYR:O	16:1P:72:GLU:HA	2.13	0.49
16:1P:79:ASP:HB3	16:1P:82:ARG:HH21	1.78	0.49
16:1P:201:VAL:HG13	16:1P:235:ARG:HB3	1.94	0.49
16:1P:244:TYR:O	16:1P:248:VAL:HG23	2.13	0.49
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.13	0.49
20:1U:6:LEU:CD1	20:1U:11:ILE:HD11	2.42	0.49
28:1c:28:TRP:NE1	29:1d:66:THR:HG22	2.28	0.49
32:1g:24:ILE:O	32:1g:26:LEU:N	2.43	0.49
32:1g:71:VAL:O	32:1g:75:THR:HG23	2.13	0.49
38:1m:55:ARG:NH1	38:1m:57:GLY:O	2.46	0.49
2:1B:116:MET:SD	2:1B:156:LEU:HD13	2.52	0.48
3:1C:39:GLN:HE21	21:1V:111:TRP:CD1	2.30	0.48
4:1D:161:ILE:HG13	4:1D:235:TRP:HZ3	1.77	0.48
4:1D:407:LYS:NZ	4:1D:408:GLY:H	2.10	0.48
5:1E:86:PHE:HD1	7:1G:177:ARG:HB3	1.78	0.48
5:1E:193:CYS:SG	6:1F:267:THR:HG22	2.53	0.48
6:1F:162:ILE:HG13	6:1F:174:ASP:HA	1.95	0.48
6:1F:302:SER:HB2	6:1F:350:LEU:HD11	1.95	0.48
10:1J:79:TYR:CE2	16:1P:325:ARG:HA	2.48	0.48
11:1K:66:PHE:HE2	14:1N:31:ILE:HG12	1.78	0.48
11:1K:94:ASN:HB3	12:1L:583:LEU:HD23	1.94	0.48
13:1M:266:MET:HA	13:1M:269:MET:HE3	1.94	0.48
13:1M:312:ALA:O	13:1M:316:MET:HG3	2.13	0.48
14:1N:236:LYS:HD3	14:1N:314:LYS:HB3	1.94	0.48
15:1O:13:ARG:O	15:1O:16:ARG:NH2	2.43	0.48
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.94	0.48
16:1P:240:ASP:OD1	16:1P:337:ALA:HB1	2.13	0.48
18:1R:84:CYS:HB3	18:1R:87:CYS:HB2	1.94	0.48
19:1S:23:CYS:HB3	19:1S:26:SER:HB3	1.95	0.48
20:1T:13:ASP:O	20:1T:17:TYR:N	2.46	0.48
20:1T:32:VAL:HG22	20:1T:74:GLN:HE21	1.78	0.48
22:1W:65:GLU:CB	22:1W:69:LYS:NZ	2.57	0.48
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.47	0.48
24:1Y:64:ALA:O	24:1Y:68:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:51:ARG:HH22	29:1d:60:ARG:CZ	2.26	0.48
38:1m:51:ASN:OD1	39:1n:168:HIS:ND1	2.44	0.48
3:1C:45:PHE:HB2	3:1C:47:GLU:HG3	1.94	0.48
4:1D:322:GLU:CD	4:1D:322:GLU:H	2.22	0.48
6:1F:318:ASP:OD1	6:1F:321:ALA:N	2.46	0.48
8:1H:134:ARG:HA	8:1H:282:TYR:OH	2.13	0.48
8:1H:189:THR:OG1	8:1H:234:MET:HB3	2.13	0.48
11:1K:96:LEU:HD12	14:1N:51:ARG:HG3	1.95	0.48
16:1P:200:THR:HG23	16:1P:290:SER:HA	1.95	0.48
23:1X:77:CYS:HB3	23:1X:80:PRO:HG2	1.93	0.48
33:1h:88:GLU:HA	33:1h:91:MET:CE	2.42	0.48
37:1l:128:VAL:HG23	40:1o:97:ARG:HB3	1.95	0.48
2:1B:66:ARG:HG3	2:1B:67:TYR:CD1	2.48	0.48
2:1B:87:ILE:HG22	2:1B:114:VAL:HB	1.94	0.48
5:1E:153:MET:HE1	5:1E:160:TYR:HE1	1.49	0.48
6:1F:171:TYR:HD2	6:1F:173:PHE:HB2	1.77	0.48
6:1F:258:ILE:HD12	6:1F:265:PRO:HA	1.95	0.48
7:1G:36:GLN:OE1	17:1Q:49:VAL:HG22	2.12	0.48
7:1G:289:GLY:O	42:1q:144:TYR:OH	2.26	0.48
11:1K:55:LEU:HD12	30:1e:24:GLN:NE2	2.28	0.48
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.48	0.48
15:1O:266:LYS:O	15:1O:269:VAL:HG22	2.14	0.48
17:1Q:126:LYS:HA	44:1s:70:ARG:HH22	1.77	0.48
26:1a:21:MET:HE1	26:1a:25:HIS:CE1	2.49	0.48
43:1r:63:MET:CE	43:1r:64:PRO:HD2	2.41	0.48
6:1F:230:VAL:O	6:1F:234:ILE:HG12	2.14	0.48
6:1F:303:SER:O	6:1F:413:TRP:HB2	2.13	0.48
7:1G:143:GLY:HA2	7:1G:190:MET:HE1	1.95	0.48
8:1H:89:LEU:HD22	8:1H:105:MET:HE1	1.96	0.48
11:1K:55:LEU:HD11	30:1e:23:GLU:O	2.14	0.48
12:1L:72:GLN:HE21	41:1p:99:GLN:HE22	1.60	0.48
14:1N:8:THR:O	14:1N:12:THR:HG23	2.13	0.48
16:1P:200:THR:HA	16:1P:290:SER:HA	1.96	0.48
22:1W:62:LYS:HZ1	22:1W:107:PHE:HA	1.78	0.48
28:1c:44:ARG:HE	28:1c:45:ARG:CA	2.26	0.48
1:1A:53:MET:HE1	11:1K:79:VAL:HG13	1.95	0.48
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.43	0.48
5:1E:60:TRP:CD1	5:1E:60:TRP:C	2.91	0.48
7:1G:336:ASN:HD21	19:1S:67:ARG:NH2	2.08	0.48
8:1H:19:PHE:CD2	8:1H:48:PRO:HG2	2.48	0.48
10:1J:110:GLU:C	10:1J:111:GLU:OE1	2.56	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:37:MET:HE1	11:1K:64:LEU:HD12	1.94	0.48
21:1V:97:LYS:HG2	21:1V:99:TRP:CD1	2.49	0.48
25:1Z:120:MET:HE2	30:1e:68:ARG:HD2	1.96	0.48
26:1a:1:MET:HE1	43:1r:0:ACE:H3	1.94	0.48
32:1g:25:ARG:C	32:1g:25:ARG:NE	2.68	0.48
32:1g:111:ASN:HB3	41:1p:161:ARG:NH2	2.25	0.48
35:1j:50:HIS:HD1	35:1j:50:HIS:H	1.61	0.48
4:1D:146:ARG:NH1	4:1D:368:GLU:O	2.29	0.48
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.95	0.48
6:1F:76:GLY:O	6:1F:80:SER:OG	2.22	0.48
6:1F:274:VAL:HG12	6:1F:275:PRO:O	2.13	0.48
7:1G:259:ASN:O	7:1G:260:GLU:HB2	2.13	0.48
8:1H:287:HIS:HE1	50:1I:203:PC1:H131	1.79	0.48
11:1K:76:SER:HA	11:1K:79:VAL:HG12	1.94	0.48
12:1L:203:MET:HE2	41:1p:113:GLN:OE1	2.13	0.48
14:1N:275:SER:OG	14:1N:278:MET:HB2	2.13	0.48
16:1P:176:ASP:OD1	16:1P:179:LEU:HB2	2.13	0.48
16:1P:292:MET:N	16:1P:292:MET:SD	2.86	0.48
21:1V:48:GLU:O	21:1V:52:ASN:ND2	2.46	0.48
25:1Z:83:VAL:HG23	25:1Z:124:LEU:HD21	1.96	0.48
29:1d:1:MET:SD	33:1h:122:TRP:CE3	3.07	0.48
33:1h:88:GLU:O	33:1h:91:MET:HE3	2.12	0.48
4:1D:136:TRP:CZ3	4:1D:314:CYS:HA	2.49	0.48
5:1E:78:MET:HA	5:1E:81:TYR:CD2	2.49	0.48
6:1F:327:THR:OG1	6:1F:328:GLY:N	2.46	0.48
6:1F:406:ALA:O	6:1F:410:GLY:N	2.41	0.48
8:1H:87:VAL:HG13	8:1H:95:LEU:HB3	1.95	0.48
8:1H:150:LEU:HD21	8:1H:241:LEU:HD11	1.94	0.48
11:1K:62:ILE:HA	11:1K:65:VAL:HG22	1.95	0.48
12:1L:95:PHE:HE1	12:1L:456:ARG:HG2	1.79	0.48
12:1L:275:THR:HA	12:1L:278:LEU:HD23	1.95	0.48
45:1L:702:3PE:H112	45:1L:702:3PE:H11	1.96	0.48
17:1Q:93:VAL:HG12	17:1Q:103:PHE:HZ	1.79	0.48
22:1W:42:GLU:O	22:1W:46:THR:HG22	2.14	0.48
22:1W:103:ILE:C	22:1W:103:ILE:HD12	2.39	0.48
32:1g:82:ASP:CG	32:1g:87:GLU:OE1	2.57	0.48
42:1q:20:LEU:HD12	42:1q:20:LEU:O	2.14	0.48
2:1B:27:GLU:OE1	2:1B:178:ARG:NH2	2.46	0.48
3:1C:180:VAL:HG21	3:1C:184:VAL:HG11	1.96	0.48
5:1E:56:ARG:HD2	44:1s:48:THR:HB	1.96	0.48
5:1E:135:LYS:N	5:1E:135:LYS:CD	2.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:108:MET:HE1	10:1J:57:PHE:CD1	2.49	0.48
8:1H:233:MET:SD	8:1H:233:MET:C	2.97	0.48
8:1H:258:ASN:OD1	8:1H:262:LYS:NZ	2.47	0.48
12:1L:286:LEU:HD11	12:1L:290:LEU:HD12	1.95	0.48
21:1V:81:LEU:O	21:1V:85:ASN:ND2	2.47	0.48
32:1g:68:ILE:O	32:1g:72:LEU:HB3	2.14	0.48
35:1j:26:GLU:OE1	35:1j:27:PHE:N	2.46	0.48
42:1q:39:VAL:HB	42:1q:50:GLU:CD	2.39	0.48
4:1D:221:ARG:CD	43:1r:24:GLN:HE21	2.26	0.48
6:1F:105:CYS:O	6:1F:109:GLU:HG2	2.12	0.48
7:1G:408:LEU:HD13	7:1G:415:LEU:HD11	1.96	0.48
8:1H:105:MET:HE2	8:1H:105:MET:HB2	1.74	0.48
8:1H:186:PHE:CD2	50:1I:203:PC1:H2E1	2.49	0.48
12:1L:405:ASN:ND2	37:1I:120:GLU:OE2	2.47	0.48
12:1L:408:ALA:HB2	37:1I:116:PHE:HZ	1.77	0.48
13:1M:378:GLU:O	13:1M:382:ILE:HG12	2.13	0.48
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD21	1.95	0.48
20:1T:24:LYS:HD3	20:1T:25:ILE:HD13	1.95	0.48
25:1Z:110:VAL:HG11	30:1e:71:THR:OG1	2.13	0.48
43:1r:8:GLN:O	43:1r:12:ASN:ND2	2.47	0.48
1:1A:90:MET:HE1	10:1J:155:ILE:HD11	1.96	0.48
1:1A:92:LEU:HD13	8:1H:302:MET:HG2	1.94	0.48
3:1C:181:LYS:HD3	3:1C:181:LYS:HA	1.69	0.48
6:1F:146:ALA:O	6:1F:150:GLN:NE2	2.43	0.48
7:1G:91:GLU:OE2	7:1G:125:SER:N	2.47	0.48
7:1G:210:SER:OG	7:1G:213:TYR:HB3	2.14	0.48
7:1G:242:THR:N	7:1G:248:MET:HE1	2.29	0.48
8:1H:272:TRP:O	8:1H:276:SER:OG	2.25	0.48
9:1I:12:MET:HE1	9:1I:20:ARG:HH12	1.78	0.48
10:1J:113:VAL:HB	10:1J:119:PHE:CZ	2.49	0.48
11:1K:20:LEU:HB3	12:1L:592:LEU:HB2	1.96	0.48
11:1K:43:MET:HB3	14:1N:75:ILE:HD12	1.96	0.48
11:1K:48:ILE:HD13	11:1K:56:ALA:CB	2.44	0.48
12:1L:226:GLN:O	12:1L:230:HIS:HB3	2.14	0.48
13:1M:111:THR:O	13:1M:111:THR:HG22	2.14	0.48
13:1M:365:THR:HG22	13:1M:374:ASN:ND2	2.29	0.48
13:1M:380:PHE:HE2	13:1M:455:LEU:HD11	1.78	0.48
37:1I:43:GLY:HA2	38:1m:78:ASN:HB3	1.95	0.48
43:1r:63:MET:CE	43:1r:64:PRO:CD	2.79	0.48
4:1D:146:ARG:CZ	4:1D:270:ARG:HH12	2.26	0.47
6:1F:101:GLU:CD	6:1F:104:THR:HG23	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:129:ARG:NE	43:1r:48:LEU:O	2.33	0.47
8:1H:96:ILE:HG23	25:1Z:144:THR:HG21	1.96	0.47
8:1H:233:MET:SD	8:1H:234:MET:N	2.87	0.47
9:1I:153:LYS:HB2	42:1q:124:TYR:CE1	2.49	0.47
13:1M:191:SER:HB2	52:1M:501:PGT:H31	1.95	0.47
16:1P:36:ASN:HD22	16:1P:36:ASN:C	2.21	0.47
20:1T:6:LEU:HD11	20:1T:14:ARG:NH1	2.29	0.47
25:1Z:75:PHE:CE1	26:1a:50:ARG:HD2	2.49	0.47
25:1Z:99:LYS:O	25:1Z:99:LYS:HD3	2.14	0.47
38:1m:7:PRO:HG3	38:1m:13:LEU:HD13	1.95	0.47
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.50	0.47
5:1E:21:PHE:CE2	5:1E:65:ALA:HA	2.49	0.47
6:1F:344:VAL:HG12	6:1F:380:VAL:HG22	1.96	0.47
7:1G:27:LEU:HD11	7:1G:69:CYS:HA	1.96	0.47
7:1G:511:VAL:HG22	7:1G:514:ILE:HB	1.96	0.47
8:1H:222:MET:HA	8:1H:225:MET:HE2	1.94	0.47
8:1H:282:TYR:HE1	8:1H:286:MET:HE1	1.78	0.47
9:1I:160:LYS:HD2	9:1I:161:TRP:NE1	2.28	0.47
11:1K:37:MET:HE3	11:1K:67:ALA:HB3	1.96	0.47
12:1L:66:TRP:CD1	50:1L:703:PC1:H11	2.49	0.47
12:1L:246:LEU:HD12	12:1L:246:LEU:O	2.14	0.47
12:1L:248:HIS:HE1	12:1L:252:MET:HE3	1.78	0.47
12:1L:325:ALA:O	12:1L:329:ILE:HG12	2.14	0.47
12:1L:483:PRO:HG2	12:1L:486:MET:HE1	1.96	0.47
13:1M:190:TRP:CD2	24:1Y:126:MET:HE1	2.49	0.47
14:1N:134:GLN:C	14:1N:134:GLN:CD	2.83	0.47
21:1V:24:LYS:O	21:1V:28:THR:HG23	2.14	0.47
35:1j:68:PRO:CD	35:1j:68:PRO:O	2.62	0.47
36:1k:18:TYR:OH	36:1k:46:ARG:NH2	2.47	0.47
42:1q:69:ASN:OD1	42:1q:112:ASN:ND2	2.46	0.47
53:1r:201:CDL:H531	53:1r:201:CDL:H711	1.96	0.47
45:1A:201:3PE:H271	8:1H:295:PRO:HB3	1.96	0.47
7:1G:195:LEU:HD13	7:1G:264:SER:HA	1.96	0.47
7:1G:375:ASP:OD1	7:1G:376:VAL:N	2.48	0.47
12:1L:61:MET:HA	34:1i:98:GLU:HA	1.95	0.47
12:1L:94:LEU:HA	12:1L:97:THR:HG22	1.97	0.47
12:1L:290:LEU:O	12:1L:523:SER:OG	2.32	0.47
13:1M:19:LYS:HE3	13:1M:20:HIS:H	1.78	0.47
13:1M:47:GLU:HB3	41:1p:92:ARG:HE	1.79	0.47
13:1M:278:ARG:NH2	37:1l:82:ASP:OD1	2.45	0.47
14:1N:95:MET:HE3	14:1N:149:ILE:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:107:GLN:HG2	15:1O:124:LEU:HD13	1.96	0.47
22:1W:44:PRO:HD3	22:1W:60:ARG:NH1	2.30	0.47
23:1X:6:LEU:HD11	25:1Z:88:ARG:HB2	1.96	0.47
34:1i:101:PRO:HG2	41:1p:16:THR:HG22	1.96	0.47
37:1l:112:MET:O	37:1l:112:MET:HE3	2.14	0.47
41:1p:88:GLU:OE1	41:1p:150:SER:OG	2.30	0.47
1:1A:82:ASN:HD21	27:1b:46:ARG:HG3	1.78	0.47
6:1F:184:TYR:HB3	6:1F:357:GLU:HB3	1.95	0.47
7:1G:55:CYS:HB3	47:1G:803:FES:S2	2.54	0.47
7:1G:378:LEU:HD21	7:1G:439:PHE:CE2	2.49	0.47
8:1H:102:VAL:HG21	8:1H:154:LEU:HD22	1.97	0.47
8:1H:133:LEU:HD13	10:1J:70:TYR:CE1	2.49	0.47
10:1J:17:PHE:CD2	11:1K:11:ALA:HB1	2.49	0.47
12:1L:130:ILE:HD12	12:1L:131:LEU:N	2.30	0.47
13:1M:310:MET:HE2	13:1M:459:TYR:HA	1.97	0.47
13:1M:329:LEU:HD11	13:1M:359:TRP:HA	1.97	0.47
15:1O:293:PHE:O	15:1O:297:THR:OG1	2.31	0.47
16:1P:180:ASN:HA	16:1P:321:HIS:NE2	2.29	0.47
17:1Q:21:THR:HG23	17:1Q:22:LEU:HD23	1.95	0.47
20:1T:53:ALA:C	20:1T:54:MET:HE2	2.38	0.47
20:1U:32:VAL:O	20:1U:74:GLN:N	2.47	0.47
50:1f:101:PC1:H322	50:1f:101:PC1:H272	1.96	0.47
37:1l:85:ILE:HG13	37:1l:88:ARG:H	1.80	0.47
40:1o:60:HIS:ND1	40:1o:61:TYR:N	2.62	0.47
41:1p:10:PRO:HD2	41:1p:108:ARG:HD2	1.97	0.47
4:1D:282:GLU:HG3	4:1D:313:GLN:HE22	1.79	0.47
6:1F:79:TRP:HE1	6:1F:223:ALA:HB2	1.79	0.47
7:1G:141:ASN:HB2	7:1G:699:GLU:HG3	1.97	0.47
7:1G:640:ASN:OD1	7:1G:640:ASN:N	2.45	0.47
10:1J:28:TYR:CE2	10:1J:82:VAL:HG23	2.50	0.47
13:1M:30:HIS:O	13:1M:34:ILE:HG12	2.15	0.47
13:1M:277:LEU:HD13	13:1M:406:TYR:HB3	1.97	0.47
13:1M:310:MET:CE	13:1M:459:TYR:HA	2.45	0.47
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.95	0.47
14:1N:218:LEU:CD1	14:1N:244:MET:HE2	2.37	0.47
16:1P:107:GLU:O	16:1P:111:VAL:HB	2.15	0.47
20:1U:26:ASP:HB3	20:1U:28:GLU:OE1	2.14	0.47
21:1V:35:GLY:CA	21:1V:44:ARG:HH12	2.26	0.47
24:1Y:139:LYS:HG2	24:1Y:140:VAL:HG13	1.95	0.47
30:1e:20:GLN:HG2	30:1e:36:GLU:OE1	2.14	0.47
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:66:ASP:CG	21:1V:85:ASN:HB2	2.40	0.47
3:1C:84:PRO:HB3	17:1Q:95:PHE:CE2	2.49	0.47
4:1D:136:TRP:HZ3	4:1D:314:CYS:HA	1.79	0.47
6:1F:15:LEU:HB2	6:1F:271:GLU:H	1.79	0.47
6:1F:137:TYR:HB2	6:1F:196:ILE:HD11	1.96	0.47
6:1F:302:SER:OG	6:1F:303:SER:N	2.47	0.47
6:1F:353:PHE:O	6:1F:357:GLU:HG2	2.14	0.47
6:1F:363:THR:HG22	7:1G:96:PHE:HB3	1.95	0.47
7:1G:447:LYS:C	7:1G:448:LYS:HD2	2.38	0.47
12:1L:313:MET:HE2	12:1L:329:ILE:HD13	1.97	0.47
12:1L:578:SER:HB3	14:1N:172:GLN:HE22	1.80	0.47
13:1M:24:TRP:HZ2	13:1M:92:LYS:HZ2	1.61	0.47
13:1M:342:MET:CE	13:1M:410:MET:HA	2.41	0.47
14:1N:254:LEU:HD21	14:1N:290:LEU:HD21	1.95	0.47
14:1N:323:MET:SD	29:1d:49:ARG:NH1	2.87	0.47
15:1O:129:TYR:CB	15:1O:214:MET:HE1	2.44	0.47
30:1e:88:GLU:HB3	30:1e:90:LYS:HE2	1.96	0.47
39:1n:25:HIS:CE1	39:1n:78:PRO:HB3	2.49	0.47
40:1o:30:PHE:CE2	40:1o:103:ARG:HD2	2.50	0.47
2:1B:125:TYR:HE1	4:1D:102:TYR:CD2	2.31	0.47
3:1C:193:GLU:OE2	17:1Q:64:ARG:HD3	2.15	0.47
4:1D:15:GLY:HA2	14:1N:228:LEU:HD11	1.97	0.47
4:1D:62:LEU:HG	4:1D:64:LEU:HG	1.96	0.47
4:1D:87:THR:O	4:1D:91:ILE:HG13	2.14	0.47
5:1E:203:THR:OG1	6:1F:17:ASP:OD2	2.21	0.47
6:1F:99:GLU:OE2	6:1F:107:ASP:N	2.43	0.47
6:1F:233:THR:HA	6:1F:236:ARG:HH21	1.80	0.47
6:1F:372:MET:HE2	6:1F:395:ILE:HG13	1.97	0.47
7:1G:254:MET:HE1	17:1Q:109:LYS:CB	2.36	0.47
7:1G:257:ASP:C	7:1G:394:ARG:HH22	2.22	0.47
7:1G:276:ARG:O	7:1G:278:ARG:HG2	2.15	0.47
7:1G:314:ASP:HB3	7:1G:520:LYS:HD2	1.96	0.47
7:1G:343:LEU:HD22	7:1G:507:TYR:CZ	2.49	0.47
7:1G:366:THR:H	7:1G:491:ASN:HD21	1.63	0.47
7:1G:494:HIS:CE1	7:1G:499:GLN:HB3	2.50	0.47
7:1G:518:PRO:HB2	7:1G:538:PRO:HB3	1.96	0.47
7:1G:675:ASP:OD2	7:1G:677:ILE:HG22	2.14	0.47
10:1J:79:TYR:HE2	16:1P:325:ARG:HA	1.80	0.47
11:1K:8:ILE:HB	11:1K:43:MET:HE3	1.97	0.47
12:1L:139:GLN:O	12:1L:142:ILE:HB	2.15	0.47
12:1L:213:LEU:HD11	12:1L:267:MET:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:226:GLN:NE2	12:1L:314:MET:SD	2.88	0.47
12:1L:364:LYS:HB2	12:1L:364:LYS:HE2	1.61	0.47
13:1M:163:ALA:O	13:1M:167:ILE:HG12	2.15	0.47
14:1N:103:ALA:O	14:1N:107:GLY:N	2.33	0.47
15:1O:109:ALA:HB1	15:1O:263:VAL:HG13	1.97	0.47
15:1O:204:ASN:HD22	15:1O:208:LYS:HE2	1.80	0.47
16:1P:206:TYR:HB3	16:1P:209:ASP:OD1	2.15	0.47
16:1P:250:TYR:CD2	16:1P:326:TRP:HB2	2.50	0.47
16:1P:313:LYS:CE	16:1P:316:GLU:HG2	2.44	0.47
17:1Q:112:LYS:HZ3	17:1Q:113:PRO:HG2	1.79	0.47
20:1T:34:SER:O	20:1T:34:SER:OG	2.27	0.47
20:1T:58:PHE:HB3	20:1T:60:PHE:CD1	2.50	0.47
20:1T:72:CYS:N	20:1T:75:GLU:OE1	2.46	0.47
20:1U:4:PRO:HA	35:1j:1:ALA:HB2	1.97	0.47
22:1W:26:ASN:C	22:1W:26:ASN:OD1	2.57	0.47
23:1X:17:VAL:HG13	26:1a:50:ARG:HH22	1.80	0.47
23:1X:76:HIS:HD2	23:1X:114:LEU:HD22	1.80	0.47
26:1a:65:GLY:N	26:1a:67:GLU:OE2	2.46	0.47
29:1d:2:MET:HE2	29:1d:5:ARG:HH11	1.80	0.47
39:1n:25:HIS:CE1	39:1n:74:GLN:HB2	2.50	0.47
40:1o:30:PHE:HE2	40:1o:103:ARG:HD2	1.79	0.47
41:1p:14:ARG:CD	41:1p:14:ARG:H	2.27	0.47
42:1q:3:LEU:HD21	53:1r:201:CDL:H551	1.97	0.47
42:1q:34:ARG:HD3	42:1q:54:GLN:NE2	2.29	0.47
42:1q:53:LYS:HD2	42:1q:53:LYS:O	2.15	0.47
2:1B:47:PRO:HD2	2:1B:75:VAL:H	1.80	0.47
3:1C:196:LYS:NZ	17:1Q:81:ASN:HD22	2.12	0.47
7:1G:140:LYS:CD	7:1G:150:MET:HE2	2.44	0.47
8:1H:266:LEU:O	8:1H:269:THR:OG1	2.27	0.47
9:1I:65:HIS:ND1	9:1I:133:GLU:OE2	2.48	0.47
9:1I:142:GLU:OE1	42:1q:118:SER:OG	2.21	0.47
9:1I:150:ASN:OD1	9:1I:150:ASN:C	2.58	0.47
14:1N:72:MET:CG	14:1N:75:ILE:HD11	2.45	0.47
16:1P:203:GLN:NE2	16:1P:234:ASN:N	2.62	0.47
17:1Q:35:VAL:HG11	17:1Q:57:MET:HE2	1.96	0.47
19:1S:82:SER:O	19:1S:86:VAL:HG23	2.15	0.47
20:1T:44:SER:O	20:1T:48:VAL:HG23	2.14	0.47
2:1B:25:ARG:HH12	2:1B:27:GLU:HB3	1.80	0.47
4:1D:148:LEU:HD22	4:1D:177:MET:HE2	1.95	0.47
5:1E:184:PRO:CD	44:1s:44:HIS:ND1	2.76	0.47
7:1G:12:PHE:O	7:1G:78:ASN:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:591:GLY:HA2	16:1P:6:ILE:HD12	1.97	0.47
12:1L:79:SER:HB3	12:1L:135:ASN:HB3	1.96	0.47
12:1L:342:CYS:O	12:1L:346:ILE:HG22	2.15	0.47
12:1L:379:ALA:O	12:1L:388:GLY:HA3	2.15	0.47
16:1P:117:ILE:HG13	16:1P:118:ALA:N	2.28	0.47
34:1i:120:LYS:HE3	34:1i:120:LYS:CA	2.35	0.47
1:1A:105:GLU:HG3	1:1A:110:GLY:HA3	1.97	0.47
4:1D:342:MET:CE	4:1D:346:ILE:HG13	2.44	0.47
6:1F:118:LEU:HD11	6:1F:225:VAL:HG13	1.97	0.47
6:1F:258:ILE:HG22	6:1F:334:VAL:HB	1.97	0.47
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.50	0.47
10:1J:82:VAL:HG13	10:1J:85:SER:H	1.79	0.47
12:1L:584:ILE:HG12	14:1N:58:LYS:HD3	1.96	0.47
14:1N:95:MET:CE	14:1N:149:ILE:HG12	2.45	0.47
19:1S:35:PHE:HA	19:1S:39:ARG:HG2	1.97	0.47
22:1W:28:ALA:HB1	22:1W:79:VAL:HG21	1.97	0.47
22:1W:57:LYS:HB3	22:1W:57:LYS:HE2	1.64	0.47
23:1X:24:LEU:HD22	23:1X:24:LEU:H	1.79	0.47
24:1Y:91:ILE:HD12	24:1Y:92:GLY:N	2.29	0.47
32:1g:63:PHE:HA	33:1h:28:TYR:CE1	2.49	0.47
32:1g:66:PHE:CD1	33:1h:28:TYR:HE2	2.33	0.47
35:1j:54:PRO:HG3	40:1o:95:VAL:HG23	1.97	0.47
40:1o:62:LEU:HD23	40:1o:86:TRP:CE2	2.50	0.47
5:1E:144:CYS:CB	5:1E:148:CYS:SG	3.02	0.46
6:1F:259:SER:HA	6:1F:265:PRO:HB3	1.96	0.46
7:1G:379:LEU:HB3	7:1G:408:LEU:HD12	1.96	0.46
10:1J:38:GLY:HA2	10:1J:57:PHE:CE2	2.50	0.46
10:1J:113:VAL:HG12	10:1J:115:ILE:HG22	1.97	0.46
10:1J:138:GLU:HG3	30:1e:28:ILE:HD13	1.96	0.46
12:1L:545:SER:HB3	13:1M:278:ARG:HG3	1.97	0.46
13:1M:281:ASP:OD2	13:1M:284:SER:N	2.46	0.46
13:1M:293:HIS:HB2	13:1M:319:HIS:CD2	2.50	0.46
15:1O:30:ASN:ND2	15:1O:174:VAL:O	2.47	0.46
36:1k:87:LEU:HD12	36:1k:88:GLU:H	1.80	0.46
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.29	0.46
3:1C:85:THR:HG21	21:1V:115:ILE:HB	1.97	0.46
4:1D:121:ALA:HB1	4:1D:378:LEU:HD21	1.97	0.46
4:1D:414:VAL:HG12	4:1D:417:ILE:HD12	1.96	0.46
6:1F:55:TRP:CZ3	6:1F:59:GLU:N	2.83	0.46
6:1F:270:GLU:HG2	6:1F:279:LEU:HD13	1.96	0.46
7:1G:12:PHE:CE2	7:1G:76:GLY:HA2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:183:MET:O	8:1H:187:ILE:HG12	2.15	0.46
10:1J:55:MET:HE2	10:1J:55:MET:HA	1.96	0.46
12:1L:89:PHE:CE2	12:1L:128:MET:HE3	2.49	0.46
15:1O:176:VAL:CG1	15:1O:177:PRO:HD3	2.44	0.46
16:1P:102:LYS:HE3	16:1P:102:LYS:HB3	1.67	0.46
17:1Q:62:ARG:HD3	17:1Q:62:ARG:HA	1.72	0.46
18:1R:3:ARG:HH22	18:1R:6:PRO:HD3	1.80	0.46
22:1W:63:VAL:HG12	22:1W:67:PHE:CE2	2.50	0.46
23:1X:6:LEU:CD1	25:1Z:88:ARG:HB2	2.45	0.46
31:1f:40:LYS:HD3	31:1f:40:LYS:HA	1.78	0.46
36:1k:83:ALA:O	36:1k:87:LEU:HG	2.15	0.46
43:1r:61:GLU:HA	43:1r:61:GLU:OE2	2.16	0.46
43:1r:105:LEU:HD12	43:1r:111:TYR:HE2	1.80	0.46
2:1B:50:PHE:HB3	2:1B:52:LEU:CD1	2.46	0.46
2:1B:52:LEU:HD23	2:1B:91:THR:O	2.15	0.46
4:1D:395:GLY:HA2	4:1D:398:HIS:HB2	1.96	0.46
6:1F:296:ALA:HB3	6:1F:306:LEU:HD12	1.96	0.46
6:1F:392:LEU:HD21	6:1F:415:VAL:HG21	1.97	0.46
7:1G:319:ALA:HB3	7:1G:345:THR:HA	1.97	0.46
8:1H:108:MET:HE1	10:1J:57:PHE:HD1	1.80	0.46
9:1I:6:ASN:O	9:1I:8:ARG:HG2	2.16	0.46
12:1L:51:LEU:HD21	12:1L:88:MET:CE	2.39	0.46
12:1L:306:THR:OG1	12:1L:307:SER:N	2.49	0.46
12:1L:383:MET:SD	35:1j:36:ILE:HD12	2.56	0.46
14:1N:54:GLU:OE2	14:1N:54:GLU:HA	2.15	0.46
14:1N:119:THR:CG2	14:1N:131:LEU:HD11	2.45	0.46
15:1O:291:ARG:NH1	32:1g:29:ASP:OD1	2.48	0.46
16:1P:93:ASN:ND2	16:1P:117:ILE:HD11	2.30	0.46
32:1g:100:ARG:HG3	32:1g:105:LEU:HD22	1.97	0.46
37:1l:77:ILE:HD12	37:1l:81:LEU:HB2	1.98	0.46
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.80	0.46
3:1C:99:LEU:HD11	4:1D:251:LEU:HD21	1.96	0.46
4:1D:261:ARG:O	4:1D:287:ILE:HG23	2.15	0.46
6:1F:309:LYS:HA	6:1F:312:CYS:SG	2.56	0.46
12:1L:296:ASN:H	39:1n:77:GLN:NE2	2.12	0.46
12:1L:366:MET:O	12:1L:370:THR:OG1	2.23	0.46
12:1L:433:GLY:H	36:1k:59:ASN:ND2	2.13	0.46
12:1L:434:LYS:HG3	36:1k:52:TYR:CD1	2.51	0.46
14:1N:95:MET:CE	14:1N:148:SER:OG	2.62	0.46
14:1N:132:THR:OG1	14:1N:209:ILE:HD12	2.15	0.46
16:1P:41:MET:SD	16:1P:41:MET:N	2.88	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:323:THR:O	16:1P:327:LEU:HB2	2.15	0.46
20:1U:78:ASP:HB3	34:1i:15:ARG:NE	2.31	0.46
23:1X:17:VAL:HG22	23:1X:19:VAL:HG22	1.96	0.46
23:1X:111:LEU:HA	23:1X:116:TRP:O	2.15	0.46
34:1i:67:SER:O	34:1i:71:VAL:HG23	2.16	0.46
34:1i:109:ILE:CD1	34:1i:114:GLU:OE2	2.46	0.46
35:1j:61:ASP:OD1	35:1j:61:ASP:N	2.40	0.46
1:1A:67:LEU:HD11	11:1K:68:ALA:HB3	1.96	0.46
3:1C:150:ARG:HH12	3:1C:155:TYR:HA	1.80	0.46
4:1D:258:VAL:O	4:1D:262:GLY:N	2.27	0.46
5:1E:52:ASP:O	5:1E:56:ARG:N	2.42	0.46
6:1F:226:GLU:OE1	6:1F:254:LYS:HD2	2.16	0.46
6:1F:280:ILE:HG21	6:1F:291:TRP:CZ3	2.50	0.46
7:1G:189:LYS:HA	7:1G:189:LYS:HD2	1.79	0.46
7:1G:363:LEU:HD21	7:1G:578:GLY:HA3	1.98	0.46
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.97	0.46
8:1H:40:VAL:HG21	8:1H:47:GLN:HE21	1.80	0.46
8:1H:86:TRP:HA	8:1H:86:TRP:CE3	2.51	0.46
10:1J:20:PHE:CE1	11:1K:32:CYS:HA	2.47	0.46
10:1J:52:LEU:HD12	11:1K:49:LEU:HD11	1.98	0.46
10:1J:52:LEU:N	10:1J:139:GLU:OE2	2.31	0.46
10:1J:56:VAL:O	10:1J:60:TYR:HB3	2.16	0.46
12:1L:51:LEU:HD11	12:1L:88:MET:HE3	1.97	0.46
12:1L:141:PHE:CD2	13:1M:370:PRO:HG3	2.51	0.46
15:1O:173:ASP:N	15:1O:223:TYR:O	2.45	0.46
15:1O:254:ARG:NH1	15:1O:255:THR:HG23	2.30	0.46
29:1d:116:PHE:HB2	41:1p:156:ALA:HB1	1.98	0.46
33:1h:56:PRO:HD3	41:1p:63:TYR:CE1	2.51	0.46
42:1q:48:TYR:HE1	42:1q:86:TRP:CG	2.33	0.46
42:1q:92:CYS:HB3	43:1r:33:ARG:HG3	1.96	0.46
5:1E:128:VAL:HA	5:1E:139:LEU:HD12	1.98	0.46
5:1E:144:CYS:HA	47:1E:301:FES:S1	2.55	0.46
6:1F:413:TRP:CD1	6:1F:413:TRP:N	2.83	0.46
7:1G:385:ARG:HB3	7:1G:415:LEU:HD23	1.98	0.46
7:1G:537:LEU:HD21	7:1G:543:ILE:HD11	1.98	0.46
8:1H:133:LEU:HD13	10:1J:70:TYR:HE1	1.81	0.46
9:1I:175:TYR:HA	43:1r:40:LEU:HD11	1.98	0.46
11:1K:20:LEU:HD23	12:1L:592:LEU:HA	1.96	0.46
24:1Y:8:TYR:HE1	24:1Y:24:SER:HB3	1.80	0.46
31:1f:45:LYS:HB3	41:1p:68:ARG:HH22	1.80	0.46
40:1o:14:LYS:HG2	40:1o:109:GLN:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:10:ASN:OD1	1:1A:10:ASN:N	2.47	0.46
2:1B:49:THR:CG2	2:1B:59:MET:HE3	2.41	0.46
4:1D:116:GLN:NE2	4:1D:276:ASP:OD2	2.49	0.46
4:1D:174:ARG:HA	4:1D:177:MET:CE	2.46	0.46
4:1D:308:LEU:HD23	4:1D:308:LEU:HA	1.82	0.46
5:1E:81:TYR:O	5:1E:85:THR:HG22	2.16	0.46
6:1F:129:MET:HE2	6:1F:131:ALA:HB2	1.98	0.46
12:1L:76:LEU:HD21	12:1L:196:TRP:HE3	1.80	0.46
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.15	0.46
19:1S:19:ARG:HG2	19:1S:53:LEU:HB2	1.98	0.46
19:1S:28:GLY:HA2	19:1S:80:ASN:HA	1.97	0.46
20:1T:20:LYS:NZ	20:1T:27:PRO:CB	2.79	0.46
20:1U:6:LEU:HD21	20:1U:84:LYS:HG2	1.98	0.46
21:1V:64:VAL:HG13	21:1V:76:ILE:HD13	1.97	0.46
22:1W:119:LEU:HD12	22:1W:119:LEU:C	2.41	0.46
45:1Y:201:3PE:H371	45:1Y:201:3PE:H231	1.98	0.46
40:1o:5:ALA:HA	40:1o:9:LEU:HD13	1.98	0.46
41:1p:74:THR:HG23	41:1p:75:GLU:HG3	1.97	0.46
1:1A:94:LEU:HD12	1:1A:94:LEU:HA	1.77	0.46
3:1C:125:LYS:HZ1	4:1D:252:ASN:HB3	1.81	0.46
6:1F:144:ASN:OD1	6:1F:144:ASN:N	2.49	0.46
6:1F:344:VAL:HA	6:1F:347:ILE:HD11	1.98	0.46
7:1G:422:LEU:H	7:1G:422:LEU:HD12	1.81	0.46
9:1I:74:GLU:OE1	18:1R:44:ILE:CG1	2.64	0.46
10:1J:64:MET:CE	11:1K:34:GLU:HG2	2.46	0.46
11:1K:5:TYR:HE1	11:1K:46:LEU:HB3	1.81	0.46
11:1K:66:PHE:CE2	14:1N:31:ILE:HG23	2.51	0.46
13:1M:305:THR:HB	13:1M:308:SER:HB2	1.98	0.46
15:1O:207:LYS:N	15:1O:207:LYS:HD2	2.31	0.46
16:1P:216:ASN:HA	16:1P:219:LYS:HG3	1.98	0.46
16:1P:325:ARG:HG3	16:1P:326:TRP:CE2	2.51	0.46
18:1R:2:VAL:HG21	18:1R:10:LYS:HE3	1.98	0.46
21:1V:22:ARG:HH12	21:1V:26:LEU:HB2	1.81	0.46
23:1X:75:ARG:HG3	23:1X:76:HIS:ND1	2.31	0.46
29:1d:40:CYS:O	29:1d:44:ILE:HD12	2.16	0.46
32:1g:48:ASP:OD1	32:1g:50:ASP:N	2.35	0.46
3:1C:75:LEU:HB2	3:1C:124:TYR:CD2	2.51	0.46
3:1C:133:GLU:HB2	3:1C:152:LEU:HD12	1.97	0.46
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.98	0.46
4:1D:293:CYS:HA	4:1D:296:ARG:HE	1.80	0.46
7:1G:255:HIS:ND1	7:1G:255:HIS:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:293:PHE:O	8:1H:297:THR:OG1	2.27	0.46
9:1I:32:ARG:HH22	25:1Z:27:ARG:HA	1.81	0.46
10:1J:3:MET:CE	25:1Z:130:ASN:HA	2.45	0.46
12:1L:9:LEU:HD23	34:1i:81:ILE:HG23	1.98	0.46
13:1M:81:GLN:HE22	32:1g:57:ASN:HD21	1.64	0.46
13:1M:121:LEU:HA	13:1M:124:ALA:HB3	1.97	0.46
15:1O:254:ARG:NH1	15:1O:254:ARG:HB3	2.31	0.46
21:1V:92:LYS:N	21:1V:95:ARG:HH21	2.14	0.46
34:1i:30:ARG:NH2	39:1n:116:ASP:OD1	2.48	0.46
41:1p:72:ASP:OD1	41:1p:72:ASP:N	2.46	0.46
42:1q:17:HIS:NE2	42:1q:33:VAL:O	2.45	0.46
7:1G:164:SER:HB3	17:1Q:132:THR:HG21	1.96	0.46
7:1G:230:VAL:CG2	7:1G:497:ALA:CB	2.94	0.46
7:1G:397:LYS:HG3	7:1G:401:HIS:CE1	2.51	0.46
7:1G:525:LEU:HD12	7:1G:546:GLN:HB3	1.98	0.46
7:1G:644:GLN:NE2	19:1S:37:GLU:O	2.48	0.46
10:1J:26:PRO:HB3	11:1K:27:MET:HG3	1.98	0.46
22:1W:24:ASP:OD1	22:1W:26:ASN:N	2.34	0.46
22:1W:92:GLU:HG2	22:1W:98:LYS:HG3	1.97	0.46
23:1X:20:SER:O	23:1X:24:LEU:HD22	2.16	0.46
23:1X:125:SER:N	25:1Z:66:GLU:OE1	2.42	0.46
29:1d:10:PRO:HB2	29:1d:11:LEU:HD12	1.96	0.46
30:1e:12:ASP:OD1	30:1e:12:ASP:N	2.40	0.46
39:1n:23:LEU:HD21	39:1n:43:MET:HE2	1.98	0.46
2:1B:40:ALA:O	2:1B:44:SER:N	2.44	0.45
5:1E:123:LYS:NZ	5:1E:173:ILE:HG23	2.31	0.45
5:1E:183:LYS:HE2	5:1E:183:LYS:HB2	1.81	0.45
6:1F:371:TRP:CH2	7:1G:129:ARG:HG3	2.50	0.45
7:1G:74:MET:SD	7:1G:77:TRP:CE3	3.09	0.45
8:1H:86:TRP:HZ2	8:1H:232:ILE:HB	1.80	0.45
9:1I:74:GLU:OE1	18:1R:44:ILE:HG13	2.16	0.45
11:1K:12:PHE:CD2	14:1N:72:MET:HE2	2.51	0.45
12:1L:81:LYS:HZ1	12:1L:262:ARG:NH1	2.14	0.45
12:1L:355:ASP:OD1	12:1L:357:ARG:NE	2.49	0.45
12:1L:594:THR:HA	12:1L:597:ILE:HG12	1.97	0.45
14:1N:75:ILE:O	14:1N:79:LEU:N	2.45	0.45
19:1S:29:SER:OG	19:1S:33:ARG:NH2	2.46	0.45
21:1V:27:TYR:O	21:1V:30:ILE:HG13	2.16	0.45
29:1d:-1:MET:HB3	29:1d:2:MET:N	2.31	0.45
42:1q:99:THR:O	42:1q:100:THR:OG1	2.32	0.45
2:1B:71:ARG:HA	8:1H:37:PRO:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:152:LEU:HD22	4:1D:84:HIS:CD2	2.50	0.45
4:1D:172:GLU:OE2	4:1D:176:LYS:NZ	2.45	0.45
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.49	0.45
4:1D:268:ASP:OD1	4:1D:368:GLU:HG2	2.16	0.45
5:1E:147:ALA:HB3	5:1E:160:TYR:OH	2.16	0.45
6:1F:140:GLY:O	6:1F:179:ARG:NH1	2.46	0.45
7:1G:492:ILE:HD12	7:1G:494:HIS:CD2	2.51	0.45
7:1G:534:ARG:HD3	42:1q:145:LYS:HE2	1.97	0.45
14:1N:41:ILE:N	14:1N:42:PRO:HD2	2.31	0.45
22:1W:88:MET:HE3	22:1W:91:GLU:OE2	2.15	0.45
22:1W:95:ASN:CG	22:1W:95:ASN:O	2.58	0.45
23:1X:43:MET:CA	23:1X:43:MET:HE2	2.46	0.45
25:1Z:76:GLN:O	25:1Z:80:ASP:HB2	2.16	0.45
29:1d:2:MET:HE1	33:1h:122:TRP:HE3	1.81	0.45
30:1e:6:GLN:HE21	30:1e:13:LEU:HB2	1.80	0.45
32:1g:64:PHE:HA	32:1g:68:ILE:HG12	1.97	0.45
32:1g:121:PRO:O	32:1g:122:GLU:HG3	2.17	0.45
37:1l:7:ASP:N	37:1l:7:ASP:OD1	2.48	0.45
39:1n:106:TRP:CE3	39:1n:110:GLU:HB3	2.52	0.45
41:1p:141:ARG:HB3	41:1p:142:TYR:H	1.60	0.45
2:1B:60:MET:HE1	4:1D:171:PHE:CZ	2.50	0.45
3:1C:64:LEU:O	3:1C:72:PHE:N	2.49	0.45
4:1D:74:ARG:HA	4:1D:407:LYS:HE2	1.97	0.45
4:1D:296:ARG:O	4:1D:300:ARG:HG3	2.16	0.45
6:1F:376:MET:HA	6:1F:379:PHE:HB2	1.97	0.45
7:1G:194:GLU:HB2	7:1G:671:PHE:CE2	2.51	0.45
7:1G:232:ASP:OD1	7:1G:233:ALA:N	2.50	0.45
9:1I:27:TRP:CD1	50:1I:203:PC1:H222	2.51	0.45
9:1I:29:GLU:OE1	9:1I:29:GLU:N	2.49	0.45
12:1L:188:TRP:CE3	12:1L:212:PRO:HG3	2.52	0.45
12:1L:279:CYS:HA	37:1l:116:PHE:HE2	1.79	0.45
13:1M:43:ASN:HB3	33:1h:80:TYR:CZ	2.51	0.45
15:1O:23:LYS:HB3	15:1O:167:HIS:CG	2.51	0.45
15:1O:90:ASP:N	15:1O:90:ASP:OD1	2.48	0.45
20:1T:17:TYR:O	20:1T:20:LYS:HB3	2.15	0.45
23:1X:23:VAL:HG21	26:1a:65:GLY:HA2	1.97	0.45
29:1d:-1:MET:HA	33:1h:123:TYR:HE1	1.82	0.45
29:1d:37:LEU:O	29:1d:41:SER:OG	2.26	0.45
33:1h:56:PRO:HD3	41:1p:63:TYR:CZ	2.52	0.45
43:1r:18:ASP:C	43:1r:18:ASP:OD1	2.59	0.45
3:1C:97:LEU:HD23	3:1C:104:GLN:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:192:GLN:HE21	17:1Q:72:TRP:CA	2.30	0.45
4:1D:15:GLY:HA2	14:1N:228:LEU:HD21	1.98	0.45
5:1E:38:TYR:HD2	5:1E:45:ALA:HB3	1.80	0.45
6:1F:105:CYS:SG	6:1F:257:ASN:CG	2.97	0.45
7:1G:283:MET:HB3	7:1G:560:ILE:HB	1.99	0.45
7:1G:399:TRP:HB2	7:1G:404:LEU:HB2	1.99	0.45
9:1I:112:ASP:OD2	9:1I:112:ASP:C	2.59	0.45
12:1L:293:ILE:HG22	12:1L:422:TYR:HB3	1.99	0.45
12:1L:528:TYR:CG	37:1L:101:MET:HG2	2.51	0.45
13:1M:5:ILE:O	13:1M:9:THR:HG22	2.16	0.45
14:1N:147:GLN:HB3	33:1h:125:TYR:CE2	2.51	0.45
14:1N:248:LEU:HD13	14:1N:297:ALA:HB2	1.98	0.45
22:1W:25:MET:C	22:1W:25:MET:SD	2.99	0.45
22:1W:31:ARG:HA	22:1W:34:GLU:OE1	2.16	0.45
22:1W:42:GLU:OE1	22:1W:90:LEU:HB2	2.16	0.45
24:1Y:43:LYS:HE2	45:1Y:201:3PE:H112	1.99	0.45
25:1Z:43:LEU:HD23	25:1Z:43:LEU:HA	1.81	0.45
36:1k:20:GLN:HA	36:1k:22:LYS:HE3	1.98	0.45
39:1n:169:ILE:O	39:1n:172:ARG:HD3	2.17	0.45
40:1o:95:VAL:HA	40:1o:98:MET:SD	2.56	0.45
41:1p:11:GLU:HG3	41:1p:14:ARG:HH22	1.80	0.45
3:1C:27:GLN:O	3:1C:31:GLU:HG2	2.17	0.45
4:1D:108:TYR:HA	4:1D:111:MET:HG3	1.98	0.45
4:1D:204:PRO:HG2	4:1D:207:LEU:HB2	1.99	0.45
6:1F:111:ILE:HG23	6:1F:149:LEU:HD12	1.97	0.45
6:1F:194:GLU:HA	6:1F:197:GLU:HB3	1.97	0.45
9:1I:69:ARG:NH1	9:1I:73:GLY:O	2.49	0.45
11:1K:12:PHE:CG	14:1N:72:MET:HE1	2.51	0.45
12:1L:441:VAL:HG23	12:1L:443:ILE:HG12	1.98	0.45
13:1M:97:THR:HG22	13:1M:98:MET:HE2	1.99	0.45
15:1O:115:LEU:HD13	15:1O:121:GLY:HA2	1.98	0.45
16:1P:193:LEU:HD22	16:1P:242:VAL:HG21	1.98	0.45
17:1Q:11:ILE:HB	22:1W:77:ARG:HH21	1.81	0.45
17:1Q:55:TRP:HB2	17:1Q:86:PHE:HB2	1.98	0.45
20:1T:20:LYS:NZ	20:1T:27:PRO:HB3	2.32	0.45
20:1T:22:TYR:CE2	20:1T:24:LYS:HB3	2.51	0.45
37:1L:23:ALA:HA	37:1L:26:LYS:HB3	1.98	0.45
37:1L:139:TYR:CD2	37:1L:150:PRO:HB3	2.51	0.45
39:1n:65:GLN:OE1	39:1n:65:GLN:N	2.49	0.45
42:1q:37:THR:HG23	42:1q:50:GLU:HG2	1.98	0.45
2:1B:94:ASN:HB3	3:1C:174:LEU:HG	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:81:TYR:OH	7:1G:187:ILE:HD12	2.17	0.45
5:1E:135:LYS:HE3	5:1E:135:LYS:CA	2.46	0.45
6:1F:237:ARG:HG2	6:1F:241:TRP:CE3	2.51	0.45
6:1F:247:ARG:HE	6:1F:320:ASP:HB2	1.81	0.45
7:1G:36:GLN:NE2	17:1Q:49:VAL:H	2.03	0.45
7:1G:632:ARG:NH2	19:1S:58:SER:O	2.48	0.45
8:1H:105:MET:HG2	8:1H:237:PHE:CE2	2.51	0.45
10:1J:145:ALA:O	10:1J:149:TYR:N	2.48	0.45
12:1L:483:PRO:HG3	35:1j:53:TYR:CE1	2.52	0.45
12:1L:492:ILE:O	12:1L:495:ILE:N	2.48	0.45
14:1N:25:HIS:O	14:1N:29:ILE:HG12	2.16	0.45
14:1N:217:MET:CE	14:1N:323:MET:HA	2.42	0.45
15:1O:78:SER:N	15:1O:92:ASN:HD21	2.12	0.45
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	1.98	0.45
16:1P:235:ARG:CZ	16:1P:291:ASP:HB3	2.47	0.45
20:1U:15:VAL:HG12	20:1U:19:LEU:HD21	1.98	0.45
20:1U:71:MET:HE3	34:1i:1:SAC:HA	1.98	0.45
22:1W:50:PHE:CD2	22:1W:103:ILE:HG12	2.49	0.45
22:1W:105:ARG:O	22:1W:108:HIS:ND1	2.50	0.45
29:1d:113:LEU:HD11	41:1p:163:LEU:HD11	1.98	0.45
37:1l:134:PRO:CB	40:1o:38:MET:HE2	2.39	0.45
1:1A:79:SER:HA	1:1A:87:MET:HE3	1.99	0.45
1:1A:104:TYR:CD1	1:1A:104:TYR:C	2.95	0.45
4:1D:303:GLU:O	4:1D:307:SER:OG	2.26	0.45
6:1F:404:ILE:HB	46:1F:502:SF4:S4	2.56	0.45
7:1G:113:GLU:OE2	17:1Q:43:ASN:ND2	2.47	0.45
7:1G:140:LYS:HD2	7:1G:150:MET:HE2	1.98	0.45
7:1G:385:ARG:NH1	7:1G:414:ASP:OD2	2.50	0.45
7:1G:574:VAL:HG12	7:1G:580:ALA:HA	1.99	0.45
7:1G:589:PRO:HA	7:1G:590:PRO:HD3	1.89	0.45
7:1G:628:PRO:HD3	19:1S:21:HIS:CE1	2.51	0.45
8:1H:55:LEU:HD13	8:1H:221:ALA:HB2	1.99	0.45
8:1H:90:PRO:HG2	8:1H:240:ILE:HG12	1.99	0.45
8:1H:158:GLY:HA2	8:1H:315:PRO:HG2	1.99	0.45
12:1L:573:MET:HB2	14:1N:167:TRP:CE2	2.52	0.45
14:1N:261:MET:HE1	14:1N:340:THR:CA	2.41	0.45
15:1O:54:ALA:O	15:1O:104:ARG:NH1	2.49	0.45
27:1b:14:LYS:HD3	27:1b:14:LYS:N	2.32	0.45
28:1c:5:ARG:NH2	28:1c:6:GLU:HB3	2.32	0.45
2:1B:71:ARG:HB2	8:1H:38:ASN:OD1	2.16	0.45
2:1B:116:MET:HG2	2:1B:151:PRO:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:49:LEU:HD22	4:1D:50:ASN:H	1.82	0.45
4:1D:228:MET:HG3	4:1D:229:LEU:HD12	1.98	0.45
5:1E:27:ASN:OD1	5:1E:27:ASN:N	2.49	0.45
5:1E:194:GLU:OE1	5:1E:194:GLU:N	2.48	0.45
6:1F:153:ILE:HG23	6:1F:175:VAL:HG13	1.98	0.45
7:1G:361:ASN:HA	7:1G:490:MET:HE1	1.99	0.45
10:1J:111:GLU:CD	10:1J:111:GLU:N	2.75	0.45
10:1J:169:MET:HA	10:1J:172:THR:HG22	1.99	0.45
12:1L:114:ILE:HD11	12:1L:118:PHE:HE1	1.82	0.45
16:1P:153:GLU:HB3	16:1P:154:LYS:HZ2	1.81	0.45
17:1Q:103:PHE:CD1	17:1Q:104:ASP:N	2.84	0.45
22:1W:65:GLU:O	22:1W:69:LYS:HE2	2.07	0.45
22:1W:66:MET:HE3	22:1W:69:LYS:HG2	1.99	0.45
23:1X:141:TYR:HA	25:1Z:115:ARG:HD3	1.99	0.45
26:1a:2:TRP:HH2	53:1r:201:CDL:H751	1.81	0.45
32:1g:113:PHE:H	41:1p:158:GLN:HE22	1.65	0.45
34:1i:15:ARG:O	34:1i:19:ARG:HG2	2.17	0.45
37:1l:126:GLN:HB2	37:1l:128:VAL:HG12	1.98	0.45
1:1A:80:GLN:NE2	8:1H:317:GLN:HB3	2.32	0.45
1:1A:106:TRP:CD2	45:1A:201:3PE:H231	2.51	0.45
1:1A:111:LEU:HD23	1:1A:111:LEU:N	2.32	0.45
2:1B:161:LEU:HD21	9:1I:51:PRO:HD3	1.98	0.45
4:1D:32:PRO:HG2	4:1D:37:ASP:HA	1.98	0.45
4:1D:267:TRP:CE3	4:1D:272:THR:HG21	2.52	0.45
6:1F:53:PRO:O	6:1F:57:LEU:HG	2.16	0.45
6:1F:96:ASN:O	6:1F:225:VAL:HG23	2.17	0.45
6:1F:249:ARG:NE	6:1F:249:ARG:O	2.50	0.45
6:1F:308:PRO:HG3	6:1F:422:PHE:CZ	2.52	0.45
6:1F:355:LYS:HD2	6:1F:373:ASN:HD22	1.81	0.45
6:1F:361:GLN:HE21	6:1F:361:GLN:HB2	1.47	0.45
6:1F:422:PHE:HB3	6:1F:425:GLU:HB2	1.99	0.45
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.49	0.45
7:1G:45:ARG:HE	7:1G:45:ARG:HB3	1.51	0.45
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.99	0.45
17:1Q:11:ILE:CG1	22:1W:77:ARG:NH2	2.78	0.45
17:1Q:126:LYS:HE2	17:1Q:126:LYS:HB2	1.72	0.45
28:1c:24:SER:HB2	29:1d:66:THR:HG21	1.98	0.45
37:1l:18:GLU:OE1	37:1l:18:GLU:N	2.45	0.45
40:1o:49:GLN:NE2	41:1p:116:GLU:O	2.49	0.45
40:1o:92:LEU:C	40:1o:96:LYS:HE2	2.42	0.45
5:1E:199:LEU:HD12	5:1E:202:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:137:TYR:HE2	6:1F:186:CYS:HB3	1.81	0.45
7:1G:232:ASP:OD2	7:1G:388:ALA:HA	2.16	0.45
7:1G:358:LEU:HD12	7:1G:358:LEU:HA	1.83	0.45
7:1G:572:THR:HG23	7:1G:633:TYR:HE1	1.82	0.45
11:1K:73:LEU:HA	11:1K:76:SER:HB2	1.99	0.45
12:1L:101:MET:HG3	12:1L:118:PHE:CE2	2.52	0.45
13:1M:168:GLN:NE2	13:1M:172:GLY:O	2.51	0.45
14:1N:341:PRO:O	29:1d:79:GLN:NE2	2.50	0.45
15:1O:180:GLN:O	15:1O:184:GLN:HG2	2.17	0.45
16:1P:171:ILE:HG12	56:1P:501:NDP:H42N	1.98	0.45
23:1X:105:LYS:HD3	23:1X:105:LYS:HA	1.65	0.45
24:1Y:18:HIS:CD2	24:1Y:19:ARG:HG2	2.52	0.45
38:1m:21:GLU:HA	38:1m:24:ILE:HD11	1.98	0.45
42:1q:41:GLU:HG2	42:1q:42:ASP:O	2.17	0.45
42:1q:59:HIS:ND1	42:1q:59:HIS:C	2.74	0.45
43:1r:102:ARG:NH2	43:1r:104:GLU:H	2.14	0.45
2:1B:38:ASN:HA	2:1B:41:ARG:HB2	2.00	0.44
3:1C:50:ILE:HB	3:1C:107:VAL:HG12	1.98	0.44
3:1C:53:HIS:NE2	21:1V:104:GLU:OE1	2.50	0.44
4:1D:103:PHE:HA	4:1D:106:LEU:HD12	1.97	0.44
4:1D:133:ARG:O	4:1D:137:ILE:HD12	2.17	0.44
4:1D:231:ASN:ND2	25:1Z:25:LEU:HD21	2.31	0.44
4:1D:256:SER:HB2	4:1D:373:GLU:HB3	2.00	0.44
7:1G:703:ILE:HB	18:1R:85:GLY:HA2	1.99	0.44
8:1H:102:VAL:HG13	8:1H:150:LEU:HD13	1.99	0.44
8:1H:286:MET:HG3	8:1H:290:TRP:HE1	1.81	0.44
10:1J:36:SER:HA	10:1J:39:VAL:HG12	1.98	0.44
12:1L:486:MET:HA	51:1L:701:MYR:H72	1.45	0.44
51:1L:701:MYR:C1	37:1l:126:GLN:HG3	2.47	0.44
13:1M:218:LYS:O	13:1M:222:GLU:HG2	2.16	0.44
16:1P:311:GLU:OE2	16:1P:311:GLU:N	2.40	0.44
29:1d:104:LYS:N	29:1d:104:LYS:CD	2.72	0.44
37:1l:83:MET:HA	37:1l:83:MET:HE3	1.99	0.44
38:1m:74:ASN:O	38:1m:74:ASN:ND2	2.40	0.44
43:1r:52:TYR:O	43:1r:55:THR:HG22	2.17	0.44
2:1B:178:ARG:HD3	2:1B:178:ARG:HA	1.72	0.44
3:1C:12:ARG:HA	4:1D:129:GLN:HB3	1.99	0.44
4:1D:98:GLN:HE21	9:1I:86:VAL:HA	1.81	0.44
4:1D:364:TYR:O	4:1D:364:TYR:CG	2.70	0.44
6:1F:92:TYR:HD1	6:1F:133:ALA:HB3	1.81	0.44
6:1F:185:ILE:HG13	6:1F:359:CYS:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:185:ILE:HD12	46:1F:502:SF4:S1	2.56	0.44
7:1G:174:THR:O	7:1G:174:THR:OG1	2.32	0.44
7:1G:176:GLY:C	7:1G:181:MET:HB3	2.43	0.44
7:1G:307:LEU:HD12	7:1G:607:ALA:HB1	1.99	0.44
13:1M:75:LEU:HA	13:1M:78:MET:HE3	1.98	0.44
13:1M:175:ASN:OD1	13:1M:178:ILE:HG13	2.17	0.44
13:1M:190:TRP:CE3	24:1Y:126:MET:HE1	2.52	0.44
14:1N:2:ASN:HB3	14:1N:5:ILE:HG13	2.00	0.44
14:1N:91:ASN:ND2	14:1N:93:VAL:HG12	2.32	0.44
14:1N:106:LEU:HD11	14:1N:139:LEU:HG	1.98	0.44
14:1N:260:PHE:CZ	14:1N:264:TRP:HB2	2.53	0.44
14:1N:344:SER:O	14:1N:347:ASN:ND2	2.50	0.44
15:1O:30:ASN:HD21	15:1O:203:GLU:HB3	1.81	0.44
21:1V:107:PRO:HB2	21:1V:110:GLN:HB2	1.99	0.44
25:1Z:93:GLU:O	25:1Z:97:ILE:HG22	2.17	0.44
29:1d:-1:MET:SD	33:1h:122:TRP:CZ3	3.11	0.44
33:1h:32:THR:C	33:1h:35:PRO:HD2	2.42	0.44
34:1i:10:ARG:HA	34:1i:13:GLN:NE2	2.32	0.44
36:1k:81:VAL:HA	36:1k:84:GLU:CB	2.45	0.44
37:1l:16:THR:O	37:1l:20:ARG:HG2	2.17	0.44
40:1o:3:HIS:HA	40:1o:6:ARG:HH21	1.82	0.44
42:1q:6:VAL:HG22	42:1q:9:ARG:HH21	1.81	0.44
1:1A:3:ILE:HG13	1:1A:4:MET:N	2.33	0.44
2:1B:168:LYS:NZ	42:1q:76:ASP:HB3	2.33	0.44
3:1C:58:ILE:HG12	3:1C:118:GLU:HG3	1.99	0.44
4:1D:362:ALA:HB2	4:1D:379:VAL:HG12	1.98	0.44
5:1E:101:GLN:HG3	5:1E:142:VAL:HG11	1.98	0.44
7:1G:397:LYS:O	7:1G:401:HIS:ND1	2.50	0.44
8:1H:37:PRO:HB2	8:1H:47:GLN:HG3	1.98	0.44
8:1H:149:ILE:HG23	8:1H:181:LEU:HD22	1.98	0.44
9:1I:175:TYR:CE2	43:1r:38:PRO:HG3	2.52	0.44
12:1L:274:GLN:O	12:1L:278:LEU:HD22	2.16	0.44
12:1L:435:PRO:HG2	36:1k:56:PHE:CE2	2.52	0.44
12:1L:511:LEU:O	12:1L:511:LEU:HD13	2.17	0.44
15:1O:176:VAL:HG13	15:1O:177:PRO:HD3	2.00	0.44
20:1T:69:LYS:NZ	20:1T:79:TYR:HB2	2.32	0.44
21:1V:92:LYS:HA	21:1V:95:ARG:CZ	2.47	0.44
33:1h:19:ARG:HH21	33:1h:23:LYS:HB2	1.82	0.44
38:1m:61:ASP:C	38:1m:61:ASP:OD1	2.60	0.44
40:1o:30:PHE:HB2	40:1o:33:ARG:HD2	1.98	0.44
41:1p:159:LYS:HA	41:1p:162:MET:SD	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:45:GLY:C	42:1q:65:THR:HB	2.43	0.44
42:1q:95:ASP:H	43:1r:34:THR:HG1	1.60	0.44
3:1C:28:TYR:CD1	3:1C:28:TYR:C	2.96	0.44
4:1D:270:ARG:HB2	4:1D:278:TYR:HD2	1.82	0.44
4:1D:305:ARG:CZ	25:1Z:23:ARG:HA	2.48	0.44
5:1E:7:PHE:HA	5:1E:92:ARG:NH1	2.30	0.44
7:1G:432:ILE:HG22	7:1G:473:ILE:HG12	1.98	0.44
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	2.00	0.44
9:1I:11:SER:O	9:1I:20:ARG:NH2	2.50	0.44
9:1I:108:ARG:HD2	9:1I:110:ASP:CG	2.43	0.44
52:1M:501:PGT:H321	52:1M:501:PGT:H352	1.80	0.44
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.41	0.44
15:1O:32:CYS:SG	15:1O:182:ARG:HB2	2.58	0.44
20:1T:69:LYS:HD2	20:1T:70:LEU:HG	2.00	0.44
21:1V:30:ILE:HG22	21:1V:87:LEU:HD23	1.99	0.44
25:1Z:87:LEU:HD23	25:1Z:87:LEU:HA	1.80	0.44
28:1c:35:HIS:CD2	29:1d:26:LEU:HB3	2.51	0.44
28:1c:43:LYS:HA	28:1c:48:LEU:HD13	2.00	0.44
30:1e:94:PRO:HB2	30:1e:96:HIS:CE1	2.53	0.44
37:1l:131:LYS:NZ	40:1o:97:ARG:HH22	2.16	0.44
40:1o:60:HIS:HD1	40:1o:61:TYR:H	1.66	0.44
43:1r:63:MET:HE3	43:1r:63:MET:HA	1.99	0.44
3:1C:68:THR:CG2	21:1V:50:ILE:HD12	2.48	0.44
4:1D:112:MET:HG3	4:1D:194:ILE:HD12	1.98	0.44
4:1D:306:GLN:O	4:1D:310:ILE:HG13	2.17	0.44
6:1F:294:LEU:HD22	6:1F:309:LYS:HG3	1.98	0.44
6:1F:411:ALA:C	6:1F:414:PRO:HD2	2.42	0.44
7:1G:622:ARG:HH21	7:1G:626:VAL:HB	1.82	0.44
9:1I:69:ARG:HD3	9:1I:73:GLY:HA2	1.99	0.44
9:1I:74:GLU:OE2	9:1I:105:ARG:NH2	2.51	0.44
12:1L:64:SER:HB2	34:1i:95:THR:HA	1.99	0.44
12:1L:178:GLY:O	12:1L:219:ALA:HA	2.17	0.44
13:1M:204:MET:HB3	13:1M:209:LEU:HD22	2.00	0.44
13:1M:412:ILE:HA	13:1M:416:ARG:HB2	1.99	0.44
13:1M:451:PRO:O	13:1M:455:LEU:HD23	2.17	0.44
14:1N:156:THR:HG22	24:1Y:135:PHE:CZ	2.53	0.44
15:1O:4:GLY:O	15:1O:6:LEU:N	2.51	0.44
16:1P:325:ARG:HH21	16:1P:326:TRP:HH2	1.64	0.44
21:1V:23:LEU:O	21:1V:27:TYR:HB2	2.18	0.44
22:1W:80:ASP:O	22:1W:84:ILE:HG12	2.18	0.44
23:1X:95:LEU:HD22	23:1X:95:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:47:ASN:OD1	34:1i:48:LYS:N	2.51	0.44
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.42	0.44
36:1k:13:MET:HE3	36:1k:13:MET:HB3	1.74	0.44
38:1m:14:PRO:HG2	38:1m:17:LEU:HD13	1.99	0.44
38:1m:128:TYR:HD1	38:1m:128:TYR:H	1.65	0.44
42:1q:86:TRP:CG	42:1q:98:PRO:HG2	2.53	0.44
2:1B:77:ARG:CZ	2:1B:82:GLN:HG3	2.48	0.44
3:1C:37:VAL:HG23	3:1C:37:VAL:O	2.18	0.44
3:1C:75:LEU:HD23	3:1C:126:ALA:HB3	2.00	0.44
3:1C:100:ARG:NH2	43:1r:100:ILE:O	2.48	0.44
4:1D:223:ASP:OD2	43:1r:17:ARG:NE	2.46	0.44
4:1D:342:MET:CG	7:1G:98:LEU:HG	2.47	0.44
5:1E:34:ILE:O	5:1E:38:TYR:CE1	2.69	0.44
5:1E:108:CYS:HA	5:1E:111:ARG:HH21	1.82	0.44
7:1G:349:PHE:CD2	7:1G:458:LEU:HD21	2.53	0.44
7:1G:380:VAL:HG23	7:1G:453:LEU:HD23	1.98	0.44
9:1I:8:ARG:NH1	43:1r:112:LEU:O	2.51	0.44
12:1L:287:PHE:CE1	12:1L:527:GLY:HA3	2.53	0.44
12:1L:530:PRO:O	12:1L:534:HIS:HB2	2.17	0.44
13:1M:319:HIS:HD1	13:1M:319:HIS:C	2.25	0.44
14:1N:112:HIS:O	14:1N:116:PRO:HD3	2.17	0.44
15:1O:28:ASP:CG	15:1O:206:TYR:OH	2.60	0.44
16:1P:325:ARG:HA	16:1P:325:ARG:HD2	1.77	0.44
18:1R:3:ARG:NH2	18:1R:6:PRO:HD3	2.33	0.44
20:1T:8:LEU:CD1	20:1T:88:GLU:CG	2.95	0.44
20:1U:35:HIS:ND1	20:1U:38:LYS:HG3	2.32	0.44
20:1U:35:HIS:CD2	20:1U:38:LYS:HE2	2.53	0.44
23:1X:129:LYS:HD3	27:1b:65:VAL:HG13	1.98	0.44
26:1a:2:TRP:CD1	26:1a:2:TRP:H	2.36	0.44
37:1l:30:ARG:NH1	38:1m:34:GLU:OE1	2.43	0.44
42:1q:8:ARG:O	42:1q:10:GLY:N	2.51	0.44
42:1q:38:LEU:HD13	42:1q:40:GLY:N	2.32	0.44
42:1q:78:ASP:OD1	42:1q:80:SER:N	2.34	0.44
43:1r:0:ACE:H1	43:1r:3:ALA:HB2	1.99	0.44
2:1B:35:ASP:O	2:1B:39:TRP:HB3	2.18	0.44
3:1C:39:GLN:HA	43:1r:69:MET:SD	2.58	0.44
4:1D:245:VAL:HB	4:1D:404:LYS:HZ2	1.83	0.44
5:1E:145:LEU:HB2	6:1F:141:GLU:HB3	1.99	0.44
6:1F:224:ASN:HB3	6:1F:227:THR:HG23	1.99	0.44
6:1F:268:VAL:HG21	6:1F:283:HIS:HB3	2.00	0.44
7:1G:647:GLU:HA	7:1G:650:LYS:HD2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:147:VAL:HG22	12:1L:252:MET:HG2	1.98	0.44
12:1L:485:TYR:HB2	51:1L:701:MYR:H121	1.98	0.44
13:1M:314:ALA:HA	13:1M:454:ILE:HG13	1.99	0.44
14:1N:247:THR:O	14:1N:251:MET:N	2.39	0.44
15:1O:185:LYS:HD2	15:1O:185:LYS:HA	1.79	0.44
20:1T:8:LEU:HD12	20:1T:88:GLU:CB	2.43	0.44
21:1V:27:TYR:OH	21:1V:54:LYS:HG2	2.18	0.44
22:1W:62:LYS:NZ	22:1W:107:PHE:HA	2.33	0.44
25:1Z:10:MET:SD	25:1Z:11:PRO:HD2	2.58	0.44
32:1g:110:SER:HA	41:1p:137:ALA:HB1	2.00	0.44
37:1l:41:GLY:N	38:1m:80:ARG:HH21	2.16	0.44
43:1r:43:GLY:H	43:1r:46:HIS:CE1	2.36	0.44
43:1r:60:ARG:HB2	43:1r:60:ARG:CZ	2.47	0.44
2:1B:113:VAL:CG2	2:1B:142:VAL:HA	2.48	0.44
4:1D:261:ARG:NH1	4:1D:268:ASP:OD2	2.51	0.44
4:1D:421:GLN:HB3	4:1D:423:ILE:HG23	2.00	0.44
5:1E:163:ASP:OD1	5:1E:190:ARG:NE	2.49	0.44
6:1F:306:LEU:HD21	6:1F:422:PHE:HE2	1.83	0.44
7:1G:28:GLN:HE22	17:1Q:115:SER:HA	1.81	0.44
7:1G:364:LEU:HG	7:1G:491:ASN:ND2	2.32	0.44
8:1H:55:LEU:HD22	8:1H:221:ALA:H	1.82	0.44
8:1H:154:LEU:HD12	8:1H:154:LEU:O	2.18	0.44
9:1I:11:SER:OG	9:1I:13:ASP:OD2	2.28	0.44
10:1J:7:PHE:O	10:1J:11:THR:HG22	2.18	0.44
10:1J:136:PHE:HB2	10:1J:141:MET:HG3	1.99	0.44
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.18	0.44
13:1M:36:LEU:O	13:1M:36:LEU:HD23	2.17	0.44
13:1M:123:GLU:OE2	14:1N:254:LEU:HB3	2.18	0.44
13:1M:131:ILE:HG22	13:1M:136:TRP:HZ3	1.82	0.44
13:1M:168:GLN:NE2	33:1h:104:ARG:HD2	2.30	0.44
13:1M:356:ALA:HA	13:1M:415:GLN:NE2	2.33	0.44
14:1N:340:THR:HG22	23:1X:169:TRP:CE2	2.52	0.44
16:1P:139:ILE:HG23	16:1P:150:ALA:HB3	2.00	0.44
16:1P:203:GLN:NE2	16:1P:233:PRO:C	2.76	0.44
17:1Q:35:VAL:HG11	17:1Q:57:MET:CE	2.47	0.44
20:1T:52:MET:HE2	20:1T:52:MET:HB2	1.77	0.44
33:1h:61:PRO:HG2	33:1h:66:TYR:OH	2.17	0.44
35:1j:6:HIS:H	35:1j:6:HIS:CD2	2.35	0.44
35:1j:12:ARG:HA	36:1k:50:TRP:CE3	2.53	0.44
39:1n:11:HIS:ND1	39:1n:12:GLN:OE1	2.51	0.44
1:1A:107:THR:HG23	1:1A:108:GLN:HG2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:84:HIS:HA	4:1D:429:ASP:HB3	1.99	0.44
6:1F:92:TYR:CD1	6:1F:133:ALA:HB3	2.53	0.44
7:1G:40:PHE:HB2	7:1G:52:CYS:SG	2.58	0.44
7:1G:197:GLY:HA3	7:1G:268:ARG:HE	1.83	0.44
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.18	0.44
11:1K:31:LEU:HD23	11:1K:31:LEU:HA	1.80	0.44
12:1L:82:MET:HE1	12:1L:133:THR:HB	1.99	0.44
12:1L:305:SER:O	12:1L:309:GLN:HG2	2.18	0.44
12:1L:577:VAL:HG21	14:1N:167:TRP:HB3	1.99	0.44
14:1N:112:HIS:CE1	14:1N:164:ILE:HD12	2.52	0.44
15:1O:77:CYS:HA	15:1O:92:ASN:OD1	2.18	0.44
15:1O:171:TYR:CE1	15:1O:173:ASP:HA	2.49	0.44
20:1T:35:HIS:CD2	20:1T:38:LYS:NZ	2.86	0.44
21:1V:111:TRP:O	21:1V:112:LYS:HB3	2.17	0.44
22:1W:65:GLU:CA	22:1W:69:LYS:HZ3	2.31	0.44
23:1X:110:VAL:HA	23:1X:114:LEU:HD23	1.98	0.44
26:1a:21:MET:HE1	26:1a:25:HIS:ND1	2.33	0.44
37:1l:96:VAL:HB	37:1l:101:MET:HE2	1.99	0.44
39:1n:137:LYS:HA	39:1n:137:LYS:HD3	1.83	0.44
40:1o:110:ARG:HA	40:1o:113:ARG:NE	2.32	0.44
3:1C:41:GLN:NE2	43:1r:65:PRO:HB2	2.33	0.43
3:1C:178:ASP:OD1	3:1C:181:LYS:HE2	2.18	0.43
4:1D:8:VAL:CG1	32:1g:25:ARG:HH12	2.29	0.43
4:1D:248:GLU:HA	4:1D:248:GLU:OE2	2.18	0.43
4:1D:428:VAL:HG23	4:1D:429:ASP:H	1.83	0.43
5:1E:10:ARG:NH2	18:1R:77:LYS:HG2	2.31	0.43
5:1E:34:ILE:O	5:1E:38:TYR:CD1	2.70	0.43
7:1G:145:LEU:HD13	7:1G:269:PHE:CE1	2.53	0.43
7:1G:243:ARG:HH12	9:1I:81:LYS:NZ	2.15	0.43
9:1I:162:GLU:HB3	42:1q:109:ILE:HG23	2.00	0.43
12:1L:304:PHE:CZ	12:1L:526:LEU:HD13	2.53	0.43
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	2.00	0.43
12:1L:576:MET:SD	45:1Y:201:3PE:H31	2.58	0.43
13:1M:73:LEU:HA	13:1M:76:MET:SD	2.58	0.43
13:1M:272:THR:HA	13:1M:275:ILE:HG12	2.00	0.43
14:1N:24:SER:HB3	30:1e:1:PRO:HD3	1.99	0.43
14:1N:296:LEU:O	14:1N:300:SER:OG	2.22	0.43
14:1N:310:ASN:HB2	15:1O:274:THR:HG22	1.99	0.43
14:1N:321:LYS:HE2	14:1N:321:LYS:HB3	1.82	0.43
26:1a:40:HIS:N	26:1a:44:GLN:OE1	2.51	0.43
29:1d:77:LYS:HB2	29:1d:77:LYS:HE3	1.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1f:101:PC1:H121	33:1h:81:ASP:OD1	2.18	0.43
33:1h:114:MET:HE3	33:1h:120:GLY:C	2.43	0.43
39:1n:161:ASP:OD1	39:1n:161:ASP:N	2.50	0.43
3:1C:76:ALA:HB1	4:1D:364:TYR:CZ	2.54	0.43
3:1C:88:ASN:HD21	21:1V:107:PRO:HG2	1.82	0.43
5:1E:121:GLN:NE2	5:1E:127:LYS:HG3	2.33	0.43
5:1E:171:GLU:O	5:1E:175:GLU:HG2	2.19	0.43
7:1G:60:GLU:OE1	7:1G:78:ASN:N	2.51	0.43
7:1G:336:ASN:OD1	19:1S:67:ARG:NE	2.44	0.43
7:1G:478:ARG:CZ	7:1G:478:ARG:HA	2.48	0.43
7:1G:478:ARG:HG3	7:1G:642:PHE:CE2	2.53	0.43
8:1H:63:PRO:O	8:1H:66:SER:OG	2.32	0.43
9:1I:98:PRO:HD3	9:1I:104:ARG:HE	1.83	0.43
9:1I:160:LYS:HE2	42:1q:110:TRP:CZ3	2.53	0.43
10:1J:33:LEU:CD1	10:1J:65:LEU:HD11	2.44	0.43
10:1J:58:LEU:CD1	10:1J:59:ILE:HG23	2.48	0.43
10:1J:153:LEU:HD12	11:1K:62:ILE:HD12	2.00	0.43
11:1K:12:PHE:O	11:1K:16:LEU:N	2.39	0.43
12:1L:128:MET:HE2	12:1L:251:THR:CG2	2.49	0.43
12:1L:241:THR:OG1	12:1L:242:PRO:HD3	2.18	0.43
12:1L:323:HIS:H	12:1L:323:HIS:CD2	2.34	0.43
12:1L:470:ASN:HB3	40:1o:76:PHE:HB2	2.00	0.43
14:1N:89:MET:HE2	14:1N:98:MET:HE2	1.99	0.43
14:1N:160:LEU:O	14:1N:164:ILE:HG12	2.18	0.43
16:1P:120:VAL:O	16:1P:124:ALA:N	2.48	0.43
18:1R:16:GLN:HE22	18:1R:33:LYS:HZ3	1.65	0.43
22:1W:75:ASP:OD1	22:1W:77:ARG:HB3	2.18	0.43
23:1X:139:ASN:OD1	23:1X:139:ASN:N	2.51	0.43
35:1j:35:TRP:CH2	35:1j:39:ARG:HD3	2.53	0.43
2:1B:92:LEU:HD12	2:1B:92:LEU:HA	1.82	0.43
2:1B:125:TYR:CD1	4:1D:102:TYR:CZ	3.05	0.43
4:1D:4:TRP:CE3	13:1M:140:THR:HA	2.53	0.43
4:1D:412:ALA:HB3	8:1H:281:ARG:HG3	1.99	0.43
5:1E:86:PHE:CD2	6:1F:200:GLN:HB2	2.53	0.43
5:1E:89:MET:HE2	5:1E:89:MET:HB3	1.82	0.43
6:1F:153:ILE:HG13	6:1F:153:ILE:H	1.69	0.43
7:1G:70:ALA:O	7:1G:72:PRO:HD3	2.19	0.43
8:1H:66:SER:HA	8:1H:122:ALA:O	2.18	0.43
9:1I:152:GLU:OE2	18:1R:12:THR:OG1	2.35	0.43
13:1M:14:MET:HG3	31:1f:12:VAL:HG22	2.00	0.43
52:1M:501:PGT:H121	52:1M:501:PGT:H32	1.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:159:MET:HE3	14:1N:159:MET:CA	2.48	0.43
15:1O:129:TYR:CE2	15:1O:166:PRO:HD3	2.53	0.43
16:1P:108:ASP:O	16:1P:113:ILE:HD12	2.19	0.43
16:1P:174:ARG:HB3	16:1P:175:GLU:OE1	2.18	0.43
16:1P:240:ASP:CG	16:1P:337:ALA:HB1	2.43	0.43
17:1Q:95:PHE:HA	17:1Q:98:LYS:HD2	2.01	0.43
20:1T:8:LEU:CD1	20:1T:88:GLU:CD	2.91	0.43
20:1T:20:LYS:HZ2	20:1T:27:PRO:CB	2.30	0.43
31:1f:18:VAL:HA	31:1f:21:VAL:HB	2.00	0.43
41:1p:116:GLU:HB2	41:1p:120:TYR:HA	1.99	0.43
2:1B:46:TRP:NE1	2:1B:73:GLY:O	2.52	0.43
2:1B:148:GLY:HA2	9:1I:118:TYR:CE1	2.53	0.43
4:1D:245:VAL:HB	4:1D:404:LYS:NZ	2.33	0.43
4:1D:329:LYS:HE2	43:1r:53:TYR:CE2	2.54	0.43
7:1G:100:ASN:HD22	7:1G:135:ARG:HD3	1.83	0.43
7:1G:337:ARG:NH2	7:1G:610:THR:O	2.41	0.43
7:1G:617:ASP:OD1	7:1G:617:ASP:N	2.51	0.43
8:1H:20:LEU:HD23	8:1H:228:TYR:HB3	2.00	0.43
8:1H:88:PRO:HG3	8:1H:104:PHE:CD2	2.54	0.43
11:1K:12:PHE:HE1	11:1K:16:LEU:HD22	1.84	0.43
15:1O:3:TYR:HD1	15:1O:7:ALA:HB3	1.83	0.43
15:1O:206:TYR:CD1	15:1O:210:PHE:HD1	2.36	0.43
16:1P:212:LYS:HE2	16:1P:212:LYS:HB3	1.91	0.43
16:1P:238:LEU:O	16:1P:242:VAL:HG22	2.18	0.43
17:1Q:95:PHE:HA	17:1Q:98:LYS:CD	2.49	0.43
18:1R:81:THR:HB	18:1R:92:ARG:HB3	2.01	0.43
20:1T:45:LEU:HB3	22:1W:36:TYR:CE2	2.53	0.43
20:1U:61:GLU:OE1	39:1n:81:PHE:HB2	2.19	0.43
22:1W:22:SER:HB2	22:1W:31:ARG:HH21	1.84	0.43
40:1o:36:ARG:HB3	40:1o:57:TYR:HE2	1.83	0.43
40:1o:50:LEU:HD12	40:1o:50:LEU:HA	1.85	0.43
42:1q:55:PHE:CZ	42:1q:58:ARG:HD3	2.53	0.43
42:1q:85:GLU:HG2	42:1q:86:TRP:N	2.33	0.43
1:1A:54:LYS:HD2	4:1D:71:GLU:OE1	2.18	0.43
1:1A:105:GLU:CG	1:1A:111:LEU:HD23	2.48	0.43
1:1A:112:GLU:O	1:1A:112:GLU:OE1	2.35	0.43
4:1D:152:MET:SD	4:1D:171:PHE:CZ	3.11	0.43
5:1E:87:TYR:CD1	6:1F:181:ALA:HB3	2.53	0.43
6:1F:25:LEU:HD13	6:1F:26:TYR:CE1	2.54	0.43
6:1F:36:ALA:HB2	6:1F:116:HIS:CD2	2.53	0.43
6:1F:419:ILE:HG12	6:1F:426:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:316:ALA:HA	7:1G:342:SER:HB3	1.99	0.43
7:1G:395:ILE:O	7:1G:399:TRP:HB3	2.18	0.43
11:1K:75:LEU:CD2	11:1K:75:LEU:N	2.81	0.43
12:1L:40:VAL:HG11	12:1L:97:THR:HG23	2.01	0.43
12:1L:545:SER:O	12:1L:550:SER:N	2.50	0.43
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.18	0.43
13:1M:299:VAL:HG12	13:1M:303:ILE:HD11	2.01	0.43
14:1N:26:TRP:HB3	14:1N:74:ILE:HD12	2.00	0.43
14:1N:154:MET:HE3	14:1N:191:THR:CG2	2.46	0.43
14:1N:174:GLN:O	14:1N:178:ILE:HD12	2.18	0.43
16:1P:133:SER:O	16:1P:167:LYS:HA	2.17	0.43
25:1Z:44:LEU:N	25:1Z:44:LEU:HD23	2.34	0.43
31:1f:49:ARG:N	31:1f:52:GLU:OE1	2.50	0.43
37:1l:132:GLN:HB3	37:1l:155:HIS:CE1	2.53	0.43
39:1n:30:CYS:O	39:1n:31:VAL:HG12	2.18	0.43
41:1p:155:LEU:HD23	41:1p:155:LEU:HA	1.81	0.43
3:1C:150:ARG:NH1	3:1C:155:TYR:HA	2.34	0.43
4:1D:37:ASP:OD1	14:1N:51:ARG:NE	2.50	0.43
4:1D:90:LEU:HD12	4:1D:90:LEU:H	1.84	0.43
4:1D:318:MET:HE2	4:1D:318:MET:HB2	1.80	0.43
4:1D:374:PHE:C	4:1D:374:PHE:CD2	2.97	0.43
6:1F:66:ARG:H	6:1F:68:ARG:NH1	2.16	0.43
6:1F:157:TYR:CE1	6:1F:162:ILE:HG23	2.54	0.43
6:1F:187:GLY:HA3	48:1F:501:FMN:N5	2.34	0.43
6:1F:206:LYS:HB3	6:1F:209:PHE:CD1	2.53	0.43
7:1G:158:ARG:HB3	7:1G:202:ILE:HD11	2.00	0.43
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.99	0.43
8:1H:150:LEU:HG	8:1H:185:TRP:CZ3	2.54	0.43
8:1H:153:VAL:HG11	8:1H:242:PHE:CZ	2.54	0.43
12:1L:560:THR:HA	12:1L:564:LYS:HB2	2.01	0.43
13:1M:458:LEU:HD23	13:1M:458:LEU:HA	1.80	0.43
15:1O:14:THR:HA	15:1O:17:LYS:HE2	1.99	0.43
16:1P:81:ILE:HG21	16:1P:117:ILE:HG22	2.00	0.43
16:1P:237:LEU:HD13	16:1P:239:PHE:H	1.83	0.43
20:1T:14:ARG:NH2	20:1T:58:PHE:HA	2.33	0.43
23:1X:43:MET:HE3	25:1Z:73:PRO:HA	2.01	0.43
23:1X:101:LYS:HB2	23:1X:101:LYS:HE2	1.61	0.43
24:1Y:47:SER:OG	24:1Y:48:PHE:N	2.51	0.43
33:1h:114:MET:HE3	33:1h:120:GLY:CA	2.47	0.43
34:1i:102:ARG:HD3	34:1i:104:PHE:CZ	2.53	0.43
35:1j:60:THR:O	35:1j:64:LEU:HD23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:46:ARG:HH12	39:1n:47:PHE:HD1	1.67	0.43
41:1p:7:ASP:OD1	41:1p:7:ASP:N	2.51	0.43
2:1B:30:VAL:HG22	2:1B:173:LEU:HB3	1.99	0.43
2:1B:141:PRO:HB3	16:1P:57:MET:O	2.18	0.43
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.37	0.43
4:1D:116:GLN:OE1	4:1D:138:ARG:HB3	2.17	0.43
4:1D:342:MET:HG3	7:1G:98:LEU:HG	2.01	0.43
5:1E:152:PRO:O	5:1E:164:LEU:HB2	2.18	0.43
7:1G:56:LEU:HD11	7:1G:65:VAL:HG23	2.01	0.43
7:1G:418:ARG:HH22	44:1s:75:HIS:CE1	2.36	0.43
7:1G:615:THR:O	7:1G:619:VAL:HG23	2.19	0.43
7:1G:632:ARG:HH12	19:1S:59:ASP:CG	2.25	0.43
10:1J:64:MET:O	10:1J:68:PHE:HD2	2.02	0.43
10:1J:79:TYR:HD1	10:1J:79:TYR:C	2.26	0.43
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	2.01	0.43
10:1J:160:SER:O	10:1J:164:GLY:N	2.49	0.43
12:1L:279:CYS:O	12:1L:283:ILE:HG22	2.18	0.43
12:1L:383:MET:SD	12:1L:384:PRO:HD2	2.58	0.43
12:1L:573:MET:HB2	14:1N:167:TRP:NE1	2.33	0.43
14:1N:76:ILE:HG22	14:1N:94:ALA:HB2	2.01	0.43
14:1N:222:SER:HB2	14:1N:233:THR:HG21	2.01	0.43
20:1T:54:MET:HE2	20:1T:54:MET:CA	2.48	0.43
23:1X:31:TYR:HB2	23:1X:69:PHE:CE2	2.54	0.43
31:1f:38:ARG:O	31:1f:40:LYS:NZ	2.51	0.43
32:1g:27:GLN:N	32:1g:27:GLN:OE1	2.52	0.43
40:1o:51:MET:HB3	40:1o:54:GLN:HG3	2.00	0.43
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	2.00	0.43
41:1p:88:GLU:CD	41:1p:151:ALA:H	2.26	0.43
43:1r:3:ALA:O	43:1r:8:GLN:NE2	2.51	0.43
1:1A:65:PHE:CD2	8:1H:290:TRP:HZ3	2.36	0.43
1:1A:66:ASP:O	1:1A:69:ILE:HG12	2.18	0.43
2:1B:120:ALA:O	2:1B:136:CYS:N	2.52	0.43
2:1B:125:TYR:HD2	9:1I:117:ILE:CG1	2.23	0.43
4:1D:300:ARG:NH1	4:1D:420:THR:OG1	2.45	0.43
5:1E:184:PRO:HD2	5:1E:184:PRO:O	2.18	0.43
7:1G:38:PRO:HG2	7:1G:90:ARG:HD3	2.01	0.43
7:1G:391:PHE:CD1	7:1G:391:PHE:C	2.96	0.43
7:1G:667:THR:HG23	7:1G:669:LYS:HG2	2.01	0.43
9:1I:43:ARG:C	26:1a:1:MET:SD	3.02	0.43
13:1M:341:THR:HG21	38:1m:64:LEU:HD11	2.01	0.43
14:1N:79:LEU:O	30:1e:67:LEU:HD11	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:35:HIS:HB2	20:1T:38:LYS:HZ2	1.82	0.43
21:1V:35:GLY:C	21:1V:44:ARG:HH12	2.27	0.43
39:1n:150:THR:HG22	39:1n:152:ALA:H	1.84	0.43
2:1B:137:ASP:OD2	9:1I:144:HIS:ND1	2.46	0.43
3:1C:52:ILE:HG12	3:1C:109:THR:HG22	2.00	0.43
4:1D:165:THR:HB	4:1D:169:TRP:CZ2	2.53	0.43
5:1E:105:THR:HG21	5:1E:144:CYS:N	2.34	0.43
5:1E:116:ILE:HD13	5:1E:152:PRO:HB3	2.01	0.43
6:1F:298:ILE:HB	6:1F:335:ILE:CG2	2.48	0.43
7:1G:10:GLU:OE1	7:1G:17:SER:HB2	2.19	0.43
7:1G:501:ALA:HB2	7:1G:574:VAL:HG22	2.01	0.43
8:1H:267:THR:O	8:1H:271:LEU:HG	2.18	0.43
12:1L:129:MET:O	12:1L:133:THR:OG1	2.18	0.43
12:1L:483:PRO:HD2	12:1L:486:MET:SD	2.59	0.43
12:1L:539:TYR:HE2	38:1m:9:ARG:HH21	1.66	0.43
14:1N:249:LEU:HD11	14:1N:294:MET:HE3	2.00	0.43
15:1O:161:CYS:SG	15:1O:162:GLU:N	2.91	0.43
15:1O:171:TYR:CE2	15:1O:206:TYR:HD1	2.36	0.43
15:1O:212:PRO:O	15:1O:215:SER:OG	2.37	0.43
16:1P:150:ALA:O	16:1P:154:LYS:NZ	2.50	0.43
16:1P:237:LEU:HD13	16:1P:238:LEU:N	2.34	0.43
18:1R:54:SER:OG	18:1R:56:VAL:O	2.37	0.43
19:1S:64:LEU:O	19:1S:75:ASN:HB2	2.19	0.43
24:1Y:69:PHE:HE2	45:1Y:202:3PE:H3F1	1.83	0.43
31:1f:14:ILE:O	31:1f:18:VAL:HG22	2.19	0.43
34:1i:105:PRO:HD3	40:1o:44:GLU:CD	2.44	0.43
39:1n:50:HIS:NE2	58:1n:201:EHZ:O1	2.52	0.43
5:1E:37:ASN:OD1	5:1E:38:TYR:CE1	2.72	0.43
6:1F:394:GLU:CD	43:1r:50:ASN:H	2.25	0.43
7:1G:208:LEU:HD11	46:1G:802:SF4:S4	2.59	0.43
7:1G:259:ASN:HB2	7:1G:262:TRP:O	2.19	0.43
7:1G:383:ASN:HD21	7:1G:413:VAL:HG11	1.84	0.43
7:1G:640:ASN:C	7:1G:641:TYR:CG	2.97	0.43
8:1H:59:GLU:HA	8:1H:60:PRO:HD3	1.89	0.43
8:1H:106:LEU:HD22	10:1J:58:LEU:HD21	2.01	0.43
8:1H:273:ILE:HD12	8:1H:274:ARG:N	2.34	0.43
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.19	0.43
12:1L:254:VAL:HG21	12:1L:329:ILE:HG23	2.01	0.43
12:1L:538:THR:O	12:1L:542:LEU:HB2	2.19	0.43
45:1L:702:3PE:H3A2	45:1L:702:3PE:H2G1	2.00	0.43
13:1M:53:SER:OG	13:1M:54:LEU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:195:THR:HG23	15:1O:198:TYR:HB2	2.01	0.43
19:1S:35:PHE:CD1	19:1S:36:ILE:HG23	2.54	0.43
20:1T:6:LEU:HD11	20:1T:14:ARG:HH12	1.83	0.43
21:1V:65:LYS:HB2	21:1V:66:LYS:NZ	2.34	0.43
24:1Y:68:ILE:HD11	24:1Y:95:ALA:HB1	2.00	0.43
29:1d:36:PHE:CD1	29:1d:36:PHE:C	2.97	0.43
33:1h:24:LEU:O	33:1h:28:TYR:HB3	2.19	0.43
36:1k:12:LYS:HE3	36:1k:12:LYS:HB3	1.80	0.43
36:1k:48:GLU:HG3	36:1k:51:ARG:HD2	2.01	0.43
1:1A:104:TYR:CE1	1:1A:108:GLN:HG3	2.54	0.42
1:1A:112:GLU:OE1	1:1A:112:GLU:C	2.62	0.42
2:1B:81:ARG:O	2:1B:81:ARG:HG2	2.18	0.42
3:1C:29:VAL:HG13	3:1C:63:PHE:HE2	1.84	0.42
3:1C:193:GLU:OE2	17:1Q:75:THR:CG2	2.61	0.42
5:1E:177:LYS:HD3	5:1E:177:LYS:HA	1.74	0.42
7:1G:189:LYS:NZ	7:1G:190:MET:H	2.17	0.42
7:1G:331:LEU:HD23	7:1G:331:LEU:HA	1.79	0.42
8:1H:233:MET:O	8:1H:237:PHE:N	2.43	0.42
8:1H:284:GLN:H	8:1H:284:GLN:HG3	1.64	0.42
9:1I:66:ALA:HB1	9:1I:158:GLY:HA2	2.01	0.42
10:1J:133:SER:HB2	10:1J:138:GLU:OE1	2.19	0.42
10:1J:150:GLY:HA2	30:1e:16:TRP:CH2	2.54	0.42
12:1L:267:MET:HE2	12:1L:267:MET:HB2	1.75	0.42
13:1M:36:LEU:HD12	32:1g:68:ILE:HG22	2.01	0.42
52:1M:501:PGT:H202	52:1M:501:PGT:H231	1.93	0.42
15:1O:79:LEU:HA	15:1O:96:LEU:HD11	2.01	0.42
17:1Q:70:MET:HG2	17:1Q:70:MET:O	2.18	0.42
22:1W:108:HIS:HB3	22:1W:111:GLU:OE1	2.19	0.42
32:1g:23:THR:C	32:1g:25:ARG:N	2.76	0.42
34:1i:21:TRP:CD1	39:1n:171:THR:HA	2.54	0.42
34:1i:93:PRO:HB3	41:1p:4:TRP:CD1	2.54	0.42
37:1l:5:THR:O	37:1l:8:MET:SD	2.77	0.42
40:1o:61:TYR:CE2	40:1o:85:ASP:HB3	2.54	0.42
1:1A:104:TYR:HE1	1:1A:108:GLN:HG3	1.83	0.42
2:1B:57:VAL:O	2:1B:61:HIS:HB2	2.19	0.42
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.19	0.42
5:1E:60:TRP:CE3	5:1E:94:PRO:CD	2.86	0.42
5:1E:78:MET:O	5:1E:82:GLU:HG2	2.19	0.42
5:1E:109:MET:HE1	6:1F:345:LYS:HZ2	1.84	0.42
6:1F:316:LEU:HG	6:1F:317:MET:H	1.84	0.42
6:1F:413:TRP:CD1	6:1F:413:TRP:H	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:44:GLU:OE1	7:1G:44:GLU:N	2.33	0.42
7:1G:192:MET:SD	7:1G:192:MET:N	2.78	0.42
7:1G:227:SER:H	7:1G:253:ARG:HH12	1.65	0.42
7:1G:474:ALA:C	7:1G:642:PHE:HZ	2.28	0.42
8:1H:157:ASN:ND2	8:1H:159:SER:H	2.16	0.42
10:1J:67:VAL:HA	10:1J:70:TYR:HB3	2.01	0.42
12:1L:101:MET:HG3	12:1L:118:PHE:HE2	1.84	0.42
12:1L:545:SER:HA	12:1L:549:ALA:HB3	2.00	0.42
13:1M:96:ILE:H	13:1M:96:ILE:HG12	1.66	0.42
14:1N:73:ALA:HB1	14:1N:98:MET:HB2	2.00	0.42
20:1T:43:ASP:HB2	58:1W:201:EHZ:P1	2.58	0.42
21:1V:2:GLY:HA3	21:1V:65:LYS:NZ	2.33	0.42
21:1V:51:THR:H	21:1V:51:THR:HG1	1.62	0.42
22:1W:127:ASP:OD1	22:1W:127:ASP:C	2.63	0.42
27:1b:10:ASN:O	27:1b:14:LYS:HG2	2.19	0.42
28:1c:1:LYS:HE3	28:1c:3:TYR:H	1.85	0.42
28:1c:43:LYS:HB3	28:1c:49:GLU:OE1	2.19	0.42
40:1o:46:ASN:HA	40:1o:55:ARG:NH2	2.34	0.42
40:1o:62:LEU:O	40:1o:62:LEU:HD13	2.19	0.42
42:1q:32:ASP:OD2	42:1q:33:VAL:N	2.51	0.42
3:1C:155:TYR:HB3	22:1W:98:LYS:HG2	2.00	0.42
4:1D:251:LEU:HD23	4:1D:260:LEU:HD11	2.01	0.42
4:1D:334:LYS:O	4:1D:338:MET:N	2.52	0.42
7:1G:230:VAL:HG22	7:1G:230:VAL:O	2.19	0.42
7:1G:381:GLY:HA3	7:1G:457:ALA:HB2	2.00	0.42
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	2.01	0.42
8:1H:173:TRP:HD1	8:1H:243:LEU:HD13	1.84	0.42
10:1J:85:SER:OG	16:1P:325:ARG:NH1	2.52	0.42
12:1L:481:THR:C	12:1L:482:MET:HE2	2.44	0.42
14:1N:320:THR:HG21	15:1O:265:ASN:HA	2.02	0.42
15:1O:145:ARG:NH2	15:1O:147:GLN:OE1	2.41	0.42
16:1P:136:ASN:O	16:1P:146:LEU:HD13	2.19	0.42
18:1R:61:GLY:HA2	18:1R:87:CYS:SG	2.59	0.42
20:1T:8:LEU:HD12	20:1T:88:GLU:CG	2.49	0.42
23:1X:157:LEU:HA	29:1d:88:HIS:HD2	1.84	0.42
32:1g:47:TYR:OH	32:1g:61:VAL:HG11	2.20	0.42
37:1l:94:THR:OG1	37:1l:101:MET:HE1	2.20	0.42
37:1l:158:ILE:H	37:1l:158:ILE:HG13	1.71	0.42
41:1p:88:GLU:O	41:1p:92:ARG:HG3	2.20	0.42
42:1q:51:ASP:O	42:1q:59:HIS:HB2	2.19	0.42
2:1B:69:MET:SD	2:1B:75:VAL:HA	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:136:TRP:NE1	4:1D:277:VAL:HG21	2.34	0.42
4:1D:138:ARG:HG2	4:1D:194:ILE:HG12	2.02	0.42
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.55	0.42
5:1E:132:THR:O	5:1E:135:LYS:CE	2.67	0.42
5:1E:194:GLU:HG2	6:1F:28:ARG:NH2	2.34	0.42
7:1G:81:THR:OG1	7:1G:82:ASN:N	2.53	0.42
7:1G:703:ILE:HD12	7:1G:704:CYS:HB3	2.00	0.42
8:1H:253:GLU:O	8:1H:256:THR:OG1	2.24	0.42
8:1H:253:GLU:OE2	26:1a:25:HIS:NE2	2.53	0.42
9:1I:97:GLU:HB2	9:1I:98:PRO:CD	2.46	0.42
10:1J:79:TYR:C	10:1J:79:TYR:CD1	2.97	0.42
10:1J:169:MET:HE2	10:1J:169:MET:HB3	1.92	0.42
12:1L:90:ILE:O	12:1L:94:LEU:HG	2.20	0.42
12:1L:107:TYR:HD1	12:1L:108:MET:SD	2.42	0.42
12:1L:273:VAL:O	12:1L:277:THR:HG23	2.19	0.42
12:1L:600:THR:O	12:1L:602:PHE:N	2.51	0.42
14:1N:47:ASN:OD1	14:1N:123:SER:HB3	2.19	0.42
14:1N:257:LEU:HD23	14:1N:334:THR:HB	2.01	0.42
15:1O:285:GLY:N	32:1g:26:LEU:HD13	2.33	0.42
18:1R:68:HIS:CG	18:1R:86:TYR:HB3	2.54	0.42
20:1T:58:PHE:CD1	20:1T:80:ILE:HG21	2.53	0.42
22:1W:34:GLU:HA	22:1W:37:ARG:HG3	2.01	0.42
25:1Z:115:ARG:HH12	30:1e:35:PHE:HE2	1.67	0.42
35:1j:45:ASP:CG	35:1j:50:HIS:HB3	2.44	0.42
37:1l:66:HIS:O	37:1l:70:ARG:N	2.53	0.42
37:1l:79:TRP:HD1	37:1l:80:ASP:OD1	2.03	0.42
42:1q:41:GLU:N	42:1q:41:GLU:OE2	2.52	0.42
42:1q:95:ASP:N	43:1r:34:THR:OG1	2.34	0.42
1:1A:54:LYS:C	1:1A:113:TRP:HE1	2.28	0.42
3:1C:129:TRP:CZ3	4:1D:399:LEU:HD22	2.55	0.42
4:1D:242:ILE:HG21	4:1D:413:ASP:CG	2.44	0.42
6:1F:28:ARG:HA	6:1F:28:ARG:HD3	1.86	0.42
6:1F:197:GLU:HA	6:1F:216:PHE:CE1	2.55	0.42
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	2.01	0.42
7:1G:142:ILE:HG22	7:1G:191:PHE:H	1.84	0.42
7:1G:406:VAL:HG21	7:1G:417:TYR:CD1	2.54	0.42
7:1G:661:LEU:HD22	7:1G:661:LEU:H	1.84	0.42
12:1L:380:LEU:HD12	12:1L:380:LEU:HA	1.93	0.42
45:1L:702:3PE:O32	45:1L:702:3PE:H252	2.19	0.42
13:1M:75:LEU:HD13	13:1M:440:HIS:NE2	2.34	0.42
13:1M:154:LEU:HD23	14:1N:287:LEU:HD21	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:204:MET:HG2	13:1M:243:MET:HE1	2.01	0.42
14:1N:88:LYS:NZ	14:1N:148:SER:HB2	2.35	0.42
14:1N:207:ILE:HD13	14:1N:207:ILE:HA	1.91	0.42
14:1N:221:HIS:ND1	14:1N:240:ILE:HG12	2.35	0.42
16:1P:209:ASP:OD2	16:1P:308:THR:HG23	2.19	0.42
18:1R:80:LYS:HE3	18:1R:80:LYS:HB3	1.67	0.42
20:1U:75:GLU:HA	20:1U:78:ASP:HB2	2.01	0.42
29:1d:86:ARG:CD	29:1d:87:ASP:OD1	2.68	0.42
41:1p:136:LYS:HE3	41:1p:136:LYS:HB3	1.73	0.42
2:1B:94:ASN:HB3	3:1C:174:LEU:CG	2.49	0.42
3:1C:125:LYS:H	3:1C:125:LYS:HD3	1.85	0.42
4:1D:165:THR:N	4:1D:166:PRO:HD2	2.35	0.42
4:1D:238:ARG:HD3	8:1H:281:ARG:HB2	2.02	0.42
4:1D:240:VAL:HG12	4:1D:294:TYR:CG	2.55	0.42
6:1F:185:ILE:HG22	6:1F:191:ALA:CB	2.49	0.42
6:1F:402:HIS:O	7:1G:53:ARG:NH1	2.53	0.42
7:1G:278:ARG:HD2	7:1G:549:HIS:CD2	2.54	0.42
8:1H:301:CYS:O	8:1H:305:ILE:HG22	2.20	0.42
9:1I:60:ARG:HG2	9:1I:172:ASP:OD2	2.20	0.42
10:1J:130:THR:OG1	10:1J:131:GLY:N	2.53	0.42
12:1L:17:ILE:O	12:1L:21:MET:HG2	2.19	0.42
12:1L:62:ILE:HG13	41:1p:114:GLN:HG3	2.01	0.42
12:1L:121:LEU:HD23	12:1L:121:LEU:HA	1.91	0.42
12:1L:482:MET:HE2	12:1L:482:MET:N	2.35	0.42
13:1M:12:LEU:HB3	13:1M:13:PRO:HD3	2.01	0.42
13:1M:346:ARG:NH1	13:1M:346:ARG:HB2	2.35	0.42
16:1P:173:GLY:N	16:1P:176:ASP:HB3	2.30	0.42
16:1P:198:LYS:HD3	16:1P:237:LEU:HD11	2.01	0.42
16:1P:203:GLN:HG2	16:1P:234:ASN:C	2.44	0.42
17:1Q:30:ILE:HD11	17:1Q:99:ASN:O	2.19	0.42
17:1Q:104:ASP:OD1	17:1Q:105:VAL:N	2.52	0.42
18:1R:16:GLN:HE22	18:1R:33:LYS:NZ	2.18	0.42
18:1R:93:GLN:HG2	18:1R:94:PRO:HD2	2.01	0.42
27:1b:79:TRP:CD1	27:1b:79:TRP:H	2.37	0.42
31:1f:22:PHE:CD1	31:1f:26:LEU:HD21	2.55	0.42
32:1g:77:VAL:HA	32:1g:80:LEU:HD23	2.01	0.42
36:1k:87:LEU:HD12	36:1k:88:GLU:N	2.35	0.42
40:1o:71:ASP:OD1	40:1o:72:SER:N	2.52	0.42
3:1C:70:ALA:HB1	3:1C:72:PHE:HD1	1.84	0.42
3:1C:85:THR:OG1	17:1Q:91:ASP:OD2	2.32	0.42
3:1C:125:LYS:HE2	3:1C:125:LYS:HB2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:141:PHE:CE2	3:1C:148:LEU:HG	2.54	0.42
3:1C:183:VAL:O	3:1C:183:VAL:HG13	2.20	0.42
4:1D:349:PHE:HZ	7:1G:218:ARG:HH21	1.68	0.42
5:1E:38:TYR:CD1	5:1E:38:TYR:N	2.88	0.42
9:1I:69:ARG:HD2	42:1q:108:TYR:CD1	2.54	0.42
11:1K:34:GLU:CD	11:1K:34:GLU:H	2.27	0.42
11:1K:46:LEU:HA	11:1K:46:LEU:HD13	1.82	0.42
12:1L:81:LYS:C	12:1L:82:MET:HE2	2.43	0.42
12:1L:83:ASP:OD1	12:1L:84:TYR:N	2.53	0.42
12:1L:149:ILE:HD11	13:1M:364:LEU:HD11	2.01	0.42
13:1M:262:LEU:HD12	13:1M:262:LEU:HA	1.89	0.42
14:1N:342:ALA:CA	29:1d:79:GLN:OE1	2.60	0.42
17:1Q:124:TRP:CH2	44:1s:68:SER:HA	2.54	0.42
21:1V:21:GLU:H	21:1V:21:GLU:CD	2.26	0.42
21:1V:111:TRP:HA	21:1V:111:TRP:CE3	2.54	0.42
25:1Z:111:PHE:HB2	25:1Z:113:THR:HG22	2.02	0.42
26:1a:54:ILE:O	26:1a:64:LYS:NZ	2.49	0.42
33:1h:89:LYS:HB3	33:1h:89:LYS:HE3	1.81	0.42
34:1i:44:GLN:HA	34:1i:47:ASN:HD21	1.84	0.42
39:1n:99:PRO:HB2	39:1n:101:TRP:CD1	2.54	0.42
40:1o:92:LEU:O	40:1o:96:LYS:HD3	2.20	0.42
42:1q:97:PRO:HG2	42:1q:99:THR:OG1	2.19	0.42
4:1D:224:GLU:HG2	9:1I:36:MET:SD	2.60	0.42
5:1E:149:VAL:HB	6:1F:257:ASN:HD21	1.85	0.42
7:1G:10:GLU:HA	7:1G:19:MET:HA	2.01	0.42
7:1G:129:ARG:H	7:1G:129:ARG:HG2	1.59	0.42
7:1G:332:LYS:HE3	7:1G:332:LYS:HB2	1.72	0.42
7:1G:534:ARG:NH2	7:1G:556:MET:O	2.52	0.42
8:1H:26:LYS:NZ	26:1a:4:GLU:HB3	2.35	0.42
8:1H:89:LEU:HA	8:1H:90:PRO:HD3	1.90	0.42
9:1I:99:ARG:HB3	9:1I:103:SER:HB2	2.01	0.42
10:1J:119:PHE:CD1	10:1J:119:PHE:C	2.97	0.42
10:1J:173:ARG:NH1	15:1O:254:ARG:HH21	2.17	0.42
11:1K:12:PHE:CG	14:1N:72:MET:CE	3.02	0.42
12:1L:42:TYR:O	12:1L:46:LEU:HD22	2.20	0.42
12:1L:413:LEU:HD12	12:1L:493:VAL:HG11	2.00	0.42
15:1O:65:ASP:HB2	28:1c:2:PHE:CD1	2.54	0.42
15:1O:174:VAL:HG13	15:1O:178:GLU:HB2	2.00	0.42
15:1O:275:ILE:O	15:1O:277:VAL:N	2.49	0.42
15:1O:303:LYS:O	15:1O:303:LYS:NZ	2.48	0.42
21:1V:34:LEU:HD23	21:1V:34:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:1Y:201:3PE:H2	45:1Y:201:3PE:H221	1.61	0.42
28:1c:41:GLU:OE2	28:1c:44:ARG:CZ	2.68	0.42
28:1c:45:ARG:HH12	29:1d:19:ARG:HB2	1.85	0.42
30:1e:64:GLU:O	30:1e:68:ARG:N	2.49	0.42
33:1h:39:GLY:O	33:1h:43:VAL:HG23	2.20	0.42
33:1h:91:MET:HB2	41:1p:85:PHE:CD2	2.54	0.42
34:1i:83:TYR:CE1	41:1p:48:ARG:HD3	2.53	0.42
37:1l:156:TYR:HB2	40:1o:33:ARG:NH2	2.34	0.42
39:1n:139:LEU:HD23	39:1n:139:LEU:HA	1.81	0.42
39:1n:176:ARG:HA	39:1n:176:ARG:HD2	1.73	0.42
41:1p:158:GLN:O	41:1p:162:MET:SD	2.77	0.42
2:1B:48:MET:O	2:1B:86:MET:HA	2.20	0.42
3:1C:151:ILE:HD11	4:1D:80:ILE:HG13	2.01	0.42
5:1E:34:ILE:HD11	5:1E:50:VAL:CG1	2.50	0.42
6:1F:121:GLY:HA3	6:1F:228:VAL:O	2.19	0.42
7:1G:283:MET:HE2	7:1G:283:MET:CA	2.32	0.42
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.55	0.42
12:1L:528:TYR:CD1	37:1l:101:MET:HG2	2.55	0.42
13:1M:243:MET:HB2	13:1M:243:MET:HE2	1.81	0.42
14:1N:245:MET:HA	14:1N:248:LEU:HD12	2.01	0.42
15:1O:86:PRO:HB2	15:1O:143:PHE:CD1	2.55	0.42
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	2.01	0.42
19:1S:15:LEU:HD11	19:1S:18:ILE:HG22	2.02	0.42
20:1U:14:ARG:HH11	20:1U:58:PHE:HE1	1.65	0.42
23:1X:18:LYS:HD2	26:1a:54:ILE:HD11	2.02	0.42
24:1Y:127:GLY:HA2	24:1Y:132:TRP:HB2	2.02	0.42
29:1d:17:GLU:CD	29:1d:17:GLU:N	2.77	0.42
29:1d:44:ILE:O	29:1d:47:ALA:N	2.52	0.42
37:1l:80:ASP:O	37:1l:83:MET:HB2	2.19	0.42
43:1r:57:ASP:OD2	43:1r:60:ARG:HB3	2.19	0.42
4:1D:85:ARG:O	4:1D:87:THR:N	2.51	0.42
4:1D:124:LYS:HB2	4:1D:124:LYS:HE3	1.62	0.42
5:1E:194:GLU:OE2	6:1F:28:ARG:NH1	2.50	0.42
6:1F:185:ILE:HD11	6:1F:357:GLU:O	2.20	0.42
6:1F:364:PRO:CB	6:1F:399:ILE:HG22	2.49	0.42
7:1G:105:CYS:HB2	7:1G:106:PRO:HD3	2.01	0.42
7:1G:201:ASP:OD2	7:1G:268:ARG:NH1	2.53	0.42
7:1G:283:MET:CB	7:1G:560:ILE:HB	2.49	0.42
7:1G:622:ARG:HA	7:1G:625:GLU:HG3	2.02	0.42
9:1I:82:LEU:HD23	9:1I:82:LEU:HA	1.91	0.42
12:1L:65:ASN:OD1	12:1L:65:ASN:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:203:MET:HE2	12:1L:203:MET:HA	2.01	0.42
12:1L:390:TYR:HD2	12:1L:465:GLY:HA3	1.84	0.42
13:1M:70:THR:HA	13:1M:103:GLN:NE2	2.35	0.42
13:1M:175:ASN:CG	33:1h:97:GLU:HG2	2.45	0.42
13:1M:459:TYR:HB3	32:1g:84:ARG:HE	1.85	0.42
15:1O:78:SER:H	15:1O:92:ASN:ND2	2.10	0.42
15:1O:171:TYR:O	15:1O:223:TYR:HB2	2.20	0.42
15:1O:214:MET:HE3	15:1O:214:MET:HB2	1.90	0.42
16:1P:110:PHE:CZ	16:1P:149:LYS:HD3	2.54	0.42
16:1P:271:GLU:HA	16:1P:277:PRO:HB3	2.00	0.42
17:1Q:35:VAL:HG22	17:1Q:59:PHE:CD1	2.55	0.42
22:1W:105:ARG:HE	22:1W:105:ARG:HB2	1.67	0.42
27:1b:77:LEU:HA	27:1b:79:TRP:NE1	2.35	0.42
32:1g:77:VAL:HA	32:1g:80:LEU:CD2	2.50	0.42
32:1g:100:ARG:CG	32:1g:105:LEU:HD22	2.50	0.42
33:1h:94:LEU:HD12	33:1h:94:LEU:HA	1.88	0.42
35:1j:67:LEU:HD22	35:1j:68:PRO:HD3	2.01	0.42
39:1n:120:LYS:HA	39:1n:123:GLN:HG2	2.02	0.42
39:1n:158:LYS:HE2	39:1n:158:LYS:HB3	1.72	0.42
40:1o:21:MET:HB3	40:1o:104:GLU:OE2	2.19	0.42
41:1p:11:GLU:OE1	41:1p:115:ARG:NE	2.53	0.42
3:1C:129:TRP:HE1	3:1C:132:ARG:NH1	2.18	0.41
4:1D:149:ASN:HD21	4:1D:371:LYS:HE3	1.84	0.41
4:1D:250:ALA:O	4:1D:255:PHE:HB2	2.20	0.41
5:1E:190:ARG:NH2	6:1F:265:PRO:HG2	2.35	0.41
6:1F:132:ARG:O	6:1F:173:PHE:HA	2.20	0.41
6:1F:378:ARG:NH2	7:1G:131:LEU:HD11	2.34	0.41
6:1F:392:LEU:HD13	6:1F:419:ILE:HD11	2.02	0.41
7:1G:347:GLU:HB2	7:1G:499:GLN:OE1	2.19	0.41
8:1H:51:ASP:N	8:1H:51:ASP:OD1	2.53	0.41
9:1I:78:ILE:HD12	18:1R:86:TYR:HD2	1.85	0.41
9:1I:96:ALA:C	9:1I:97:GLU:OE1	2.63	0.41
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.34	0.41
12:1L:500:LEU:O	12:1L:504:LEU:HD12	2.20	0.41
13:1M:189:SER:O	13:1M:193:ILE:HG13	2.20	0.41
15:1O:169:VAL:HG22	15:1O:220:VAL:HA	2.02	0.41
16:1P:138:ASP:H	16:1P:146:LEU:HB3	1.84	0.41
19:1S:63:LYS:HZ2	19:1S:75:ASN:ND2	2.18	0.41
20:1T:35:HIS:HE1	20:1T:37:MET:HG2	1.84	0.41
21:1V:40:ASN:OD1	21:1V:40:ASN:N	2.50	0.41
25:1Z:7:LYS:HZ3	43:1r:37:PRO:C	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:24:ASN:ND2	25:1Z:24:ASN:C	2.76	0.41
27:1b:44:ILE:HG22	27:1b:79:TRP:HZ3	1.85	0.41
29:1d:102:PRO:HD2	29:1d:104:LYS:NZ	2.34	0.41
29:1d:116:PHE:CD2	29:1d:116:PHE:C	2.98	0.41
32:1g:26:LEU:CD1	32:1g:28:GLU:HB2	2.49	0.41
40:1o:60:HIS:O	40:1o:63:ILE:HG22	2.20	0.41
40:1o:114:ARG:NE	40:1o:117:ARG:HH22	2.16	0.41
42:1q:14:VAL:HA	42:1q:23:TYR:CD1	2.55	0.41
44:1s:71:GLN:HB2	44:1s:75:HIS:CD2	2.54	0.41
4:1D:100:LEU:HB3	4:1D:101:PRO:HD3	2.01	0.41
4:1D:287:ILE:HD12	9:1I:2:TYR:HB2	2.01	0.41
5:1E:153:MET:CE	5:1E:154:VAL:C	2.93	0.41
6:1F:68:ARG:NE	6:1F:254:LYS:HB2	2.28	0.41
6:1F:311:VAL:O	6:1F:315:VAL:HG23	2.20	0.41
7:1G:211:LYS:NZ	7:1G:699:GLU:OE2	2.53	0.41
7:1G:272:ASP:O	7:1G:276:ARG:HG2	2.19	0.41
7:1G:285:ARG:HG3	7:1G:558:ASP:O	2.19	0.41
7:1G:594:ARG:NH2	22:1W:122:PHE:O	2.52	0.41
8:1H:92:PRO:HB3	8:1H:247:HIS:HE1	1.85	0.41
8:1H:154:LEU:HD11	8:1H:159:SER:O	2.20	0.41
9:1I:98:PRO:HD3	9:1I:104:ARG:NH2	2.34	0.41
10:1J:9:LEU:HB3	10:1J:43:ILE:HG13	2.03	0.41
12:1L:61:MET:SD	12:1L:63:ILE:HD11	2.60	0.41
12:1L:361:GLY:N	12:1L:431:PHE:O	2.51	0.41
13:1M:457:PRO:HA	32:1g:84:ARG:HH22	1.85	0.41
14:1N:218:LEU:HB2	14:1N:244:MET:CE	2.50	0.41
14:1N:336:VAL:O	14:1N:336:VAL:HG12	2.19	0.41
16:1P:191:VAL:HG11	16:1P:253:PHE:CE1	2.52	0.41
17:1Q:40:PRO:HG3	17:1Q:56:LYS:CD	2.45	0.41
20:1U:70:LEU:HD12	20:1U:70:LEU:HA	1.88	0.41
20:1U:76:ILE:O	20:1U:80:ILE:HG22	2.20	0.41
21:1V:102:LEU:H	21:1V:102:LEU:HD22	1.86	0.41
23:1X:81:PHE:CE2	26:1a:66:LEU:HD23	2.54	0.41
33:1h:119:ASP:OD1	33:1h:119:ASP:N	2.44	0.41
38:1m:38:ILE:O	38:1m:42:LEU:HD12	2.20	0.41
39:1n:38:TYR:CE2	39:1n:42:LEU:HD11	2.55	0.41
40:1o:43:GLN:H	40:1o:43:GLN:CD	2.27	0.41
41:1p:30:THR:O	41:1p:34:LYS:HG2	2.21	0.41
41:1p:91:TRP:HZ2	41:1p:154:CYS:HG	1.64	0.41
42:1q:72:ASP:OD1	42:1q:72:ASP:N	2.53	0.41
1:1A:71:LEU:HB3	1:1A:94:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:144:ILE:HG22	9:1I:142:GLU:CG	2.50	0.41
3:1C:138:PHE:HE1	4:1D:388:ARG:HH22	1.69	0.41
3:1C:203:TRP:HZ3	7:1G:36:GLN:HG2	1.86	0.41
4:1D:100:LEU:HD11	4:1D:195:ARG:HA	2.03	0.41
6:1F:267:THR:O	6:1F:267:THR:OG1	2.32	0.41
6:1F:291:TRP:CH2	6:1F:294:LEU:HD13	2.56	0.41
6:1F:376:MET:O	6:1F:380:VAL:HG23	2.21	0.41
7:1G:25:THR:HG22	7:1G:28:GLN:HB2	2.01	0.41
8:1H:264:LEU:HD11	26:1a:13:ALA:HA	2.01	0.41
9:1I:2:TYR:CE1	43:1r:105:LEU:HD22	2.55	0.41
9:1I:74:GLU:OE2	9:1I:99:ARG:NH2	2.53	0.41
10:1J:12:ILE:HG13	10:1J:39:VAL:HG21	2.02	0.41
12:1L:81:LYS:NZ	12:1L:262:ARG:HD3	2.35	0.41
12:1L:378:LEU:HD21	36:1k:66:LEU:HD11	2.01	0.41
16:1P:132:ILE:HG22	16:1P:166:ILE:HB	2.02	0.41
17:1Q:127:ARG:CG	44:1s:70:ARG:CZ	2.97	0.41
23:1X:94:GLN:HE22	26:1a:37:ARG:HD3	1.85	0.41
24:1Y:85:ASP:HB3	24:1Y:88:ASN:ND2	2.35	0.41
43:1r:40:LEU:H	43:1r:40:LEU:HG	1.68	0.41
1:1A:83:ASN:ND2	50:1J:201:PC1:H122	2.36	0.41
3:1C:136:ASP:CG	3:1C:150:ARG:HA	2.45	0.41
3:1C:192:GLN:NE2	17:1Q:72:TRP:CE3	2.88	0.41
4:1D:110:SER:OG	4:1D:145:THR:HB	2.20	0.41
4:1D:160:ASP:O	8:1H:279:ARG:NH1	2.51	0.41
7:1G:200:ILE:HD13	7:1G:210:SER:HB3	2.03	0.41
7:1G:230:VAL:CG2	7:1G:322:LEU:HG	2.51	0.41
7:1G:327:ALA:HB1	7:1G:525:LEU:HD21	2.02	0.41
7:1G:364:LEU:CB	7:1G:576:THR:HG22	2.51	0.41
7:1G:409:ILE:HD12	7:1G:409:ILE:O	2.20	0.41
7:1G:524:LEU:HB2	7:1G:545:TYR:HA	2.03	0.41
7:1G:688:VAL:HA	7:1G:691:VAL:HG22	2.02	0.41
8:1H:235:ASN:ND2	8:1H:266:LEU:HB3	2.35	0.41
9:1I:18:THR:HG21	25:1Z:33:TYR:CD1	2.55	0.41
12:1L:49:VAL:CG1	12:1L:50:PRO:HD3	2.50	0.41
13:1M:88:THR:HG23	13:1M:91:ARG:H	1.84	0.41
13:1M:374:ASN:O	13:1M:378:GLU:HG3	2.20	0.41
16:1P:148:SER:HA	16:1P:151:VAL:HB	2.03	0.41
20:1U:12:LYS:O	20:1U:16:LEU:HG	2.20	0.41
22:1W:43:VAL:N	22:1W:44:PRO:HD2	2.36	0.41
26:1a:4:GLU:O	26:1a:7:PRO:HD2	2.20	0.41
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:89:SER:O	39:1n:89:SER:OG	2.32	0.41
2:1B:150:PRO:HG3	4:1D:189:MET:SD	2.61	0.41
3:1C:40:VAL:HG23	3:1C:50:ILE:HD13	2.03	0.41
4:1D:169:TRP:HB2	4:1D:170:MET:HE3	2.02	0.41
6:1F:194:GLU:CD	6:1F:204:ARG:HE	2.29	0.41
6:1F:399:ILE:HG23	7:1G:96:PHE:CZ	2.56	0.41
7:1G:356:THR:OG1	7:1G:503:LEU:O	2.38	0.41
8:1H:85:MET:HG2	8:1H:233:MET:HE2	2.02	0.41
10:1J:59:ILE:CD1	11:1K:64:LEU:HD23	2.50	0.41
11:1K:58:MET:H	11:1K:58:MET:HG2	1.53	0.41
11:1K:76:SER:O	11:1K:79:VAL:HG12	2.21	0.41
12:1L:84:TYR:CD2	12:1L:475:MET:HE1	2.55	0.41
12:1L:292:ALA:HB2	12:1L:304:PHE:HB3	2.03	0.41
12:1L:508:THR:O	39:1n:35:LYS:HD2	2.20	0.41
14:1N:128:LEU:O	14:1N:132:THR:HG22	2.21	0.41
14:1N:154:MET:HE2	14:1N:154:MET:HB2	1.81	0.41
14:1N:163:LEU:O	14:1N:167:TRP:HB2	2.21	0.41
14:1N:217:MET:HG3	14:1N:326:LEU:HD22	2.03	0.41
15:1O:135:LEU:HD21	15:1O:149:VAL:HA	2.03	0.41
15:1O:138:MET:HB3	15:1O:143:PHE:HB2	2.03	0.41
16:1P:107:GLU:OE1	16:1P:108:ASP:N	2.54	0.41
16:1P:200:THR:HB	16:1P:238:LEU:CG	2.46	0.41
16:1P:289:MET:HE2	16:1P:289:MET:HB3	1.72	0.41
19:1S:81:PHE:N	19:1S:81:PHE:CD2	2.88	0.41
20:1U:79:TYR:CZ	20:1U:83:LYS:HE3	2.55	0.41
31:1f:2:ASN:O	31:1f:5:GLN:N	2.53	0.41
31:1f:22:PHE:CD1	31:1f:22:PHE:C	2.96	0.41
33:1h:94:LEU:HG	41:1p:81:ILE:HD12	2.01	0.41
38:1m:120:LEU:HD12	38:1m:120:LEU:HA	1.81	0.41
44:1s:70:ARG:HB3	44:1s:75:HIS:CB	2.49	0.41
3:1C:25:PHE:CE1	43:1r:96:PRO:HD3	2.56	0.41
3:1C:79:THR:HB	4:1D:390:LYS:HG2	2.02	0.41
4:1D:112:MET:HA	4:1D:115:GLU:OE1	2.20	0.41
5:1E:146:GLY:HA3	6:1F:142:PHE:HE1	1.85	0.41
5:1E:196:ALA:HB3	6:1F:264:HIS:ND1	2.36	0.41
6:1F:66:ARG:HG2	6:1F:249:ARG:HH21	1.85	0.41
6:1F:153:ILE:HG23	6:1F:175:VAL:CG1	2.51	0.41
6:1F:194:GLU:OE2	17:1Q:133:LYS:HE2	2.20	0.41
7:1G:71:MET:HE2	7:1G:71:MET:HA	2.01	0.41
7:1G:496:ILE:HG22	7:1G:499:GLN:N	2.34	0.41
8:1H:103:LEU:HD21	10:1J:51:PHE:CE1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1I:204:PC1:H12	25:1Z:29:GLY:HA3	2.02	0.41
12:1L:381:THR:HG21	12:1L:498:PHE:CZ	2.56	0.41
12:1L:385:TYR:HA	12:1L:390:TYR:HE1	1.84	0.41
13:1M:389:SER:OG	13:1M:392:THR:HG23	2.20	0.41
14:1N:25:HIS:ND1	14:1N:27:LEU:HB3	2.34	0.41
17:1Q:97:GLU:CD	17:1Q:97:GLU:C	2.89	0.41
19:1S:72:GLN:HA	19:1S:72:GLN:NE2	2.35	0.41
20:1T:8:LEU:HD11	20:1T:87:TYR:C	2.46	0.41
20:1T:35:HIS:CD2	20:1T:38:LYS:CE	3.04	0.41
20:1T:46:ASP:O	20:1T:50:ILE:HG12	2.21	0.41
21:1V:34:LEU:O	21:1V:44:ARG:NH1	2.54	0.41
22:1W:58:GLN:O	22:1W:62:LYS:HG2	2.21	0.41
24:1Y:72:THR:HA	24:1Y:75:ILE:HG22	2.02	0.41
25:1Z:45:PHE:C	25:1Z:45:PHE:CD1	2.98	0.41
30:1e:29:PRO:HB3	33:1h:138:LYS:HE2	2.02	0.41
35:1j:59:TRP:CD2	40:1o:99:LYS:HE3	2.56	0.41
39:1n:135:GLU:OE2	39:1n:166:TRP:HD1	2.04	0.41
41:1p:142:TYR:O	41:1p:145:LEU:HG	2.21	0.41
1:1A:16:LEU:O	1:1A:20:ILE:HG23	2.21	0.41
2:1B:35:ASP:O	2:1B:39:TRP:N	2.54	0.41
2:1B:127:HIS:CD2	2:1B:134:ARG:HG2	2.56	0.41
2:1B:132:VAL:O	2:1B:134:ARG:NH1	2.53	0.41
3:1C:172:VAL:CG2	3:1C:185:ALA:HB1	2.50	0.41
4:1D:204:PRO:HA	9:1I:175:TYR:CZ	2.55	0.41
4:1D:343:GLU:OE1	7:1G:128:SER:HB3	2.21	0.41
5:1E:145:LEU:HD12	5:1E:145:LEU:C	2.46	0.41
7:1G:57:VAL:HG12	7:1G:68:ALA:HB2	2.03	0.41
7:1G:88:LYS:HD3	7:1G:88:LYS:HA	1.94	0.41
7:1G:194:GLU:O	7:1G:265:ASP:N	2.52	0.41
7:1G:228:ILE:CD1	7:1G:581:GLN:O	2.63	0.41
7:1G:274:LEU:HD11	7:1G:677:ILE:HD11	2.02	0.41
7:1G:377:ILE:HD12	7:1G:377:ILE:HA	1.85	0.41
7:1G:385:ARG:HB2	7:1G:392:ASN:ND2	2.36	0.41
7:1G:431:ASP:O	7:1G:436:ASN:N	2.49	0.41
7:1G:433:ALA:O	7:1G:476:ASN:ND2	2.53	0.41
9:1I:14:MET:HE2	27:1b:9:LYS:HE2	2.03	0.41
9:1I:29:GLU:HG2	9:1I:30:LEU:HD23	2.02	0.41
9:1I:46:ALA:HB2	43:1r:25:LEU:HD22	2.02	0.41
10:1J:163:ILE:HG13	14:1N:12:THR:HG21	2.02	0.41
11:1K:1:FME:HG2	11:1K:5:TYR:HD2	1.85	0.41
12:1L:154:LEU:HA	12:1L:154:LEU:HD12	1.79	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:196:TRP:CD1	13:1M:253:LEU:HB3	2.56	0.41
13:1M:240:GLY:O	13:1M:244:MET:HE2	2.20	0.41
13:1M:282:LEU:O	13:1M:286:ILE:HG13	2.21	0.41
13:1M:304:GLN:HA	13:1M:309:PHE:HE1	1.86	0.41
14:1N:308:THR:O	14:1N:311:MET:HB3	2.21	0.41
15:1O:1:LEU:HD12	15:1O:2:GLN:O	2.21	0.41
16:1P:200:THR:OG1	16:1P:287:VAL:O	2.33	0.41
16:1P:242:VAL:HG23	16:1P:253:PHE:CZ	2.56	0.41
19:1S:77:SER:C	19:1S:78:LEU:HD22	2.46	0.41
20:1T:11:ILE:HG22	20:1T:77:VAL:HG22	2.03	0.41
20:1T:35:HIS:HE1	20:1T:37:MET:CG	2.33	0.41
20:1U:48:VAL:HG11	39:1n:16:LEU:HD22	2.02	0.41
21:1V:113:TRP:CG	21:1V:114:PRO:HA	2.56	0.41
23:1X:22:SER:OG	23:1X:89:ASP:HB3	2.21	0.41
23:1X:51:ASP:OD1	23:1X:53:ARG:NE	2.48	0.41
32:1g:82:ASP:CG	32:1g:87:GLU:CD	2.89	0.41
40:1o:80:LYS:HD3	40:1o:80:LYS:HA	1.84	0.41
41:1p:118:GLU:H	41:1p:118:GLU:CD	2.19	0.41
43:1r:100:ILE:HD12	43:1r:100:ILE:HA	1.84	0.41
2:1B:100:LEU:O	2:1B:100:LEU:HD23	2.21	0.41
2:1B:152:THR:HG1	2:1B:154:GLU:CD	2.29	0.41
3:1C:133:GLU:OE1	3:1C:134:ILE:N	2.51	0.41
4:1D:169:TRP:CZ3	8:1H:33:LEU:HG	2.55	0.41
4:1D:291:GLY:O	4:1D:296:ARG:NH1	2.54	0.41
5:1E:6:LEU:O	5:1E:92:ARG:NH1	2.51	0.41
5:1E:48:LEU:HD22	5:1E:83:VAL:HG13	2.03	0.41
5:1E:74:GLN:HB3	44:1s:74:ARG:NH1	2.35	0.41
5:1E:106:THR:O	5:1E:110:LEU:HG	2.21	0.41
6:1F:302:SER:CB	6:1F:350:LEU:HD11	2.51	0.41
7:1G:478:ARG:HG3	7:1G:642:PHE:HE2	1.85	0.41
7:1G:625:GLU:O	19:1S:65:TRP:NE1	2.54	0.41
8:1H:77:LEU:HA	8:1H:80:SER:OG	2.20	0.41
8:1H:85:MET:HE1	8:1H:108:MET:HB3	2.01	0.41
9:1I:1:THR:HG22	43:1r:104:GLU:HB3	2.03	0.41
10:1J:17:PHE:HA	10:1J:20:PHE:HE2	1.85	0.41
12:1L:237:MET:CE	12:1L:244:SER:OG	2.64	0.41
12:1L:434:LYS:HD3	12:1L:434:LYS:HA	1.82	0.41
12:1L:466:PHE:HE1	12:1L:470:ASN:ND2	2.19	0.41
13:1M:22:MET:HB3	13:1M:26:ASN:HD21	1.86	0.41
13:1M:182:TRP:NE1	41:1p:79:LYS:HA	2.34	0.41
13:1M:333:ASN:OD1	13:1M:334:TYR:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:108:LEU:HA	14:1N:161:SER:HB2	2.02	0.41
14:1N:119:THR:HG22	14:1N:131:LEU:HD11	2.03	0.41
14:1N:147:GLN:HB3	33:1h:125:TYR:CZ	2.55	0.41
15:1O:303:LYS:HB3	15:1O:309:ASN:HD21	1.85	0.41
18:1R:14:THR:HG21	42:1q:129:THR:HG22	2.03	0.41
21:1V:35:GLY:O	21:1V:44:ARG:NH1	2.52	0.41
22:1W:85:LYS:HE3	22:1W:85:LYS:HB2	1.93	0.41
22:1W:87:LYS:HA	22:1W:90:LEU:HD22	2.02	0.41
22:1W:87:LYS:HA	22:1W:90:LEU:CD2	2.50	0.41
22:1W:99:GLN:OE1	22:1W:99:GLN:HA	2.20	0.41
27:1b:59:ASP:OD1	27:1b:59:ASP:N	2.52	0.41
31:1f:26:LEU:H	31:1f:26:LEU:HD22	1.85	0.41
50:1f:101:PC1:C2A	50:1f:101:PC1:H381	2.51	0.41
32:1g:26:LEU:HD12	32:1g:27:GLN:N	2.35	0.41
32:1g:66:PHE:HB3	33:1h:29:ILE:HG13	2.02	0.41
32:1g:110:SER:O	41:1p:141:ARG:HG3	2.21	0.41
36:1k:75:ALA:O	36:1k:79:VAL:HG12	2.21	0.41
37:1l:8:MET:HA	37:1l:26:LYS:HE2	2.02	0.41
37:1l:138:LEU:HD12	37:1l:142:ARG:NH2	2.36	0.41
42:1q:86:TRP:CH2	42:1q:99:THR:HG23	2.56	0.41
43:1r:33:ARG:HA	43:1r:33:ARG:HD2	1.85	0.41
1:1A:66:ASP:OD1	1:1A:66:ASP:C	2.64	0.41
2:1B:82:GLN:C	2:1B:82:GLN:HE21	2.17	0.41
2:1B:101:ARG:HH12	2:1B:104:TYR:HB3	1.86	0.41
3:1C:12:ARG:HH22	4:1D:124:LYS:HE2	1.85	0.41
3:1C:56:GLY:O	3:1C:60:VAL:HG22	2.20	0.41
3:1C:88:ASN:HA	3:1C:112:ASP:OD2	2.20	0.41
3:1C:192:GLN:NE2	17:1Q:72:TRP:HB3	2.35	0.41
4:1D:23:LYS:HG3	4:1D:24:GLU:N	2.35	0.41
4:1D:220:PHE:HD1	43:1r:17:ARG:HH12	1.68	0.41
4:1D:378:LEU:HA	4:1D:389:CYS:HA	2.03	0.41
6:1F:203:PRO:HD2	6:1F:361:GLN:NE2	2.36	0.41
6:1F:252:GLY:O	6:1F:272:MET:HG3	2.20	0.41
6:1F:322:LEU:HG	6:1F:329:LEU:HA	2.03	0.41
7:1G:185:THR:O	7:1G:185:THR:HG22	2.21	0.41
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.54	0.41
7:1G:365:ASN:HB2	7:1G:488:LYS:HD3	2.03	0.41
7:1G:379:LEU:HD12	7:1G:452:VAL:CG1	2.49	0.41
7:1G:672:TYR:O	7:1G:678:SER:OG	2.36	0.41
7:1G:678:SER:OG	7:1G:684:MET:HE1	2.20	0.41
8:1H:22:LEU:HB2	8:1H:48:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:28:LEU:O	8:1H:32:GLN:HB2	2.21	0.41
8:1H:75:PRO:O	8:1H:222:MET:HE1	2.20	0.41
8:1H:85:MET:O	8:1H:88:PRO:HD2	2.20	0.41
8:1H:141:SER:C	8:1H:289:LEU:HD11	2.46	0.41
9:1I:148:LEU:HD11	16:1P:65:LEU:HD11	2.02	0.41
10:1J:35:VAL:O	10:1J:39:VAL:HG12	2.21	0.41
12:1L:137:LEU:C	12:1L:186:MET:HE1	2.46	0.41
12:1L:151:SER:HB2	12:1L:252:MET:HE2	2.02	0.41
12:1L:400:ASN:O	37:1I:126:GLN:NE2	2.54	0.41
12:1L:439:PRO:HG2	20:1U:57:GLU:OE1	2.21	0.41
12:1L:489:THR:O	12:1L:493:VAL:HG22	2.21	0.41
12:1L:576:MET:HG2	12:1L:577:VAL:HG13	2.03	0.41
13:1M:101:LEU:HD23	13:1M:101:LEU:HA	1.83	0.41
13:1M:156:GLY:O	13:1M:159:PRO:HD2	2.21	0.41
13:1M:329:LEU:HD22	13:1M:359:TRP:CE3	2.56	0.41
13:1M:434:ASN:HB3	33:1h:21:PHE:CE2	2.55	0.41
14:1N:9:LEU:HA	14:1N:9:LEU:HD12	1.76	0.41
14:1N:113:PHE:O	14:1N:116:PRO:HD2	2.21	0.41
14:1N:255:PRO:HG3	14:1N:260:PHE:CD1	2.56	0.41
15:1O:207:LYS:HE3	15:1O:207:LYS:CA	2.49	0.41
15:1O:282:ILE:HD12	15:1O:282:ILE:HA	1.92	0.41
16:1P:40:ARG:NH2	22:1W:110:THR:O	2.53	0.41
16:1P:54:TYR:HA	16:1P:57:MET:HG2	2.03	0.41
16:1P:106:PHE:CZ	16:1P:145:TYR:CD2	3.09	0.41
16:1P:179:LEU:HD12	16:1P:318:LEU:HD21	2.03	0.41
17:1Q:26:PRO:HD2	17:1Q:29:HIS:HB2	2.03	0.41
20:1T:58:PHE:CE1	20:1T:80:ILE:HG21	2.56	0.41
20:1U:9:GLU:HA	20:1U:12:LYS:HE3	2.03	0.41
20:1U:83:LYS:HD3	20:1U:83:LYS:HA	1.83	0.41
23:1X:18:LYS:HA	26:1a:54:ILE:HD11	2.03	0.41
30:1e:49:ILE:HD12	30:1e:50:ARG:N	2.35	0.41
31:1f:22:PHE:HD1	31:1f:22:PHE:C	2.29	0.41
31:1f:31:ASP:OD1	31:1f:31:ASP:N	2.53	0.41
32:1g:47:TYR:HB3	32:1g:57:ASN:ND2	2.36	0.41
32:1g:98:LYS:HB3	32:1g:98:LYS:HE2	1.87	0.41
33:1h:95:GLN:HB2	41:1p:82:LEU:CD2	2.41	0.41
34:1i:79:TRP:NE1	41:1p:40:VAL:HA	2.34	0.41
35:1j:34:PHE:C	35:1j:34:PHE:CD1	2.98	0.41
37:1l:16:THR:O	37:1l:19:GLU:HG2	2.21	0.41
39:1n:154:PRO:HD2	39:1n:164:PRO:HG2	2.03	0.41
43:1r:104:GLU:OE2	43:1r:107:LYS:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:81:VAL:O	3:1C:81:VAL:CG1	2.69	0.41
4:1D:116:GLN:NE2	4:1D:120:LEU:HD21	2.36	0.41
4:1D:146:ARG:CZ	4:1D:270:ARG:HH22	2.34	0.41
5:1E:51:LEU:HB3	5:1E:90:TYR:CE1	2.56	0.41
6:1F:8:LYS:HA	6:1F:8:LYS:HD2	1.90	0.41
6:1F:94:VAL:HG23	6:1F:220:THR:HG21	2.02	0.41
6:1F:264:HIS:N	6:1F:284:ALA:O	2.50	0.41
6:1F:279:LEU:HA	6:1F:279:LEU:HD12	1.81	0.41
7:1G:429:LEU:O	7:1G:473:ILE:HD11	2.21	0.41
8:1H:252:PRO:O	8:1H:256:THR:HG23	2.22	0.41
9:1I:27:TRP:NE1	50:1I:203:PC1:H331	2.36	0.41
10:1J:119:PHE:HB2	11:1K:1:FME:O	2.20	0.41
12:1L:1:FME:HE3	34:1i:86:LYS:HE2	2.03	0.41
12:1L:341:MET:HE3	12:1L:341:MET:CA	2.51	0.41
12:1L:363:TYR:CD1	12:1L:370:THR:HG21	2.56	0.41
12:1L:399:VAL:HG12	12:1L:409:LEU:HD23	2.03	0.41
13:1M:14:MET:HE2	13:1M:26:ASN:HB3	2.03	0.41
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	2.03	0.41
13:1M:361:MET:HA	13:1M:364:LEU:HB2	2.01	0.41
14:1N:78:LEU:HD22	14:1N:84:TRP:CZ2	2.56	0.41
14:1N:287:LEU:HA	14:1N:287:LEU:HD23	1.81	0.41
16:1P:24:PHE:HB3	16:1P:95:VAL:HG23	2.03	0.41
16:1P:79:ASP:O	16:1P:82:ARG:NH2	2.54	0.41
16:1P:313:LYS:HE3	16:1P:316:GLU:HG2	2.02	0.41
17:1Q:10:LEU:HD21	22:1W:16:SER:OG	2.21	0.41
20:1T:51:ILE:HB	20:1T:62:ILE:HD11	2.03	0.41
23:1X:70:PHE:O	23:1X:73:ILE:HG13	2.21	0.41
28:1c:4:ILE:HG13	28:1c:5:ARG:N	2.36	0.41
28:1c:41:GLU:OE1	28:1c:45:ARG:NH2	2.53	0.41
35:1j:12:ARG:HD3	36:1k:50:TRP:CD1	2.56	0.41
42:1q:27:LEU:HB2	42:1q:33:VAL:CG1	2.51	0.41
43:1r:4:THR:HG23	43:1r:6:VAL:CG1	2.51	0.41
1:1A:1:FME:O1	1:1A:2:ASN:N	2.54	0.40
2:1B:125:TYR:HD1	4:1D:102:TYR:CE1	2.39	0.40
2:1B:171:LYS:H	16:1P:52:GLU:CD	2.27	0.40
3:1C:17:VAL:HA	3:1C:20:LYS:NZ	2.36	0.40
3:1C:141:PHE:CZ	3:1C:148:LEU:HG	2.56	0.40
3:1C:211:GLN:HG3	3:1C:212:PRO:HD2	2.03	0.40
4:1D:143:GLU:OE2	4:1D:270:ARG:NH2	2.54	0.40
4:1D:364:TYR:O	4:1D:365:THR:C	2.65	0.40
4:1D:390:LYS:HD3	4:1D:391:ILE:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:26:GLU:HA	5:1E:29:LYS:HE2	2.02	0.40
5:1E:63:ILE:HG23	7:1G:187:ILE:HD11	2.02	0.40
6:1F:120:GLU:O	6:1F:124:VAL:HG12	2.21	0.40
6:1F:345:LYS:HE3	6:1F:345:LYS:HB3	1.75	0.40
6:1F:351:ILE:HA	6:1F:354:TYR:HB2	2.03	0.40
6:1F:376:MET:HE2	6:1F:377:ALA:N	2.36	0.40
7:1G:21:GLU:CD	7:1G:22:PRO:HD2	2.46	0.40
7:1G:107:ILE:HG22	9:1I:78:ILE:HG21	2.02	0.40
7:1G:385:ARG:HD3	7:1G:416:THR:HG23	2.03	0.40
9:1I:8:ARG:HA	9:1I:8:ARG:CZ	2.51	0.40
10:1J:152:TRP:O	10:1J:156:VAL:HG23	2.20	0.40
10:1J:167:VAL:HG23	14:1N:42:PRO:HD3	2.03	0.40
12:1L:313:MET:CE	12:1L:329:ILE:HD13	2.52	0.40
12:1L:395:ILE:HD13	12:1L:395:ILE:HA	1.89	0.40
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.20	0.40
13:1M:11:LEU:O	13:1M:15:THR:HG23	2.21	0.40
13:1M:16:TRP:O	13:1M:93:LYS:NZ	2.41	0.40
13:1M:71:TRP:CZ3	32:1g:69:VAL:HG11	2.56	0.40
13:1M:154:LEU:HD12	13:1M:154:LEU:HA	1.78	0.40
13:1M:364:LEU:O	13:1M:367:LEU:HB2	2.20	0.40
15:1O:28:ASP:HA	15:1O:35:LYS:HD3	2.03	0.40
16:1P:169:SER:OG	16:1P:203:GLN:O	2.32	0.40
20:1T:12:LYS:O	20:1T:16:LEU:HD23	2.21	0.40
20:1T:14:ARG:CZ	20:1T:58:PHE:CD2	3.04	0.40
20:1U:72:CYS:H	20:1U:75:GLU:HG2	1.85	0.40
23:1X:43:MET:HE2	23:1X:43:MET:HA	2.02	0.40
23:1X:76:HIS:HB3	23:1X:77:CYS:H	1.79	0.40
25:1Z:127:LEU:HD22	30:1e:97:HIS:NE2	2.36	0.40
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.21	0.40
29:1d:30:ARG:NH1	29:1d:76:LEU:HD13	2.37	0.40
30:1e:9:LEU:HB3	30:1e:11:LEU:HD23	2.03	0.40
37:1l:33:ASP:OD1	37:1l:33:ASP:N	2.51	0.40
41:1p:79:LYS:HB3	41:1p:79:LYS:HE2	1.87	0.40
41:1p:139:GLN:HA	41:1p:143:SER:OG	2.20	0.40
41:1p:159:LYS:O	41:1p:163:LEU:HG	2.21	0.40
41:1p:167:LYS:NZ	41:1p:171:GLU:HB2	2.36	0.40
2:1B:84:ASP:OD1	8:1H:58:LYS:NZ	2.51	0.40
2:1B:158:TYR:HB2	9:1I:50:TYR:OH	2.21	0.40
6:1F:64:GLY:HA3	6:1F:251:SER:OG	2.22	0.40
6:1F:176:PHE:HE1	44:1s:62:ARG:HD3	1.86	0.40
6:1F:347:ILE:HG12	6:1F:418:LEU:HG	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:354:ALA:HB3	7:1G:361:ASN:ND2	2.33	0.40
7:1G:386:PHE:HZ	7:1G:668:ILE:HD12	1.86	0.40
7:1G:407:ALA:HB1	7:1G:422:LEU:HD11	2.04	0.40
7:1G:462:ASP:OD1	7:1G:466:ILE:HD11	2.20	0.40
8:1H:17:VAL:HG21	8:1H:229:ALA:HB2	2.01	0.40
13:1M:12:LEU:HD23	13:1M:100:ILE:HD11	2.04	0.40
13:1M:114:GLU:OE2	13:1M:174:LEU:HB2	2.21	0.40
14:1N:128:LEU:HD11	14:1N:213:LEU:HD13	2.03	0.40
14:1N:155:LEU:HD23	14:1N:155:LEU:HA	1.96	0.40
14:1N:246:VAL:HG22	45:1N:401:3PE:H3E1	2.02	0.40
14:1N:304:MET:HE1	15:1O:290:ASP:HB2	2.03	0.40
15:1O:308:TYR:CD1	29:1d:51:ARG:HG2	2.56	0.40
16:1P:23:VAL:O	16:1P:48:PRO:HD2	2.22	0.40
16:1P:166:ILE:HG23	16:1P:230:PHE:CD2	2.56	0.40
16:1P:325:ARG:HG3	16:1P:326:TRP:CE3	2.56	0.40
17:1Q:36:ARG:HA	17:1Q:104:ASP:HB3	2.03	0.40
17:1Q:108:ARG:HH22	17:1Q:110:VAL:HA	1.85	0.40
18:1R:25:ARG:HH11	18:1R:25:ARG:HG2	1.86	0.40
26:1a:28:LYS:HG3	26:1a:33:GLY:O	2.21	0.40
26:1a:35:GLU:H	26:1a:35:GLU:HG3	1.76	0.40
29:1d:48:ILE:HD12	29:1d:49:ARG:N	2.36	0.40
34:1i:122:PHE:HD1	40:1o:60:HIS:CD2	2.38	0.40
39:1n:67:GLU:H	39:1n:67:GLU:HG3	1.61	0.40
1:1A:14:ALA:O	1:1A:18:VAL:HG13	2.22	0.40
2:1B:48:MET:N	2:1B:85:VAL:O	2.53	0.40
2:1B:62:MET:HE2	2:1B:62:MET:HB3	1.76	0.40
3:1C:38:GLN:HG2	21:1V:106:PRO:HD3	2.03	0.40
4:1D:202:ASP:HA	4:1D:323:ILE:HG21	2.03	0.40
4:1D:232:ASN:O	4:1D:236:ARG:HG2	2.21	0.40
6:1F:80:SER:HA	6:1F:83:ASN:ND2	2.36	0.40
6:1F:202:LYS:HE3	6:1F:202:LYS:HB3	1.80	0.40
7:1G:43:HIS:NE2	7:1G:261:GLU:OE1	2.52	0.40
7:1G:230:VAL:HG22	7:1G:322:LEU:HG	2.02	0.40
7:1G:668:ILE:HG22	7:1G:691:VAL:HG21	2.03	0.40
8:1H:256:THR:O	8:1H:260:VAL:HG22	2.21	0.40
12:1L:127:THR:HG21	12:1L:147:VAL:N	2.36	0.40
12:1L:128:MET:HE2	12:1L:251:THR:HG22	2.02	0.40
12:1L:190:LEU:O	12:1L:194:ASN:HA	2.22	0.40
13:1M:281:ASP:OD1	13:1M:340:ARG:HB2	2.21	0.40
14:1N:319:HIS:O	29:1d:49:ARG:NH2	2.55	0.40
15:1O:37:ARG:NH1	15:1O:40:ARG:HE	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:65:ASP:HB2	28:1c:2:PHE:CE1	2.56	0.40
15:1O:183:ILE:HG22	15:1O:186:LYS:HZ2	1.86	0.40
16:1P:93:ASN:O	16:1P:94:LEU:HD13	2.20	0.40
20:1U:36:PHE:HB2	20:1U:71:MET:SD	2.61	0.40
34:1i:86:LYS:O	34:1i:90:THR:OG1	2.39	0.40
38:1m:16:THR:O	38:1m:22:TYR:OH	2.40	0.40
41:1p:34:LYS:HA	41:1p:34:LYS:HD3	1.81	0.40
1:1A:1:FME:HCN	1:1A:4:MET:HE3	2.03	0.40
1:1A:105:GLU:HG2	1:1A:111:LEU:HD21	2.03	0.40
2:1B:39:TRP:O	2:1B:42:ARG:NE	2.55	0.40
4:1D:201:GLN:HG3	4:1D:202:ASP:H	1.87	0.40
5:1E:16:ASN:O	5:1E:19:THR:OG1	2.38	0.40
5:1E:21:PHE:O	5:1E:68:LYS:HE2	2.21	0.40
5:1E:79:ARG:HD2	17:1Q:131:SER:O	2.21	0.40
6:1F:118:LEU:HD23	6:1F:118:LEU:HA	1.94	0.40
6:1F:248:GLU:C	6:1F:250:ASN:H	2.29	0.40
7:1G:56:LEU:HG	7:1G:89:ALA:HB1	2.02	0.40
7:1G:367:THR:O	7:1G:369:ALA:N	2.55	0.40
8:1H:125:SER:O	8:1H:129:LEU:HG	2.21	0.40
9:1I:136:ASN:OD1	9:1I:137:PHE:N	2.55	0.40
10:1J:65:LEU:HA	10:1J:65:LEU:HD13	1.89	0.40
11:1K:61:ILE:O	11:1K:65:VAL:HG13	2.22	0.40
12:1L:546:GLN:HA	12:1L:550:SER:HB3	2.02	0.40
12:1L:574:SER:HA	12:1L:577:VAL:HG22	2.02	0.40
13:1M:354:LEU:HB2	33:1h:18:ASP:OD1	2.22	0.40
14:1N:245:MET:SD	14:1N:245:MET:C	3.05	0.40
15:1O:148:CYS:HA	15:1O:279:LEU:HD21	2.03	0.40
16:1P:274:PRO:HG2	16:1P:275:PHE:CZ	2.57	0.40
20:1T:36:PHE:O	20:1T:42:LEU:HD12	2.22	0.40
23:1X:37:LYS:HE3	23:1X:38:PRO:HD3	2.04	0.40
23:1X:161:LYS:HA	23:1X:161:LYS:HD2	1.78	0.40
24:1Y:133:GLN:HG3	24:1Y:136:ALA:HB2	2.02	0.40
25:1Z:22:LYS:HB2	25:1Z:22:LYS:HE3	1.75	0.40
26:1a:23:THR:O	26:1a:27:HIS:ND1	2.55	0.40
29:1d:2:MET:CE	33:1h:122:TRP:HE3	2.35	0.40
31:1f:25:TYR:O	31:1f:28:ARG:HG2	2.21	0.40
31:1f:48:LEU:HD23	31:1f:49:ARG:O	2.21	0.40
34:1i:23:LYS:O	34:1i:23:LYS:HD3	2.21	0.40
36:1k:24:GLU:HA	36:1k:29:GLU:CD	2.46	0.40
39:1n:16:LEU:HD23	39:1n:16:LEU:HA	1.94	0.40
40:1o:111:LYS:O	40:1o:115:GLU:HG2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:47:LYS:H	43:1r:47:LYS:CD	2.34	0.40
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.46	0.40
4:1D:150:HIS:HD2	4:1D:300:ARG:HB3	1.86	0.40
5:1E:100:ILE:HD13	5:1E:100:ILE:HA	2.01	0.40
6:1F:161:LEU:HA	6:1F:167:CYS:HB3	2.04	0.40
7:1G:74:MET:SD	7:1G:74:MET:N	2.94	0.40
7:1G:554:ALA:HA	7:1G:560:ILE:HD11	2.04	0.40
9:1I:5:VAL:HG23	9:1I:6:ASN:N	2.37	0.40
9:1I:69:ARG:NH2	9:1I:155:LEU:CD1	2.80	0.40
12:1L:105:MET:HE3	12:1L:449:LEU:HD22	2.03	0.40
12:1L:314:MET:HA	12:1L:317:ILE:HD13	2.03	0.40
12:1L:500:LEU:HD13	45:1L:704:3PE:H382	2.04	0.40
14:1N:262:PRO:O	14:1N:266:ILE:HG12	2.22	0.40
15:1O:146:LYS:HD2	15:1O:147:GLN:H	1.87	0.40
15:1O:164:LEU:HB2	15:1O:248:TRP:CH2	2.57	0.40
16:1P:100:GLU:OE2	16:1P:106:PHE:HB2	2.21	0.40
17:1Q:17:LEU:O	17:1Q:97:GLU:OE2	2.39	0.40
19:1S:17:GLU:OE2	19:1S:17:GLU:HA	2.20	0.40
19:1S:35:PHE:CD1	19:1S:35:PHE:C	3.00	0.40
22:1W:84:ILE:O	22:1W:88:MET:HB2	2.21	0.40
23:1X:8:THR:HA	25:1Z:88:ARG:NE	2.36	0.40
23:1X:75:ARG:HD3	23:1X:75:ARG:C	2.47	0.40
25:1Z:40:ILE:O	25:1Z:44:LEU:HG	2.21	0.40
25:1Z:53:TRP:NE1	25:1Z:57:ARG:HD2	2.37	0.40
25:1Z:129:THR:OG1	25:1Z:130:ASN:N	2.54	0.40
26:1a:3:PHE:HA	26:1a:6:LEU:HD13	2.03	0.40
29:1d:102:PRO:O	29:1d:104:LYS:CD	2.68	0.40
31:1f:49:ARG:NH2	31:1f:52:GLU:HB2	2.37	0.40
33:1h:91:MET:C	33:1h:91:MET:SD	3.04	0.40
39:1n:116:ASP:OD1	39:1n:116:ASP:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	84/115 (73%)	80 (95%)	4 (5%)	0	100	100
2	1B	153/258 (59%)	137 (90%)	16 (10%)	0	100	100
3	1C	207/264 (78%)	194 (94%)	13 (6%)	0	100	100
4	1D	427/476 (90%)	394 (92%)	33 (8%)	0	100	100
5	1E	212/249 (85%)	191 (90%)	21 (10%)	0	100	100
6	1F	430/464 (93%)	398 (93%)	31 (7%)	1 (0%)	43	72
7	1G	697/727 (96%)	643 (92%)	50 (7%)	4 (1%)	21	52
8	1H	293/318 (92%)	279 (95%)	12 (4%)	2 (1%)	18	50
9	1I	174/239 (73%)	163 (94%)	11 (6%)	0	100	100
10	1J	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	21	52
11	1K	96/98 (98%)	91 (95%)	5 (5%)	0	100	100
12	1L	604/606 (100%)	556 (92%)	45 (8%)	3 (0%)	24	56
13	1M	457/459 (100%)	440 (96%)	16 (4%)	1 (0%)	43	72
14	1N	345/347 (99%)	319 (92%)	26 (8%)	0	100	100
15	1O	318/357 (89%)	295 (93%)	23 (7%)	0	100	100
16	1P	340/377 (90%)	305 (90%)	35 (10%)	0	100	100
17	1Q	127/175 (73%)	111 (87%)	15 (12%)	1 (1%)	16	48
18	1R	94/123 (76%)	92 (98%)	2 (2%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	78 (94%)	5 (6%)	0	100	100
20	1U	84/156 (54%)	81 (96%)	3 (4%)	0	100	100
21	1V	113/116 (97%)	104 (92%)	8 (7%)	1 (1%)	14	45
22	1W	113/128 (88%)	103 (91%)	9 (8%)	1 (1%)	14	45
23	1X	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	78 (96%)	3 (4%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	90 (92%)	7 (7%)	1 (1%)	12	43
33	1h	136/189 (72%)	128 (94%)	8 (6%)	0	100	100
34	1i	124/128 (97%)	115 (93%)	9 (7%)	0	100	100
35	1j	69/105 (66%)	65 (94%)	4 (6%)	0	100	100
36	1k	79/98 (81%)	72 (91%)	7 (9%)	0	100	100
37	1l	154/186 (83%)	145 (94%)	9 (6%)	0	100	100
38	1m	126/129 (98%)	121 (96%)	5 (4%)	0	100	100
39	1n	170/179 (95%)	160 (94%)	9 (5%)	1 (1%)	21	52
40	1o	120/137 (88%)	112 (93%)	8 (7%)	0	100	100
41	1p	171/176 (97%)	163 (95%)	8 (5%)	0	100	100
42	1q	143/145 (99%)	129 (90%)	11 (8%)	3 (2%)	5	31
43	1r	90/114 (79%)	83 (92%)	7 (8%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	8142/9744 (84%)	7572 (93%)	550 (7%)	20 (0%)	44	72

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	1G	259	ASN
8	1H	92	PRO
12	1L	406	ALA
13	1M	2	LEU
17	1Q	20	THR
32	1g	24	ILE
39	1n	31	VAL
6	1F	302	SER
7	1G	260	GLU
10	1J	116	ILE
12	1L	230	HIS
12	1L	601	LEU
22	1W	76	PRO
7	1G	696	GLN
42	1q	75	TRP
8	1H	170	GLU
21	1V	112	LYS

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Mol	Chain	Res	Type
42	1q	100	THR
42	1q	102	PRO
7	1G	368	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	76/99 (77%)	76 (100%)	0	100	100
2	1B	131/212 (62%)	129 (98%)	2 (2%)	57	68
3	1C	190/227 (84%)	189 (100%)	1 (0%)	81	80
4	1D	371/405 (92%)	370 (100%)	1 (0%)	86	83
5	1E	183/207 (88%)	182 (100%)	1 (0%)	81	80
6	1F	346/368 (94%)	343 (99%)	3 (1%)	70	75
7	1G	588/610 (96%)	581 (99%)	7 (1%)	63	72
8	1H	257/274 (94%)	256 (100%)	1 (0%)	84	81
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/140 (100%)	138 (99%)	2 (1%)	59	70
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	536 (99%)	3 (1%)	78	79
13	1M	408/408 (100%)	402 (98%)	6 (2%)	57	68
14	1N	310/310 (100%)	308 (99%)	2 (1%)	78	79
15	1O	283/307 (92%)	283 (100%)	0	100	100
16	1P	296/323 (92%)	293 (99%)	3 (1%)	68	74
17	1Q	117/152 (77%)	117 (100%)	0	100	100
18	1R	79/97 (81%)	79 (100%)	0	100	100
19	1S	77/82 (94%)	75 (97%)	2 (3%)	40	60
20	1T	79/133 (59%)	79 (100%)	0	100	100
20	1U	79/133 (59%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	1V	100/101 (99%)	100 (100%)	0	100	100
22	1W	107/112 (96%)	106 (99%)	1 (1%)	70	75
23	1X	153/154 (99%)	152 (99%)	1 (1%)	76	77
24	1Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	121 (98%)	2 (2%)	55	68
26	1a	58/58 (100%)	57 (98%)	1 (2%)	53	67
27	1b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	107/109 (98%)	106 (99%)	1 (1%)	70	75
30	1e	87/94 (93%)	86 (99%)	1 (1%)	65	73
31	1f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	92 (100%)	0	100	100
33	1h	121/158 (77%)	121 (100%)	0	100	100
34	1i	119/120 (99%)	118 (99%)	1 (1%)	73	76
35	1j	62/84 (74%)	62 (100%)	0	100	100
36	1k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	140 (99%)	1 (1%)	76	77
38	1m	113/114 (99%)	113 (100%)	0	100	100
39	1n	156/160 (98%)	156 (100%)	0	100	100
40	1o	110/120 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	154 (100%)	0	100	100
42	1q	131/131 (100%)	129 (98%)	2 (2%)	57	68
43	1r	85/98 (87%)	85 (100%)	0	100	100
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7179/8272 (87%)	7134 (99%)	45 (1%)	76	79

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

Mol	Chain	Res	Type
2	1B	82	GLN
2	1B	156	LEU
3	1C	45	PHE
4	1D	2	ARG
5	1E	58	ASN

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Mol	Chain	Res	Type
6	1F	25	LEU
6	1F	416	GLN
6	1F	437	HIS
7	1G	35	MET
7	1G	211	LYS
7	1G	363	LEU
7	1G	570	SER
7	1G	579	ARG
7	1G	641	TYR
7	1G	699	GLU
8	1H	133	LEU
10	1J	78	MET
10	1J	166	VAL
12	1L	125	LEU
12	1L	486	MET
12	1L	491	LEU
13	1M	277	LEU
13	1M	366	ASN
13	1M	375	LEU
13	1M	376	ILE
13	1M	391	ILE
13	1M	452	LYS
14	1N	284	MET
14	1N	330	ILE
16	1P	16	VAL
16	1P	178	PHE
16	1P	234	ASN
19	1S	41	VAL
19	1S	60	VAL
22	1W	88	MET
23	1X	36	ASP
25	1Z	24	ASN
25	1Z	117	VAL
26	1a	3	PHE
29	1d	58	LEU
30	1e	91	TYR
34	1i	55	PRO
37	1l	25	LYS
42	1q	35	VAL
42	1q	72	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	1A	80	GLN
2	1B	127	HIS
2	1B	164	GLN
3	1C	41	GLN
3	1C	46	ASN
3	1C	192	GLN
4	1D	46	ASN
4	1D	84	HIS
4	1D	149	ASN
4	1D	150	HIS
4	1D	231	ASN
5	1E	9	HIS
5	1E	121	GLN
5	1E	214	GLN
6	1F	37	GLN
6	1F	83	ASN
6	1F	148	ASN
6	1F	224	ASN
6	1F	257	ASN
6	1F	326	GLN
7	1G	494	HIS
7	1G	548	HIS
7	1G	549	HIS
7	1G	618	GLN
7	1G	682	GLN
8	1H	287	HIS
9	1I	6	ASN
11	1K	92	ASN
12	1L	109	HIS
12	1L	175	ASN
12	1L	295	GLN
12	1L	323	HIS
12	1L	470	ASN
12	1L	506	ASN
12	1L	603	ASN
13	1M	30	HIS
13	1M	103	GLN
13	1M	168	GLN
13	1M	169	ASN
13	1M	180	HIS
13	1M	319	HIS
13	1M	366	ASN
13	1M	390	ASN

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Mol	Chain	Res	Type
14	1N	150	ASN
14	1N	186	HIS
15	1O	30	ASN
15	1O	76	ASN
15	1O	97	GLN
15	1O	153	ASN
15	1O	222	GLN
16	1P	3	HIS
16	1P	37	HIS
16	1P	67	GLN
16	1P	89	ASN
16	1P	234	ASN
17	1Q	81	ASN
18	1R	32	GLN
19	1S	30	GLN
19	1S	75	ASN
21	1V	70	GLN
21	1V	82	GLN
21	1V	85	ASN
22	1W	58	GLN
22	1W	70	ASN
23	1X	63	ASN
24	1Y	88	ASN
24	1Y	133	GLN
27	1b	51	ASN
28	1c	35	HIS
29	1d	46	ASN
29	1d	61	GLN
29	1d	88	HIS
30	1e	33	HIS
32	1g	57	ASN
34	1i	13	GLN
37	1l	55	GLN
37	1l	87	ASN
37	1l	126	GLN
37	1l	136	ASN
40	1o	3	HIS
40	1o	60	HIS
40	1o	116	GLN
41	1p	53	GLN
41	1p	55	HIS
41	1p	99	GLN

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Mol	Chain	Res	Type
41	1p	103	ASN
41	1p	122	GLN
41	1p	158	GLN
42	1q	13	GLN
42	1q	54	GLN
42	1q	59	HIS
42	1q	69	ASN
42	1q	87	HIS
42	1q	112	ASN
43	1r	24	GLN
43	1r	51	ASN
44	1s	35	ASN
44	1s	40	ASN
44	1s	43	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	$\# Z > 2$
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	0.99	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	1.02	1 (12%)
10	FME	1J	1	10	8,9,10	0.57	0	8,9,11	0.93	1 (12%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
34	SAC	1i	1	-	7,8,9	0.57	0	7,9,11	1.13	1 (14%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	0.89	1 (12%)
8	FME	1H	1	8	8,9,10	0.56	0	8,9,11	0.92	1 (12%)
14	FME	1N	1	14	8,9,10	0.57	0	8,9,11	0.99	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	FME	1A	1	1	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
10	FME	1J	1	10	-	3/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
34	SAC	1i	1	-	-	2/7/8/10	-
11	FME	1K	1	11	-	1/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
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	-2.92	117.26	124.77
12	1L	1	FME	O-C-CA	-2.66	117.93	124.77
13	1M	1	FME	O-C-CA	-2.57	118.15	124.77
10	1J	1	FME	O-C-CA	-2.55	118.20	124.77
1	1A	1	FME	O-C-CA	-2.54	118.23	124.77
14	1N	1	FME	O-C-CA	-2.53	118.26	124.77
8	1H	1	FME	O-C-CA	-2.53	118.28	124.77
11	1K	1	FME	O-C-CA	-2.45	118.47	124.77

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	N-CA-CB-CG
11	1K	1	FME	CB-CG-SD-CE
10	1J	1	FME	CB-CG-SD-CE
34	1i	1	SAC	C-CA-N-C1A
10	1J	1	FME	C-CA-CB-CG
34	1i	1	SAC	CB-CA-N-C1A

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	1A	1	FME	2	0
12	1L	1	FME	1	0
13	1M	1	FME	3	0
34	1i	1	SAC	2	0
11	1K	1	FME	2	0
14	1N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
58	EHZ	1n	201	-	31,36,37	0.20	0	36,44,47	1.24	1 (2%)
50	PC1	1I	203	-	53,53,53	0.27	0	59,61,61	0.32	0
45	3PE	1L	702	-	45,45,50	0.28	0	48,50,55	0.31	0
56	NDP	1P	501	-	51,52,52	0.54	0	71,80,80	0.87	2 (2%)
50	PC1	1L	703	-	43,43,53	0.30	0	49,51,61	0.38	0
46	SF4	1G	802	7	0,12,12	-	-	-		
52	PGT	1M	501	-	50,50,50	0.50	0	53,56,56	0.50	0
54	GTP	1O	401	55	33,34,34	0.59	0	50,54,54	0.59	0
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.64	1 (2%)
58	EHZ	1W	201	-	31,36,37	0.18	0	36,44,47	1.31	1 (2%)
46	SF4	1F	502	6	0,12,12	-	-	-		
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.45	0
46	SF4	1I	201	9	0,12,12	-	-	-		
47	FES	1G	803	7	0,4,4	-	-	-		
50	PC1	1f	101	-	45,45,53	0.26	0	51,53,61	0.35	0
53	CDL	1N	402	-	76,76,99	0.30	0	82,88,111	0.37	0
47	FES	1E	301	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	3PE	1Y	202	-	50,50,50	0.27	0	53,55,55	0.32	0
45	3PE	1Y	201	-	30,30,50	0.35	0	33,35,55	0.66	1 (3%)
45	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.38	0
45	3PE	1L	704	-	41,41,50	0.31	0	44,46,55	1.29	5 (11%)
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.38	0
51	MYR	1L	701	-	13,14,15	0.31	0	12,13,15	0.34	0
46	SF4	1G	801	7	0,12,12	-	-	-		
46	SF4	1B	201	2	0,12,12	-	-	-		
53	CDL	1r	201	-	60,60,99	0.86	3 (5%)	66,72,111	1.11	4 (6%)
50	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.39	0
46	SF4	1I	202	9	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	EHZ	1n	201	-	-	8/42/44/45	-
50	PC1	1I	203	-	-	15/57/57/57	-
45	3PE	1L	702	-	-	4/49/49/54	-
56	NDP	1P	501	-	-	10/34/77/77	0/5/5/5
50	PC1	1L	703	-	-	7/47/47/57	-
46	SF4	1G	802	7	-	-	0/6/5/5
52	PGT	1M	501	-	-	24/55/55/55	-
54	GTP	1O	401	55	-	0/22/38/38	0/3/3/3
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
58	EHZ	1W	201	-	-	8/42/44/45	-
46	SF4	1F	502	6	-	-	0/6/5/5
50	PC1	1J	201	-	-	3/38/38/57	-
46	SF4	1I	201	9	-	-	0/6/5/5
47	FES	1G	803	7	-	-	0/1/1/1
50	PC1	1f	101	-	-	9/49/49/57	-
53	CDL	1N	402	-	-	9/87/87/110	-
45	3PE	1Y	202	-	-	7/54/54/54	-
45	3PE	1Y	201	-	-	8/34/34/54	-
47	FES	1E	301	5	-	-	0/1/1/1
45	3PE	1N	401	-	-	9/54/54/54	-
45	3PE	1L	704	-	-	6/45/45/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1A	201	-	-	3/50/50/54	-
51	MYR	1L	701	-	-	1/12/12/13	-
46	SF4	1G	801	7	-	-	0/6/5/5
46	SF4	1B	201	2	-	-	0/6/5/5
53	CDL	1r	201	-	-	13/71/71/110	-
50	PC1	1I	204	-	-	4/47/47/57	-
46	SF4	1I	202	9	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	1r	201	CDL	OB5-CB3	4.86	1.63	1.44
53	1r	201	CDL	OB2-CB2	2.27	1.53	1.44
53	1r	201	CDL	PB2-OB4	-2.21	1.45	1.55

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1n	201	EHZ	C10-S1-C9	7.16	123.01	101.84
58	1W	201	EHZ	C10-S1-C9	7.11	122.86	101.84
45	1L	704	3PE	O21-C21-C22	6.29	125.08	111.48
53	1r	201	CDL	OB4-PB2-OB2	4.60	128.41	107.57
56	1P	501	NDP	P2B-O2B-C2B	-4.27	112.04	123.43
53	1r	201	CDL	OB5-PB2-OB3	-4.15	92.48	108.94
53	1r	201	CDL	OB2-PB2-OB3	-3.83	93.76	108.94
53	1r	201	CDL	OB4-PB2-OB5	3.43	123.09	107.57
56	1P	501	NDP	O4D-C1D-C2D	-3.37	99.41	106.62
45	1L	704	3PE	O21-C21-O22	-2.77	117.22	123.70
45	1L	704	3PE	C2-O21-C21	2.64	124.10	117.80
45	1Y	201	3PE	O21-C21-C22	2.45	116.79	111.48
45	1L	704	3PE	O21-C2-C1	2.33	116.70	108.34
48	1F	501	FMN	C4-N3-C2	-2.07	121.97	125.64
45	1L	704	3PE	O21-C2-C3	2.06	115.73	108.34

There are no chirality outliers.

All (149) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	704	3PE	O22-C21-O21-C2
45	1L	704	3PE	C22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	1N	401	3PE	C1-O11-P-O14
45	1Y	201	3PE	C1-O11-P-O14
45	1Y	201	3PE	O32-C31-O31-C3
45	1Y	201	3PE	C32-C31-O31-C3
45	1Y	201	3PE	O22-C21-O21-C2
45	1Y	201	3PE	C22-C21-O21-C2
45	1Y	202	3PE	C1-O11-P-O14
50	1I	203	PC1	C11-O13-P-O11
50	1I	203	PC1	O13-C11-C12-N
50	1I	204	PC1	C11-O13-P-O14
50	1I	204	PC1	C11-O13-P-O11
50	1J	201	PC1	C1-O11-P-O14
50	1L	703	PC1	C1-O11-P-O14
52	1M	501	PGT	O31-C31-O2-C2
52	1M	501	PGT	C1-O3P-P-O1P
52	1M	501	PGT	C1-O3P-P-O4P
52	1M	501	PGT	C4-O4P-P-O3P
52	1M	501	PGT	C4-O4P-P-O1P
52	1M	501	PGT	C4-O4P-P-O2P
52	1M	501	PGT	C12-C11-O3-C3
53	1r	201	CDL	CA2-C1-CB2-OB2
53	1r	201	CDL	CA3-OA5-PA1-OA3
53	1r	201	CDL	CB2-OB2-PB2-OB3
53	1r	201	CDL	CB3-OB5-PB2-OB2
53	1r	201	CDL	CB3-OB5-PB2-OB3
56	1P	501	NDP	C5D-O5D-PN-O3
56	1P	501	NDP	C5D-O5D-PN-O1N
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	1n	201	EHZ	C16-C17-C20-O6
58	1n	201	EHZ	C18-C17-C20-O6
58	1n	201	EHZ	C19-C17-C20-O6
58	1n	201	EHZ	O2-C9-S1-C10
58	1n	201	EHZ	C8-C9-S1-C10
52	1M	501	PGT	O11-C11-O3-C3
52	1M	501	PGT	C32-C31-O2-C2
58	1W	201	EHZ	C13-C12-N1-C11
53	1r	201	CDL	O1-C1-CB2-OB2
45	1Y	202	3PE	C2-C1-O11-P
58	1W	201	EHZ	O3-C12-N1-C11
58	1W	201	EHZ	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
52	1M	501	PGT	C15-C16-C17-C18
56	1P	501	NDP	C2D-C1D-N1N-C2N
52	1M	501	PGT	C5-C4-O4P-P
56	1P	501	NDP	C2D-C1D-N1N-C6N
52	1M	501	PGT	C40-C41-C42-C43
52	1M	501	PGT	C14-C15-C16-C17
50	1I	203	PC1	C24-C25-C26-C27
45	1A	201	3PE	O21-C2-C3-O31
53	1N	402	CDL	OA6-CA4-CA6-OA8
53	1r	201	CDL	CB4-CB3-OB5-PB2
50	1f	101	PC1	C25-C26-C27-C28
58	1W	201	EHZ	O4-C15-C16-O5
58	1n	201	EHZ	C1-C21-C22-C23
45	1A	201	3PE	C1-C2-C3-O31
45	1Y	202	3PE	C3C-C3D-C3E-C3F
52	1M	501	PGT	C34-C35-C36-C37
52	1M	501	PGT	C21-C22-C23-C24
45	1Y	202	3PE	C35-C36-C37-C38
53	1N	402	CDL	C75-C76-C77-C78
53	1N	402	CDL	C55-C56-C57-C58
50	1f	101	PC1	C31-C32-C33-C34
53	1r	201	CDL	OB6-CB4-CB6-OB8
50	1I	203	PC1	O31-C31-C32-C33
52	1M	501	PGT	C22-C23-C24-C25
52	1M	501	PGT	C44-C45-C46-C47
53	1N	402	CDL	CA3-CA4-CA6-OA8
53	1r	201	CDL	CB3-CB4-CB6-OB8
45	1L	704	3PE	O11-C1-C2-O21
45	1N	401	3PE	O31-C31-C32-C33
56	1P	501	NDP	PN-O3-PA-O5B
45	1N	401	3PE	O11-C1-C2-O21
45	1Y	202	3PE	O11-C1-C2-O21
50	1f	101	PC1	C1-C2-C3-O31
45	1A	201	3PE	C12-C11-O13-P
50	1J	201	PC1	O13-C11-C12-N
53	1N	402	CDL	C33-C34-C35-C36
50	1I	204	PC1	C34-C35-C36-C37
58	1W	201	EHZ	C5-C6-C7-O1
45	1N	401	3PE	C34-C35-C36-C37
56	1P	501	NDP	C3B-C2B-O2B-P2B
50	1I	203	PC1	C38-C39-C3A-C3B
45	1N	401	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
50	1J	201	PC1	C1-O11-P-O13
50	1L	703	PC1	C11-O13-P-O14
50	1L	703	PC1	C1-O11-P-O12
50	1L	703	PC1	C1-O11-P-O13
50	1f	101	PC1	C1-O11-P-O14
53	1r	201	CDL	CB3-OB5-PB2-OB4
56	1P	501	NDP	C5D-O5D-PN-O2N
51	1L	701	MYR	C7-C8-C9-C10
52	1M	501	PGT	C16-C17-C18-C19
45	1N	401	3PE	C2-C1-O11-P
53	1r	201	CDL	CA4-CA3-OA5-PA1
56	1P	501	NDP	O4D-C1D-N1N-C2N
56	1P	501	NDP	O4D-C1D-N1N-C6N
56	1P	501	NDP	C1B-C2B-O2B-P2B
45	1Y	202	3PE	O11-C1-C2-C3
53	1N	402	CDL	C32-C33-C34-C35
52	1M	501	PGT	C18-C19-C20-C21
45	1N	401	3PE	C3A-C3B-C3C-C3D
45	1L	702	3PE	C33-C34-C35-C36
50	1I	204	PC1	O21-C2-C3-O31
45	1N	401	3PE	C39-C3A-C3B-C3C
45	1N	401	3PE	C2-C3-O31-C31
58	1n	201	EHZ	S1-C10-C11-N1
50	1I	203	PC1	C11-C12-N-C14
45	1L	702	3PE	C22-C23-C24-C25
50	1I	203	PC1	C3B-C3C-C3D-C3E
50	1I	203	PC1	O32-C31-C32-C33
45	1L	704	3PE	C1-C2-O21-C21
45	1Y	201	3PE	C21-C22-C23-C24
50	1f	101	PC1	C21-C22-C23-C24
52	1M	501	PGT	C2-C1-O3P-P
53	1r	201	CDL	C12-C13-C14-C15
50	1f	101	PC1	O21-C2-C3-O31
50	1I	203	PC1	C23-C24-C25-C26
50	1L	703	PC1	C1-C2-C3-O31
52	1M	501	PGT	O3P-C1-C2-O2
53	1r	201	CDL	CB2-C1-CA2-OA2
52	1M	501	PGT	O3P-C1-C2-C3
45	1L	704	3PE	C1-C2-C3-O31
45	1Y	202	3PE	C12-C11-O13-P
53	1N	402	CDL	C53-C54-C55-C56
45	1L	704	3PE	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
50	1I	203	PC1	C33-C34-C35-C36
50	1I	203	PC1	C3A-C3B-C3C-C3D
45	1Y	201	3PE	O21-C2-C3-O31
52	1M	501	PGT	C35-C36-C37-C38
50	1L	703	PC1	O31-C31-C32-C33
50	1I	203	PC1	C11-C12-N-C13
50	1I	203	PC1	C39-C3A-C3B-C3C
45	1L	702	3PE	C37-C38-C39-C3A
50	1I	203	PC1	C11-C12-N-C15
58	1n	201	EHZ	C3-C4-C5-C6
48	1F	501	FMN	N10-C1'-C2'-O2'
50	1f	101	PC1	C27-C28-C29-C2A
45	1L	702	3PE	C35-C36-C37-C38
50	1I	203	PC1	C32-C33-C34-C35
53	1N	402	CDL	C52-C53-C54-C55
53	1N	402	CDL	C12-C13-C14-C15
52	1M	501	PGT	C32-C33-C34-C35
45	1Y	201	3PE	C32-C33-C34-C35
50	1f	101	PC1	O31-C31-C32-C33
50	1f	101	PC1	O32-C31-C32-C33
50	1L	703	PC1	O32-C31-C32-C33

There are no ring outliers.

25 monomers are involved in 90 short contacts:

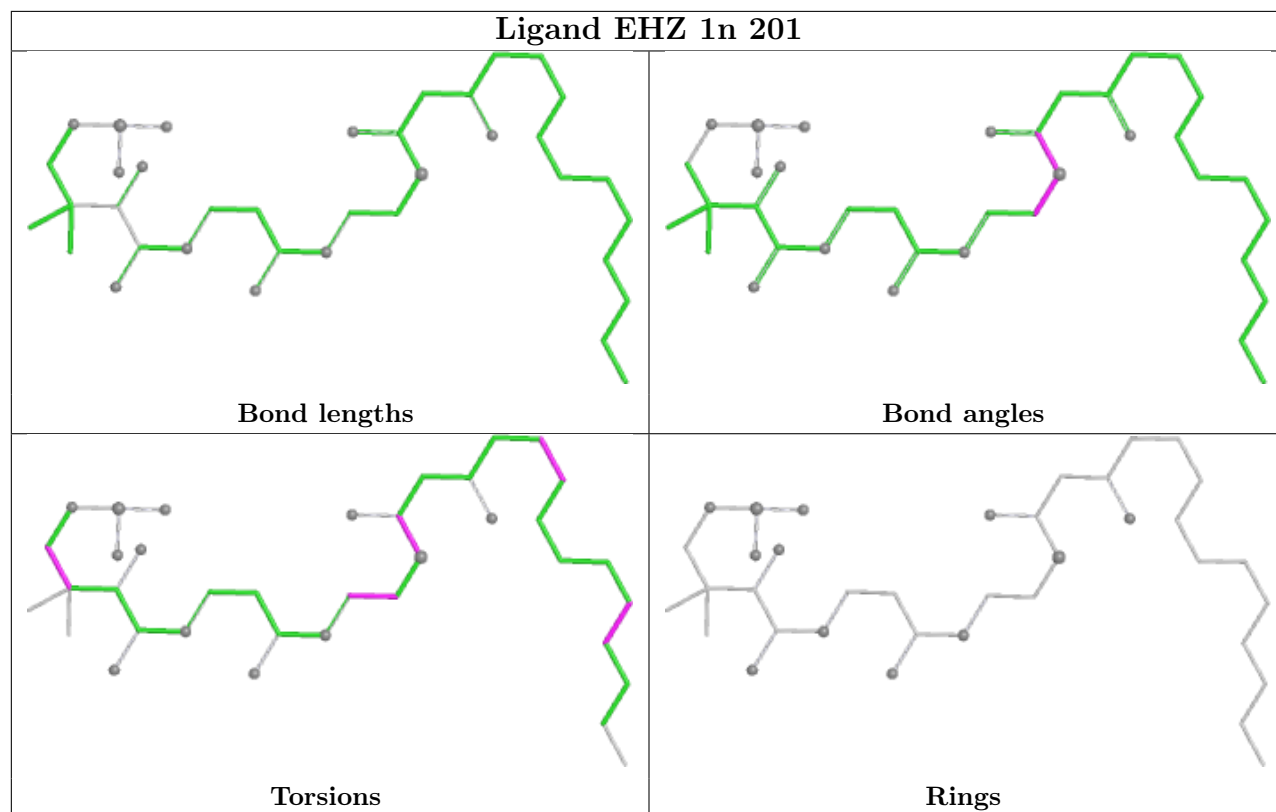
Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	1n	201	EHZ	1	0
50	1I	203	PC1	8	0
45	1L	702	3PE	6	0
56	1P	501	NDP	3	0
50	1L	703	PC1	2	0
46	1G	802	SF4	1	0
52	1M	501	PGT	9	0
54	1O	401	GTP	2	0
48	1F	501	FMN	2	0
58	1W	201	EHZ	5	0
46	1F	502	SF4	4	0
50	1J	201	PC1	4	0
47	1G	803	FES	1	0
50	1f	101	PC1	3	0
53	1N	402	CDL	6	0
47	1E	301	FES	4	0

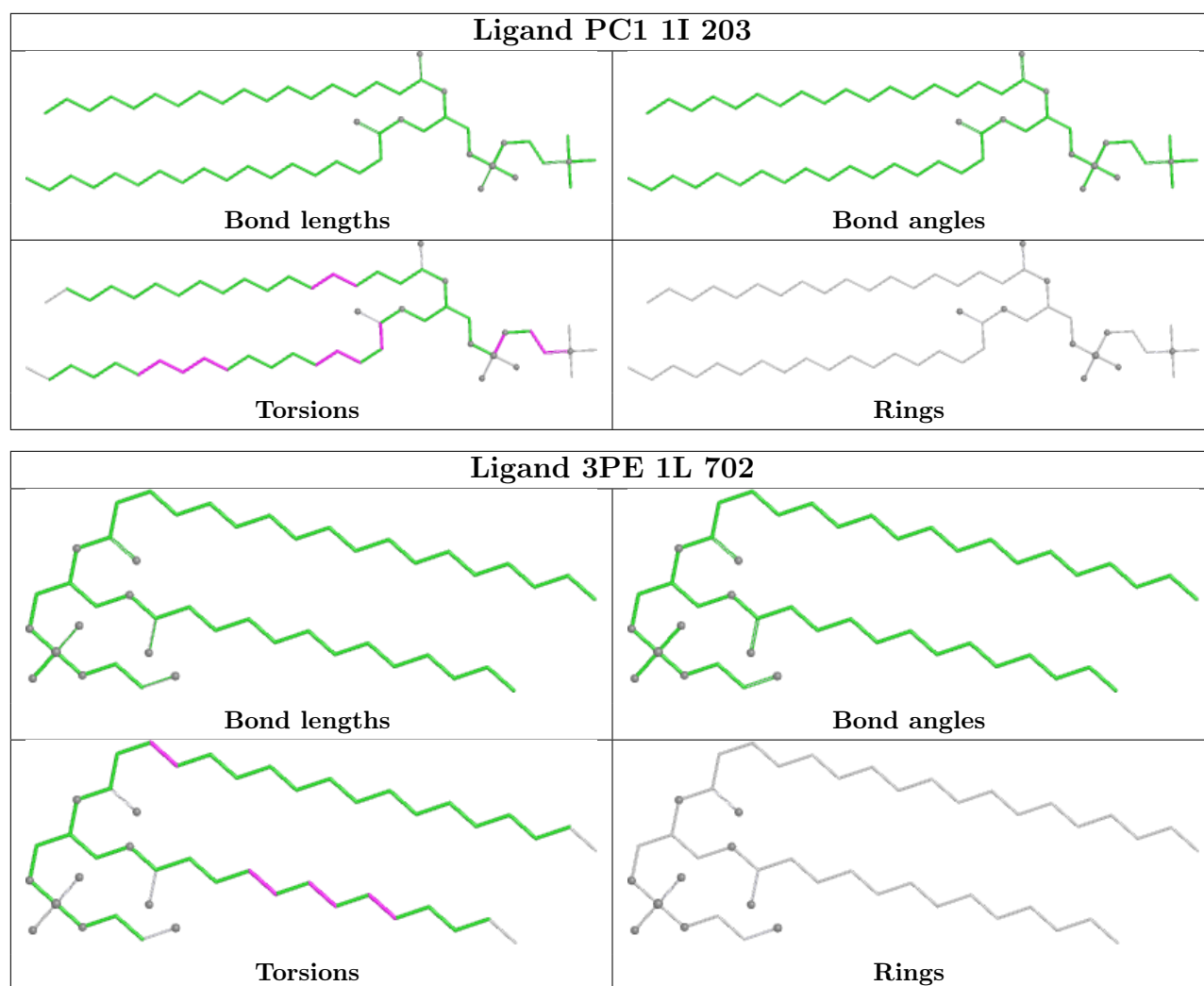
Continued on next page...

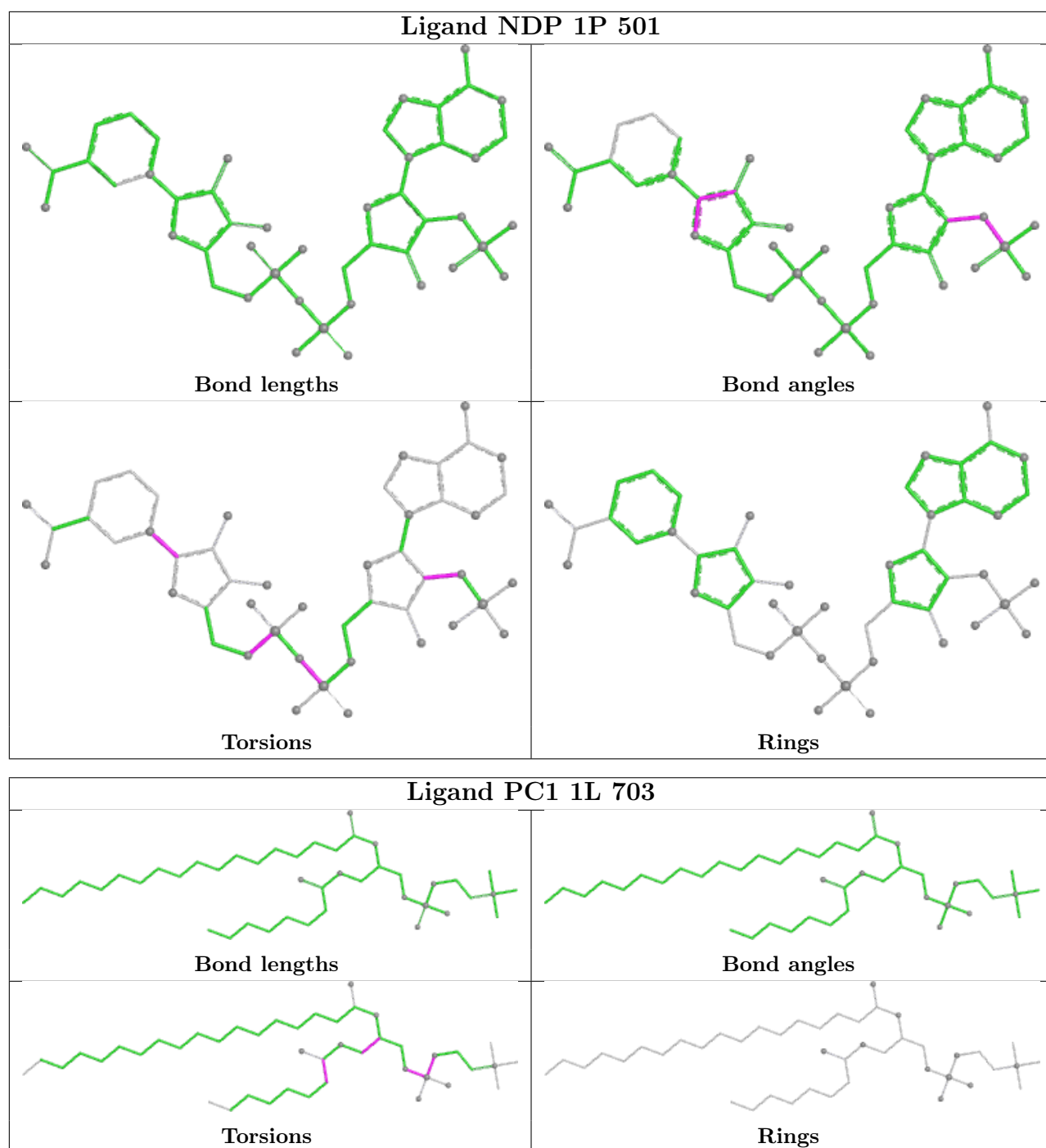
Continued from previous page...

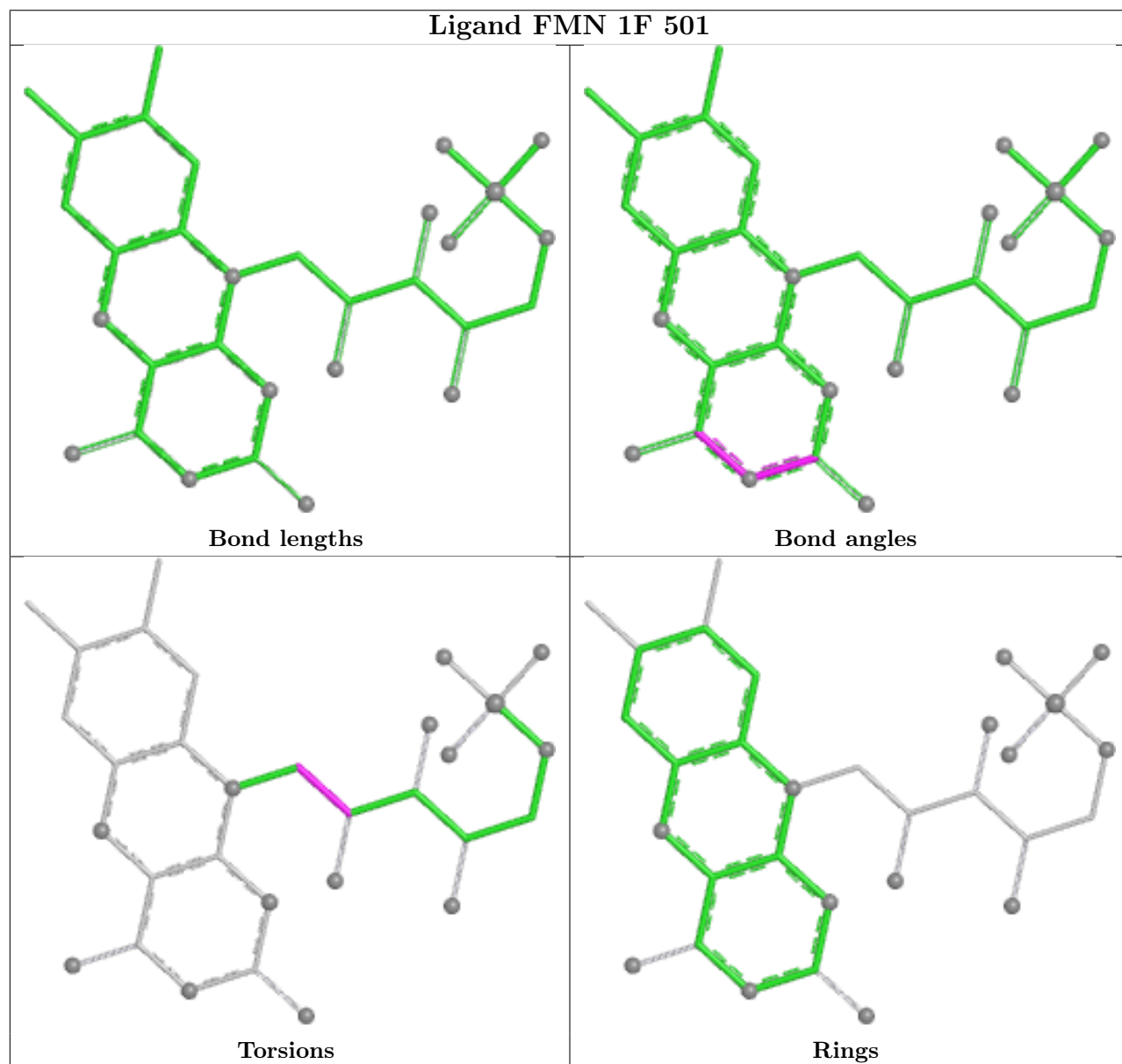
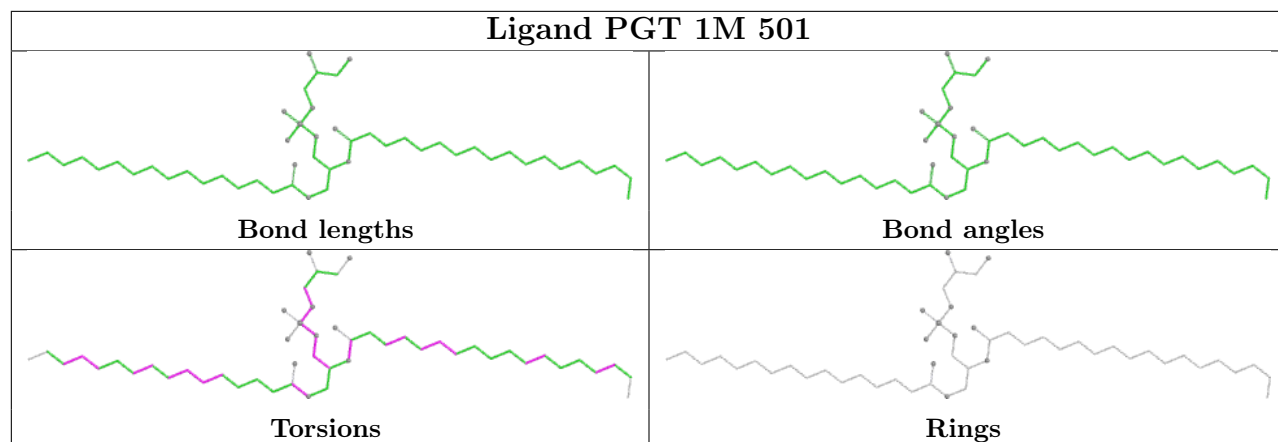
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1Y	202	3PE	1	0
45	1Y	201	3PE	5	0
45	1N	401	3PE	2	0
45	1L	704	3PE	4	0
45	1A	201	3PE	3	0
51	1L	701	MYR	5	0
46	1B	201	SF4	1	0
53	1r	201	CDL	6	0
50	1I	204	PC1	2	0

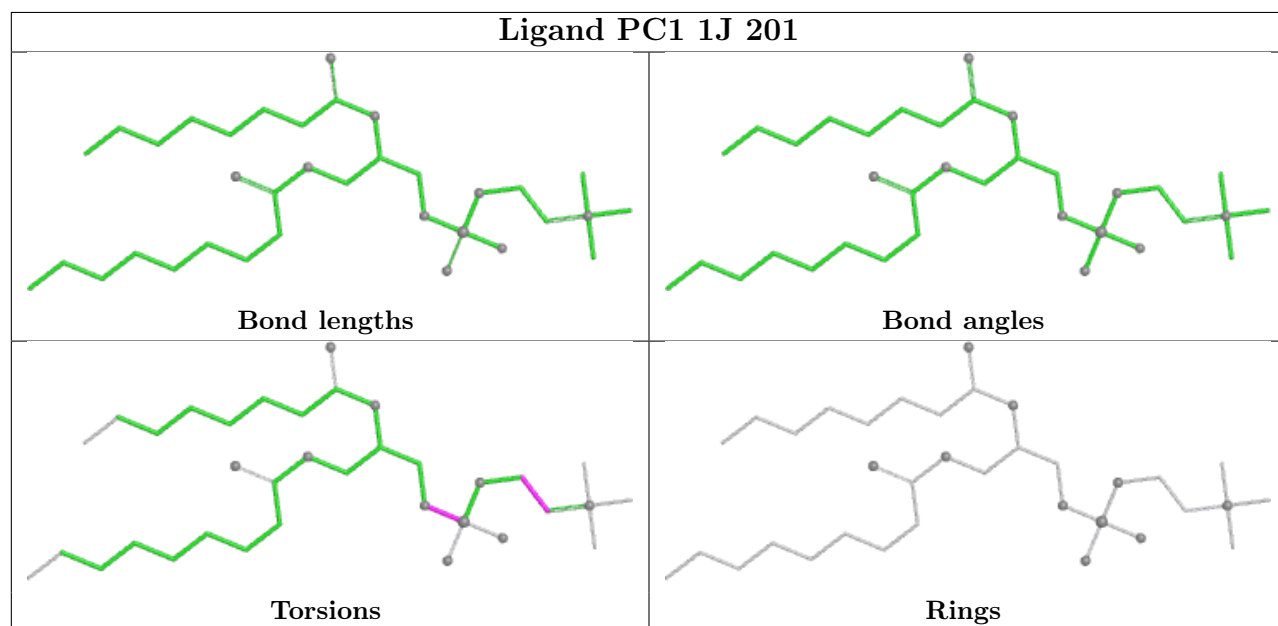
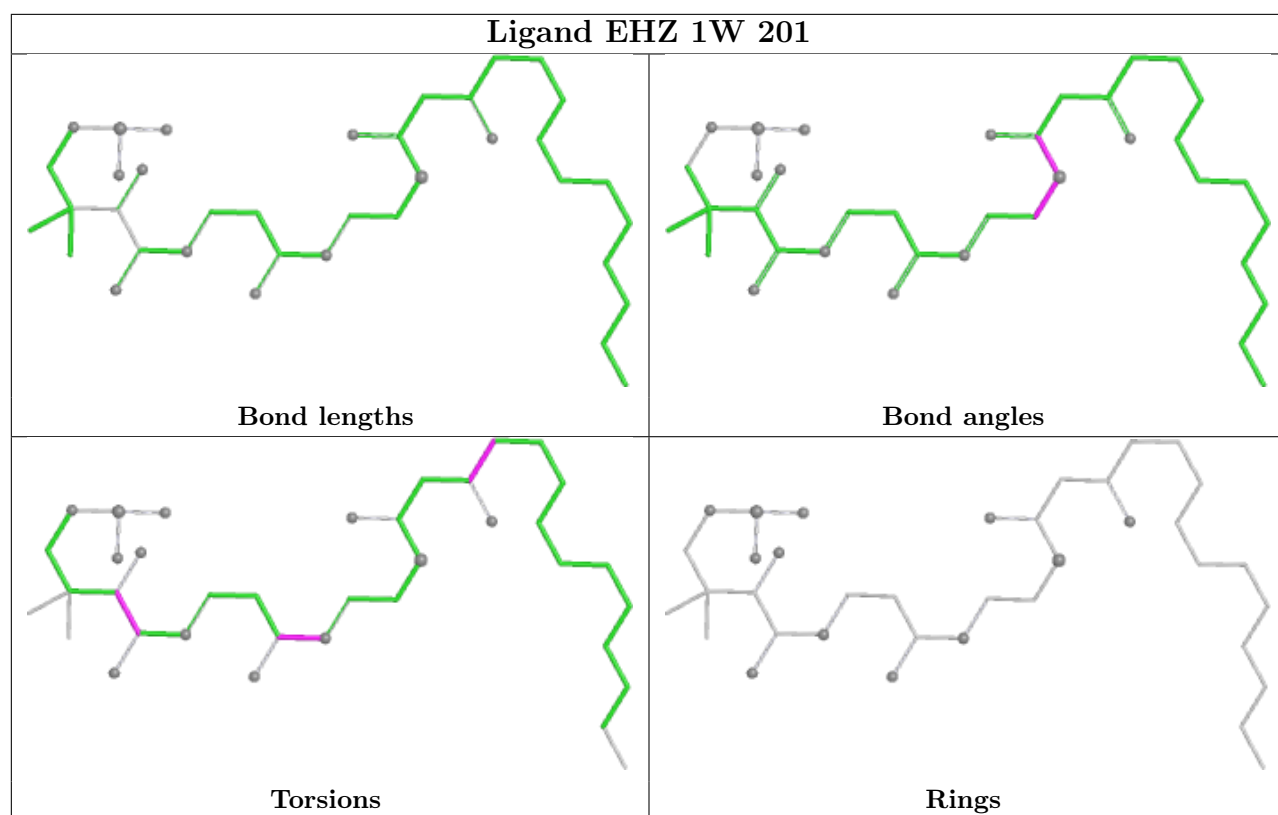
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

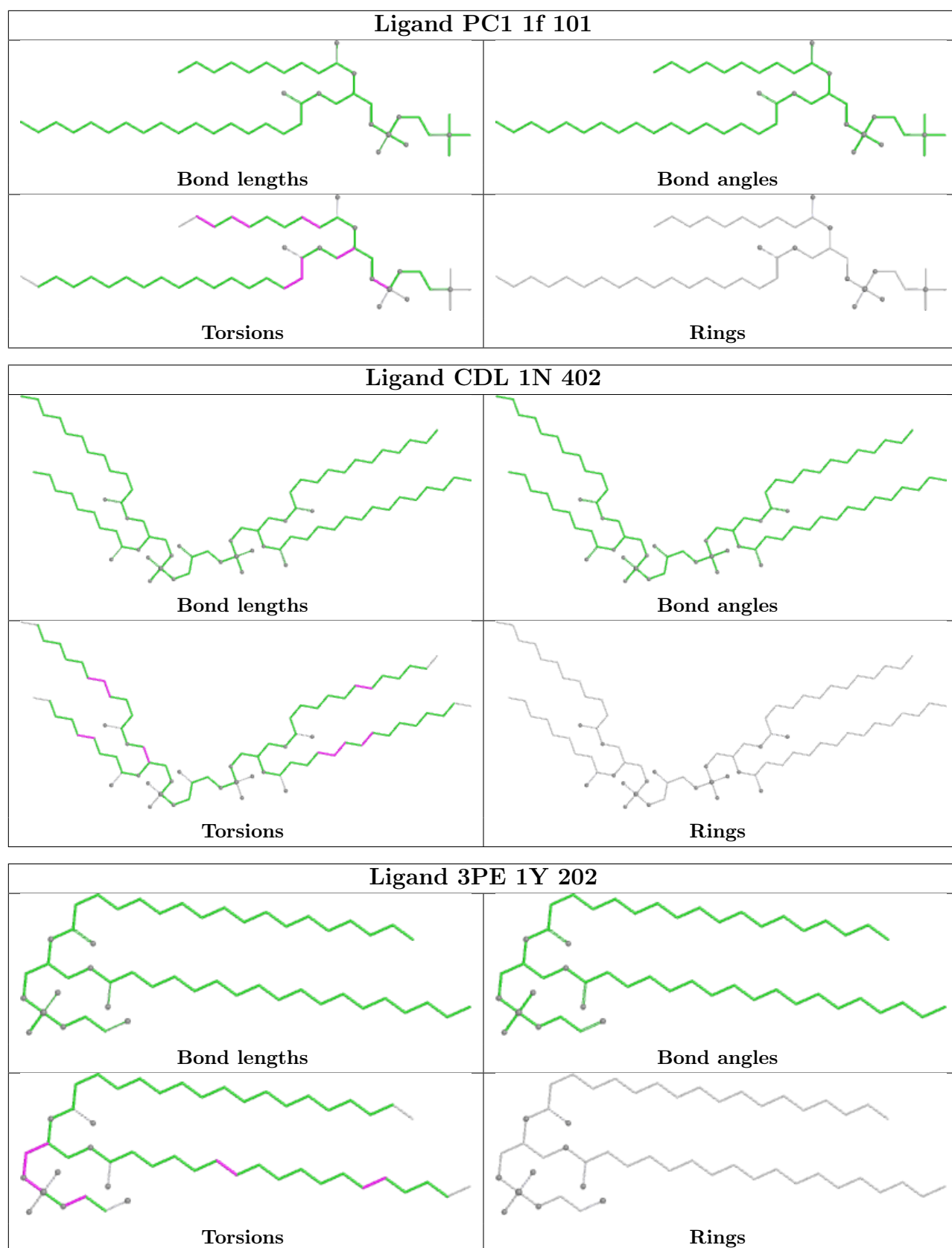


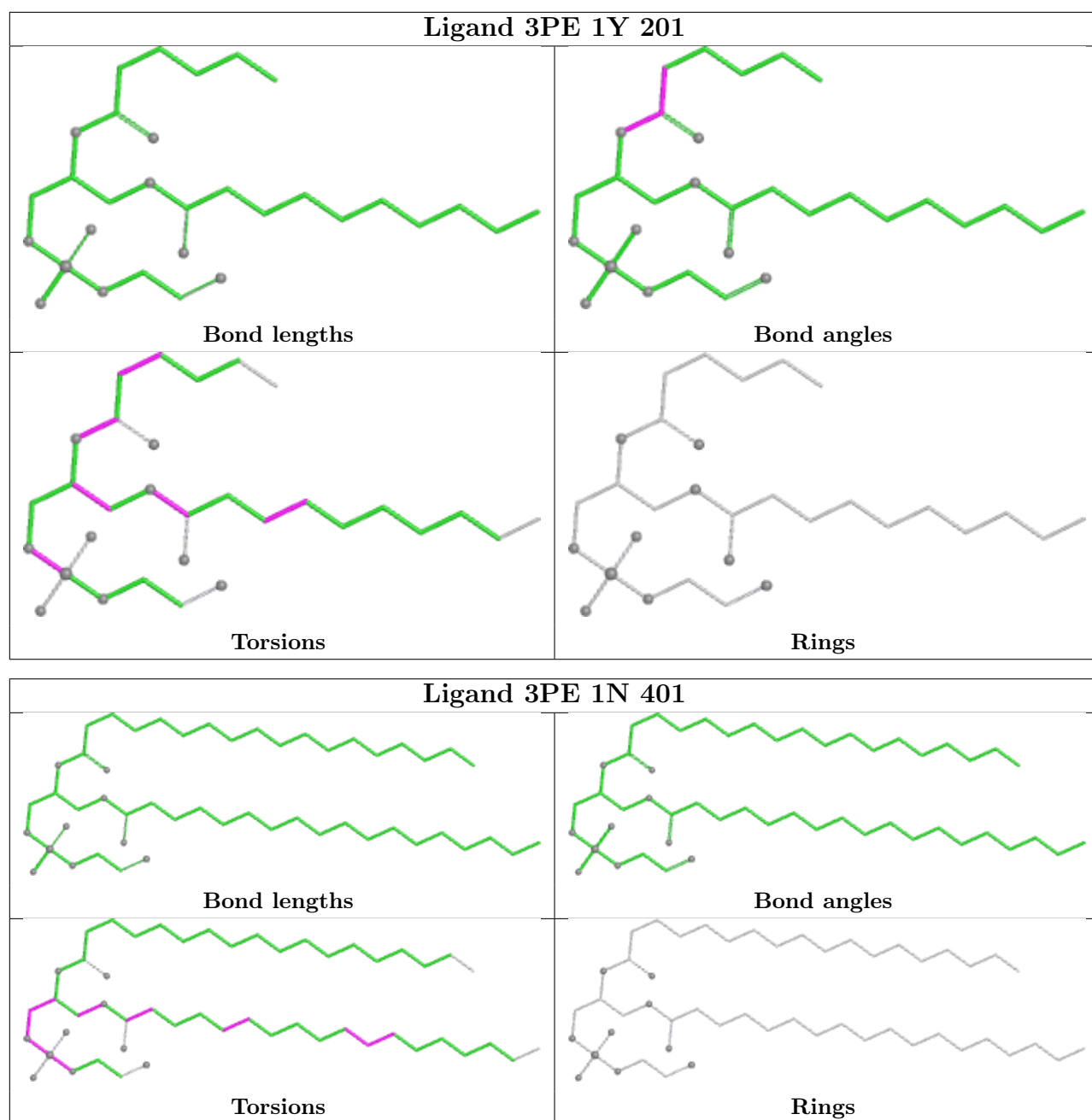


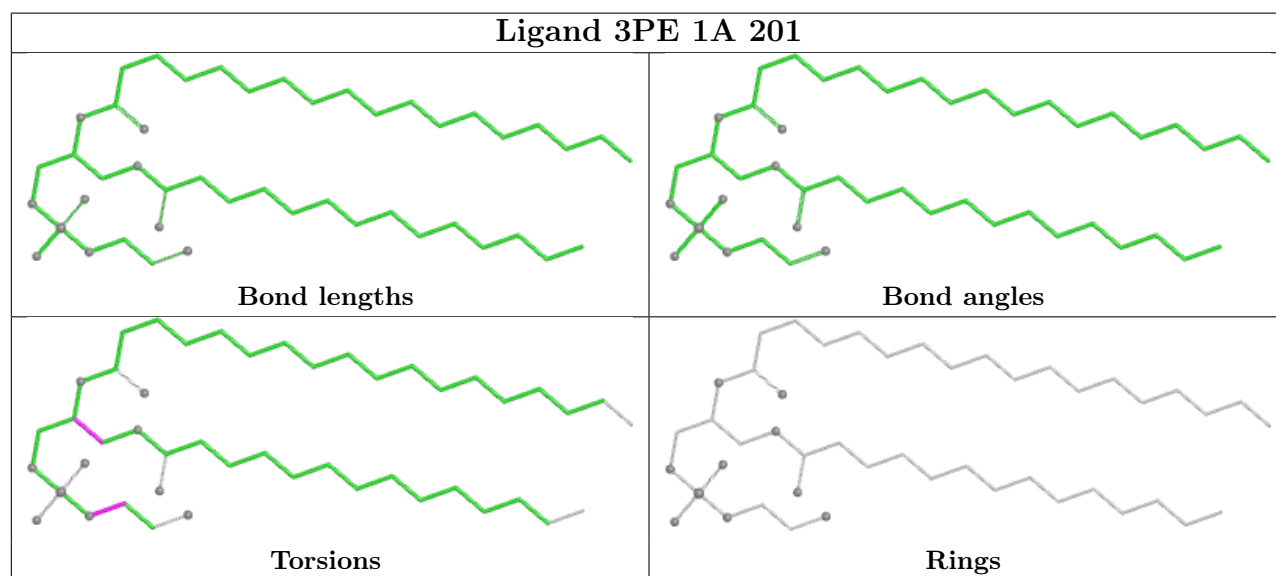
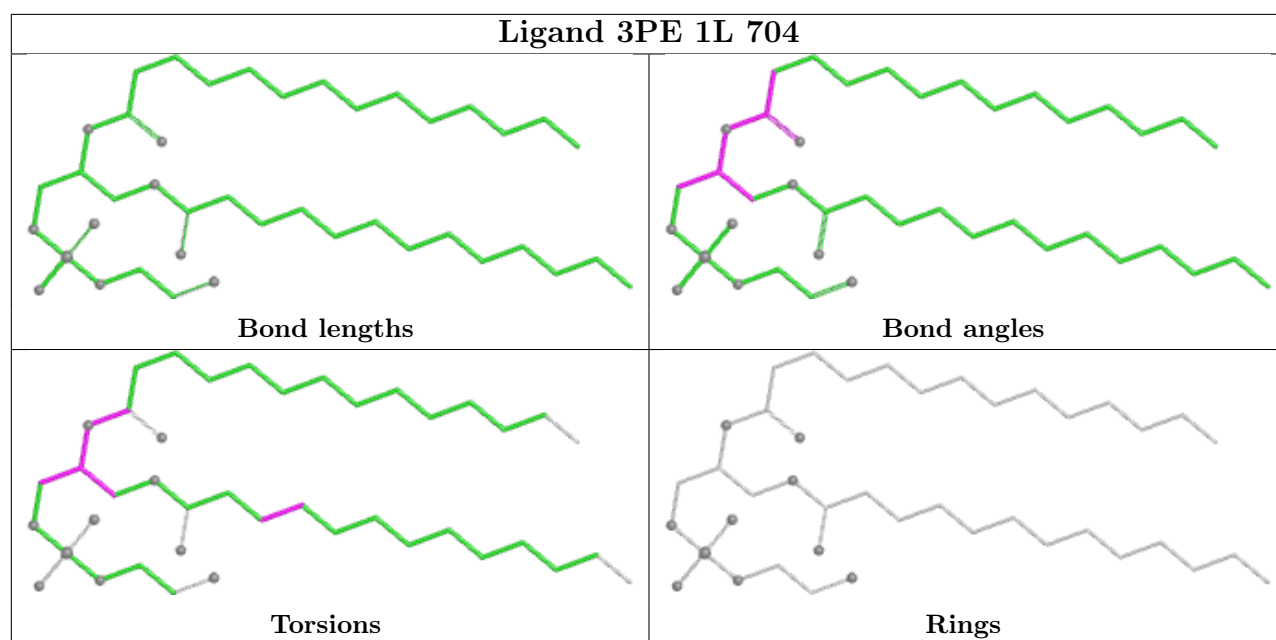


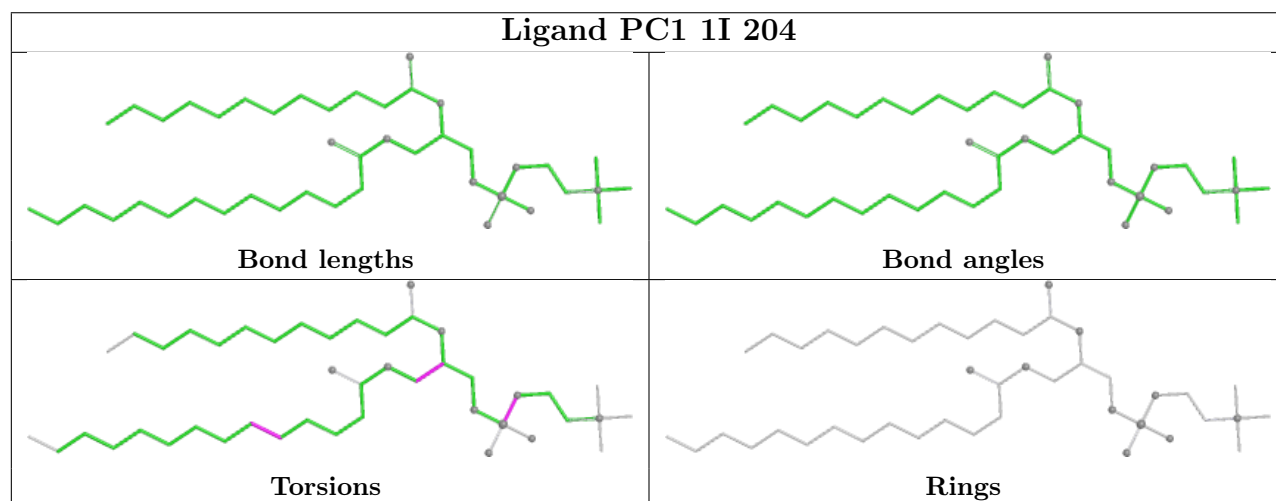
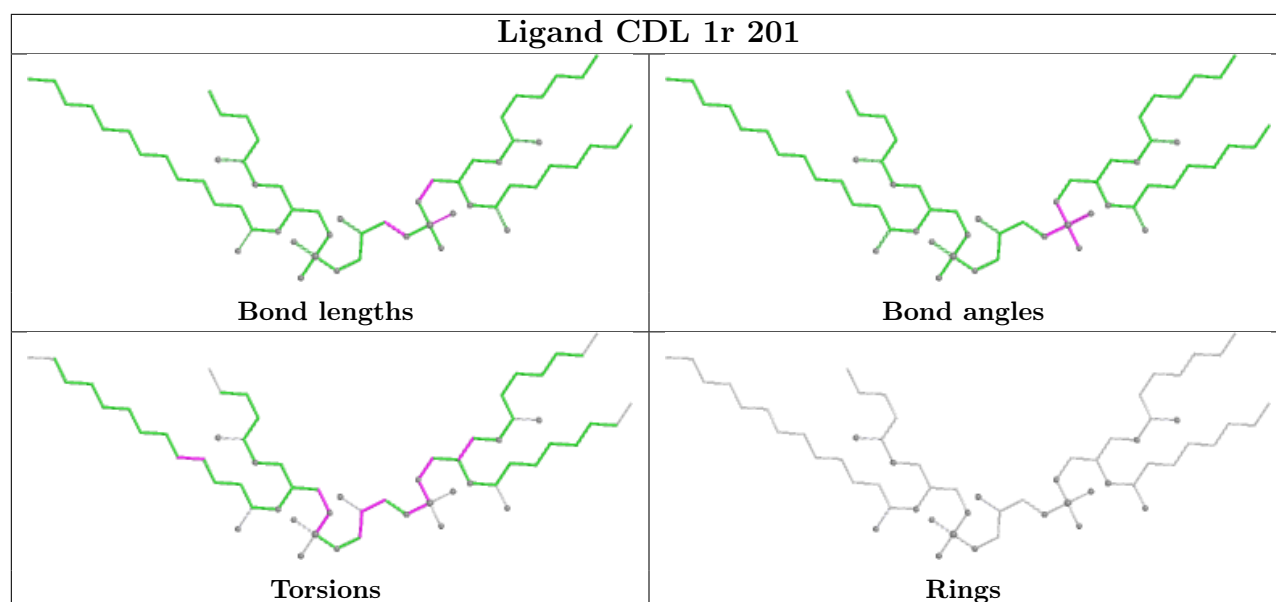












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1i	2
43	1r	1
22	1W	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	4.03
1	1r	1:ALA	C	2:SER	N	3.12
1	1i	54:ALA	C	55:PRO	N	1.79
1	1W	75:ASP	C	76:PRO	N	1.72

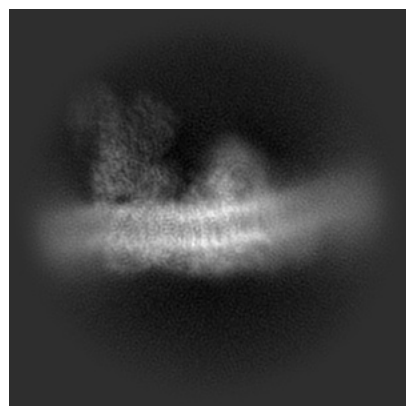
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42172. These allow visual inspection of the internal detail of the map and identification of artifacts.

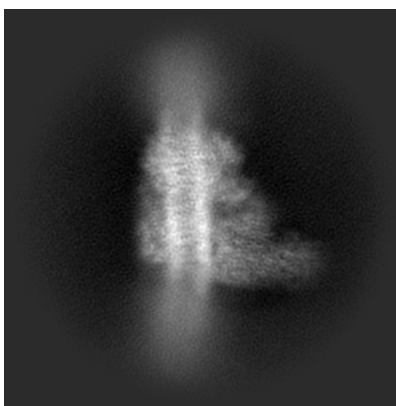
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

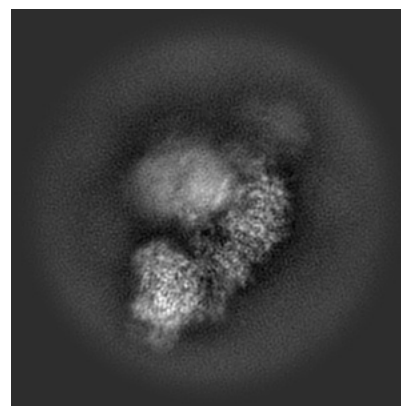
6.1.1 Primary map



X

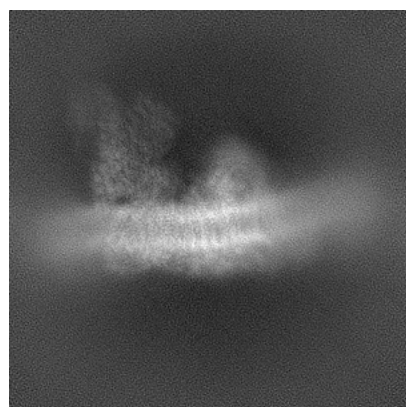


Y

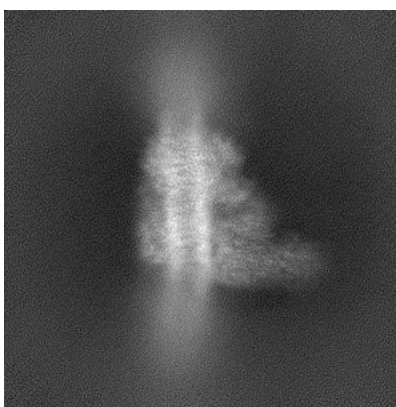


Z

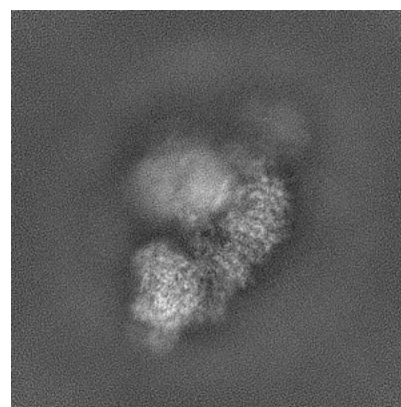
6.1.2 Raw map



X



Y

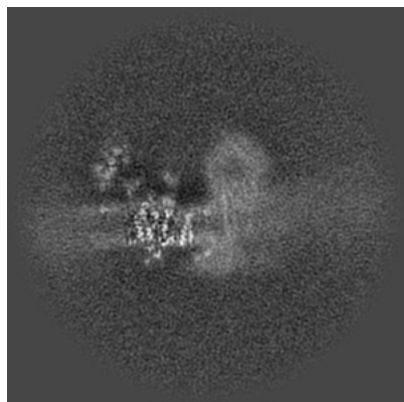


Z

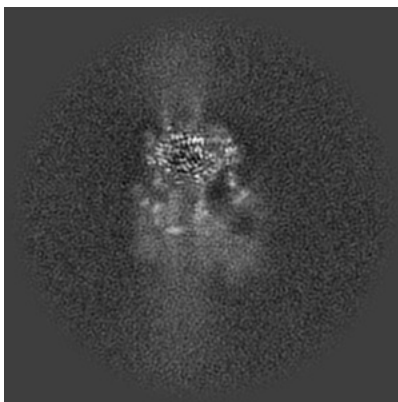
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

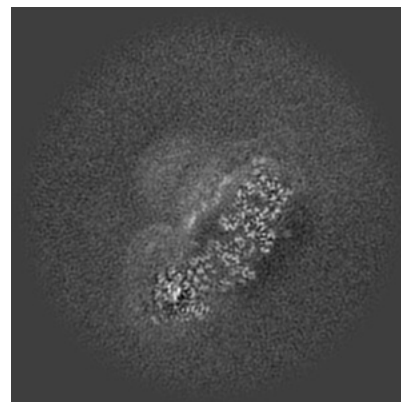
6.2.1 Primary map



X Index: 160

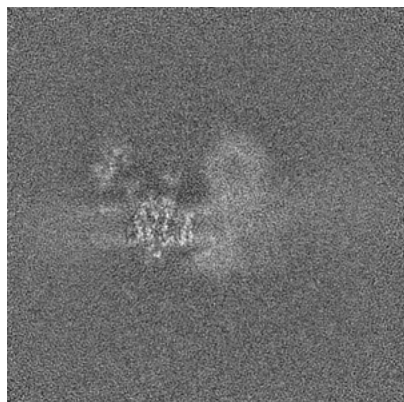


Y Index: 160

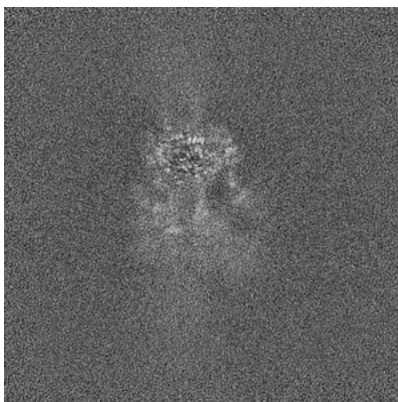


Z Index: 160

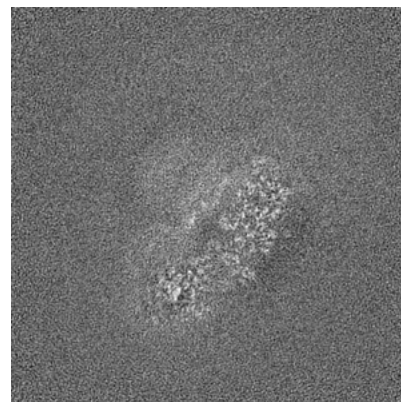
6.2.2 Raw map



X Index: 160



Y Index: 160

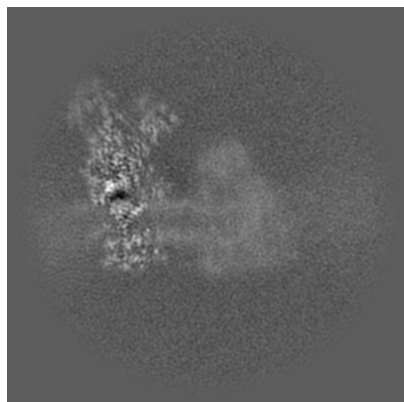


Z Index: 160

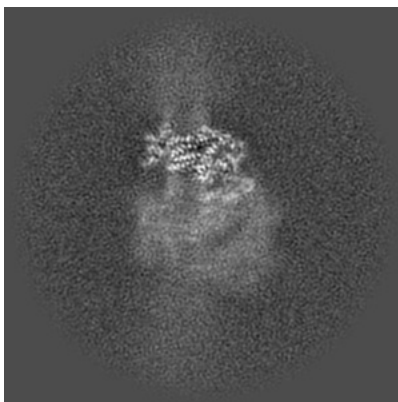
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

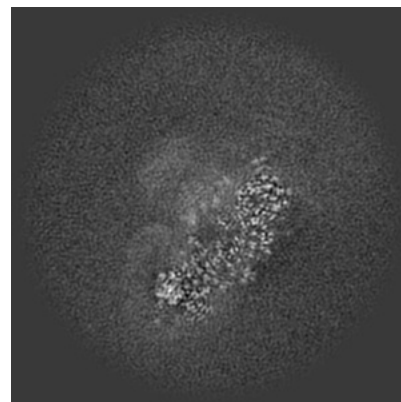
6.3.1 Primary map



X Index: 129

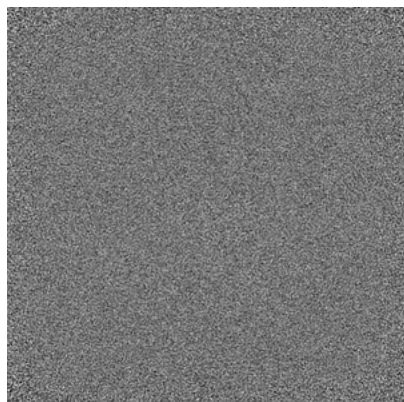


Y Index: 171

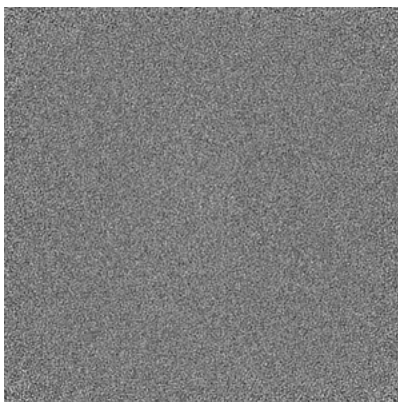


Z Index: 158

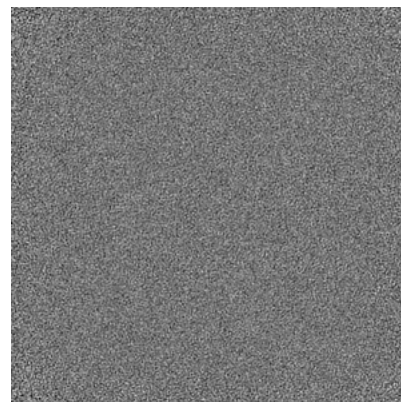
6.3.2 Raw map



X Index: 0



Y Index: 0

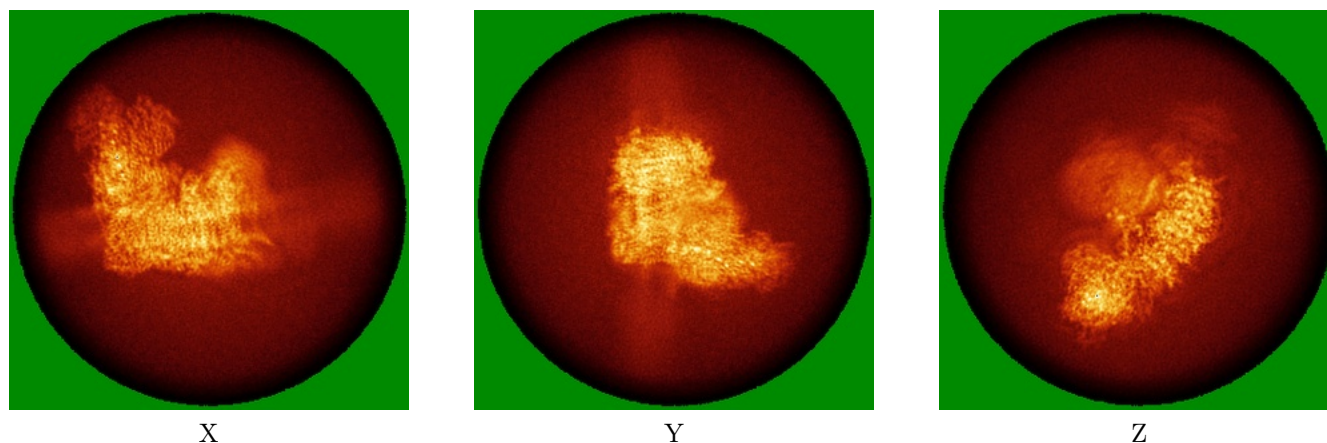


Z Index: 0

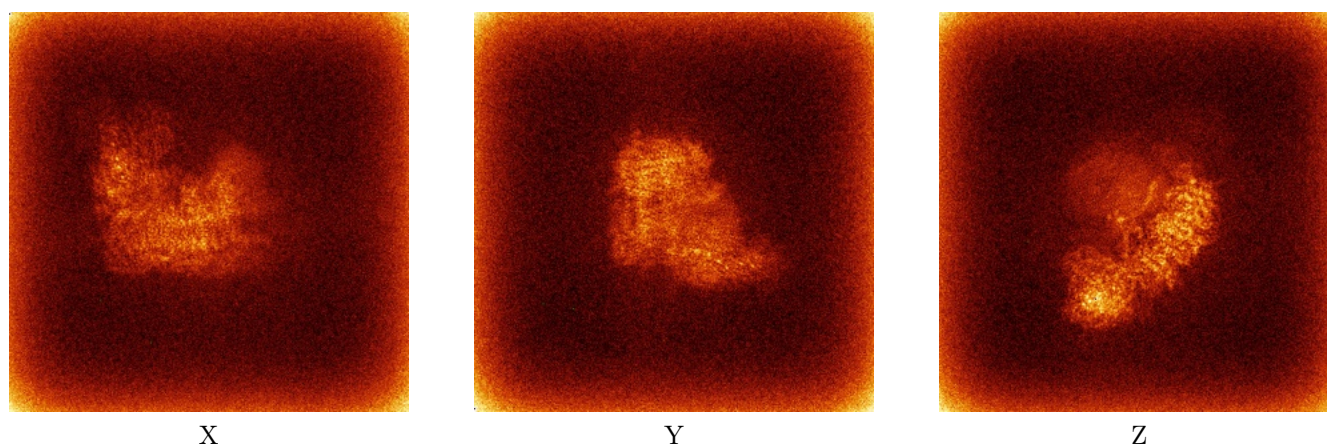
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

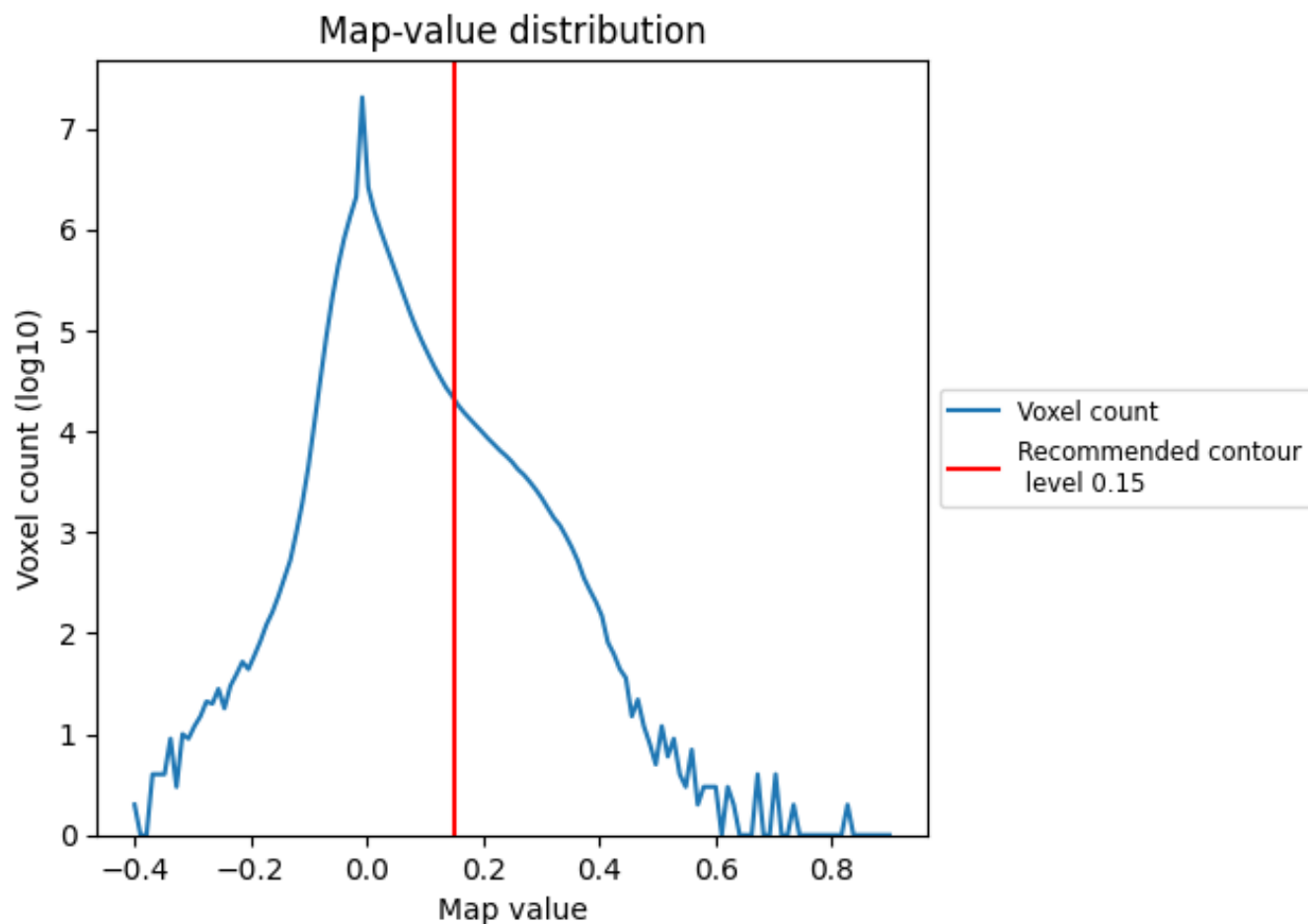
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

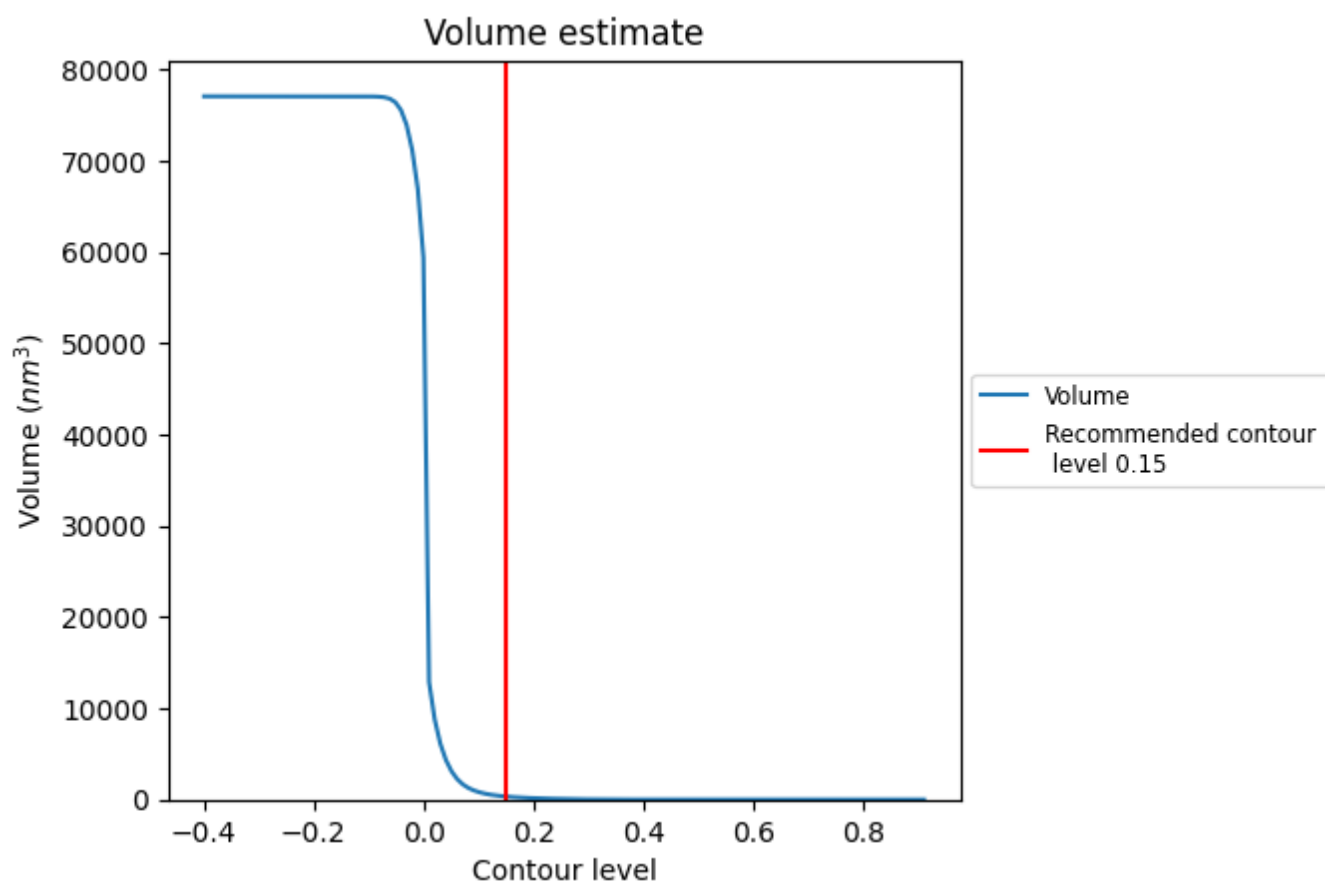
This section contains the results of statistical analysis of the map.

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.

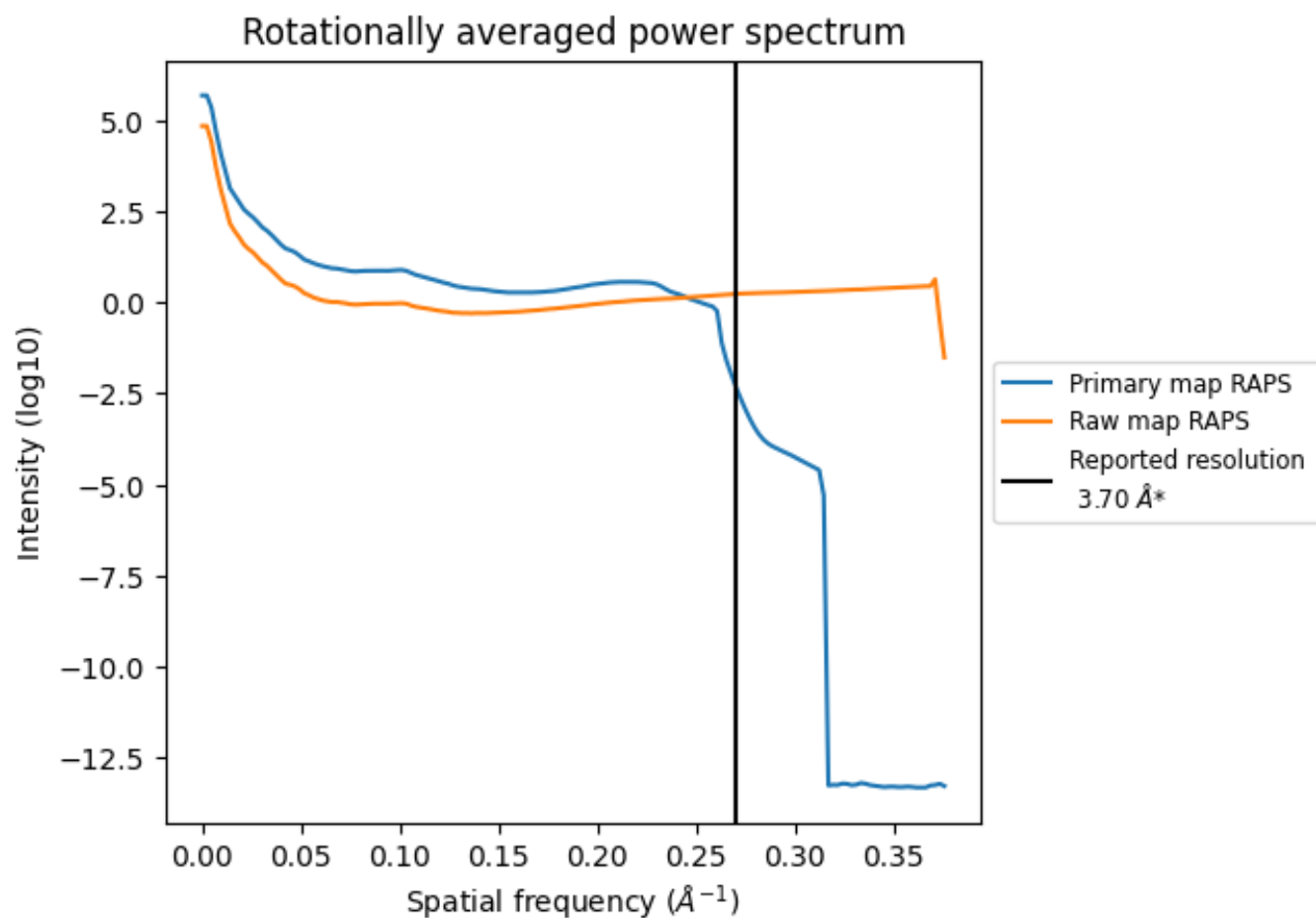
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 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 ⓘ

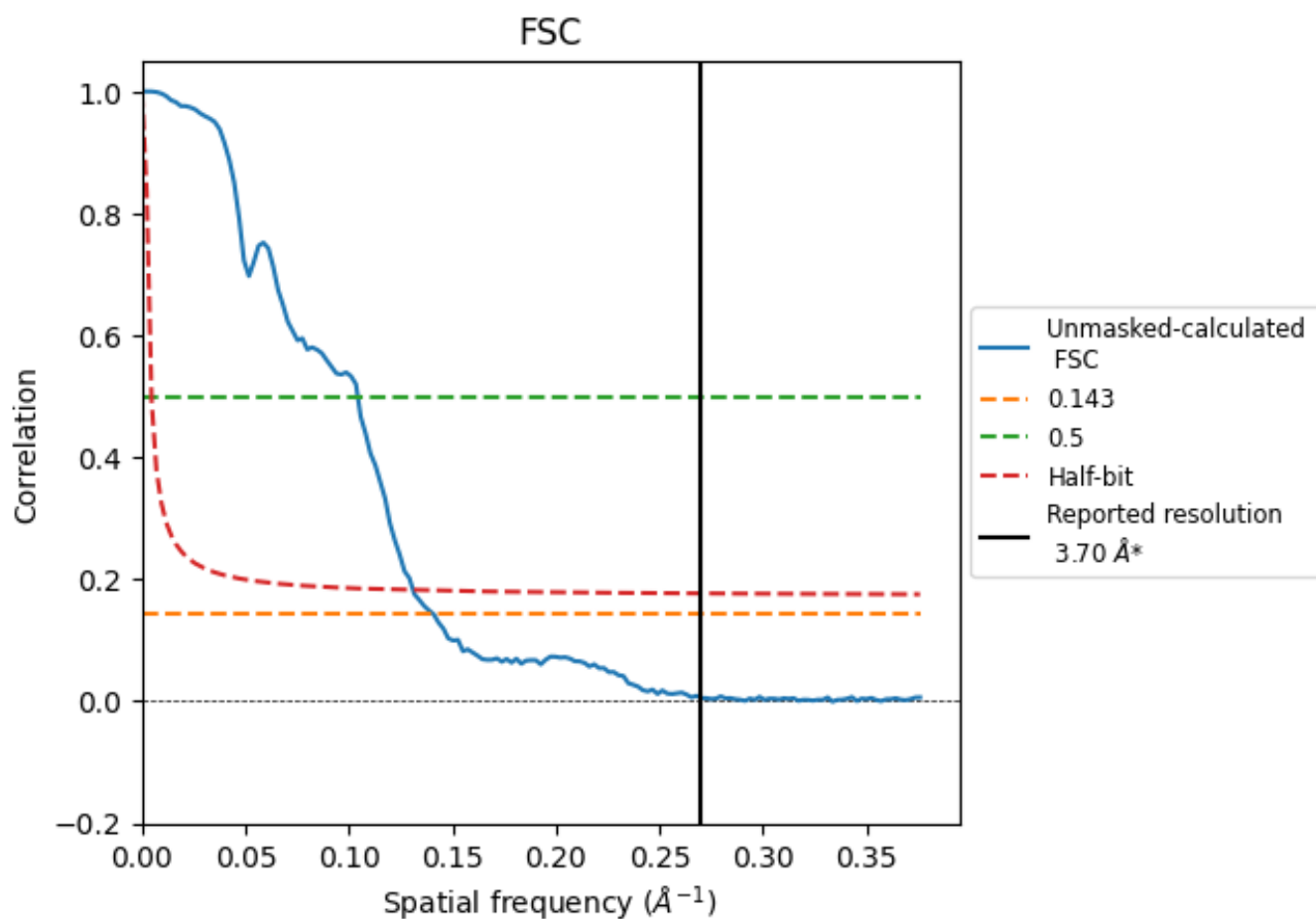


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

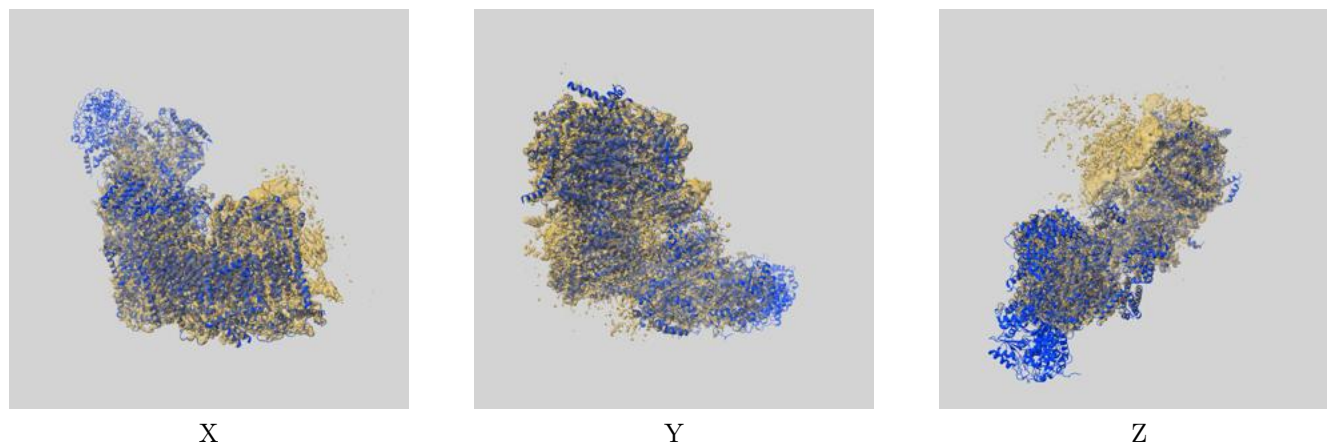
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.11	9.59	7.63

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.11 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

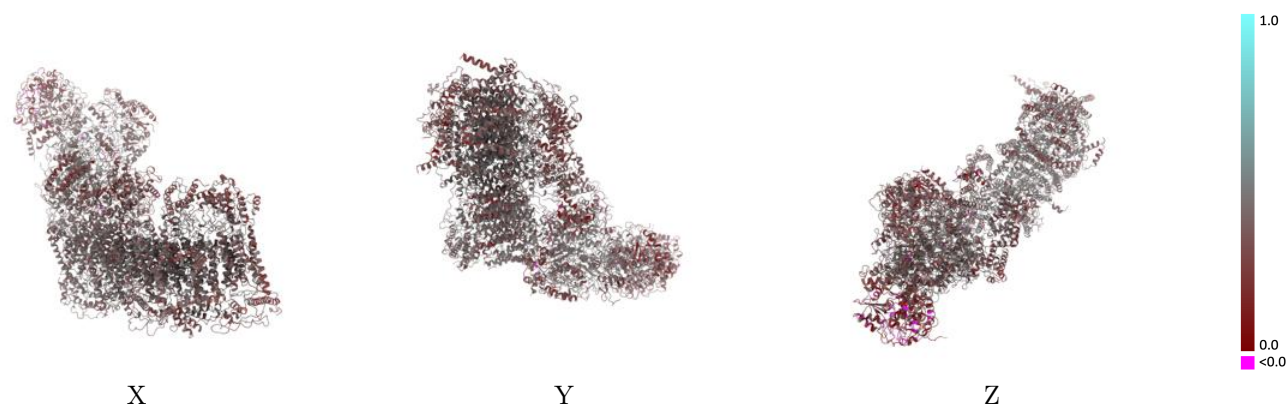
This section contains information regarding the fit between EMDB map EMD-42172 and PDB model 8UEV. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



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

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

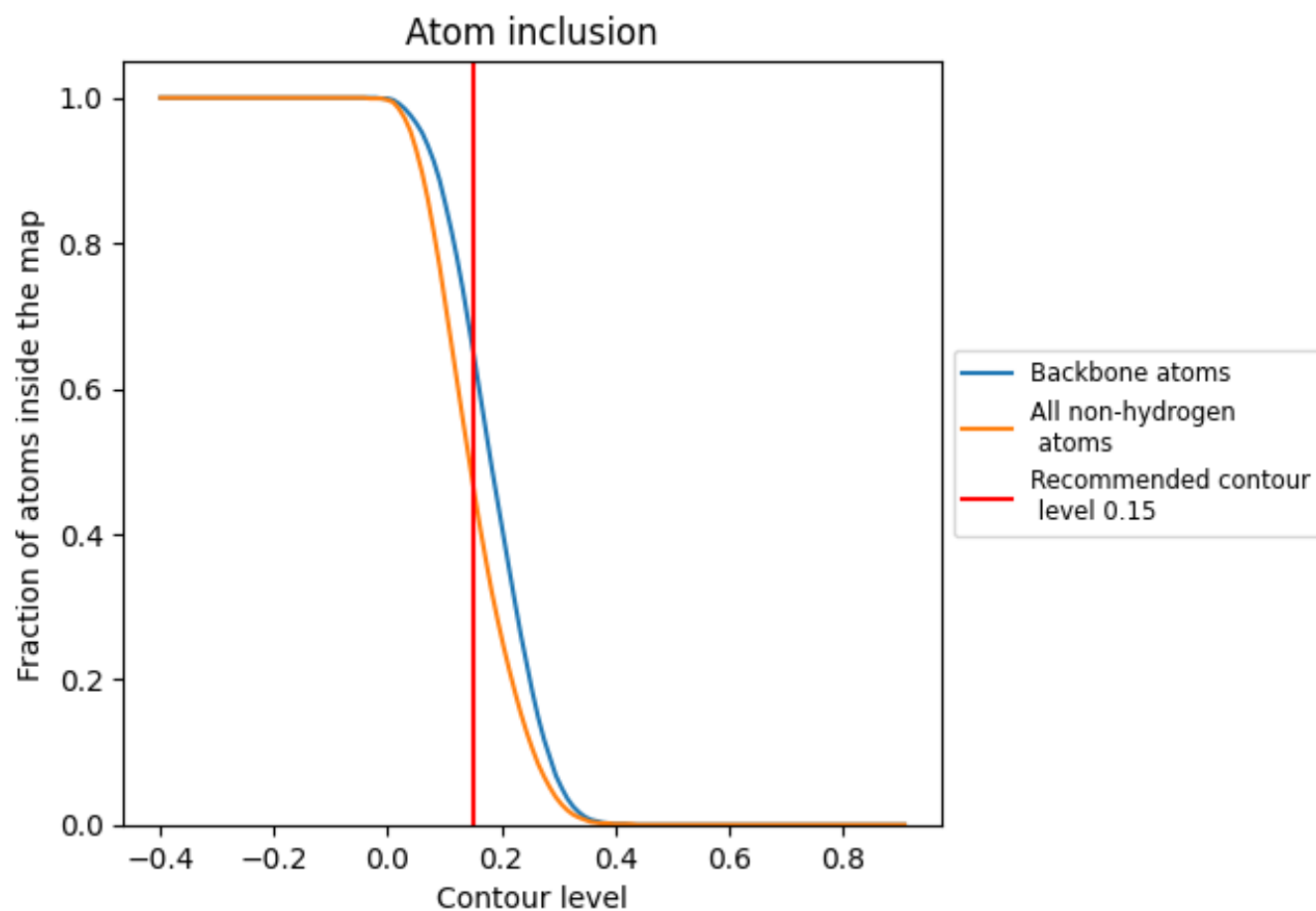


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 47% 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	 0.4700	 0.3720
1A	 0.5330	 0.3980
1B	 0.5360	 0.4120
1C	 0.3790	 0.4050
1D	 0.5130	 0.3900
1E	 0.0170	 0.2640
1F	 0.0260	 0.2420
1G	 0.2700	 0.3560
1H	 0.6000	 0.4040
1I	 0.5430	 0.4040
1J	 0.4900	 0.3710
1K	 0.5900	 0.4010
1L	 0.7030	 0.4000
1M	 0.7470	 0.4290
1N	 0.6660	 0.4180
1O	 0.3710	 0.3540
1P	 0.2900	 0.3420
1Q	 0.2780	 0.3820
1R	 0.2670	 0.4000
1S	 0.1250	 0.2970
1T	 0.2030	 0.2660
1U	 0.6350	 0.3460
1V	 0.2070	 0.3340
1W	 0.2910	 0.3410
1X	 0.5300	 0.4010
1Y	 0.6650	 0.3700
1Z	 0.5480	 0.4060
1a	 0.6560	 0.4080
1b	 0.5310	 0.4090
1c	 0.4360	 0.3760
1d	 0.6810	 0.4150
1e	 0.5760	 0.4250
1f	 0.4550	 0.3590
1g	 0.6000	 0.3840
1h	 0.6400	 0.3980



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Chain	Atom inclusion	Q-score
1i	 0.3950	 0.3490
1j	 0.5200	 0.3690
1k	 0.5260	 0.3480
1l	 0.6480	 0.3910
1m	 0.6980	 0.3850
1n	 0.6530	 0.3660
1o	 0.4940	 0.3250
1p	 0.6120	 0.3770
1q	 0.4190	 0.4040
1r	 0.3430	 0.3900
1s	 0.0000	 0.2230