



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:21 PM EDT

PDB ID : 8UET / pdb_00008uet
EMDB ID : EMD-42170
Title : In-situ complex I, Deactive class02
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:

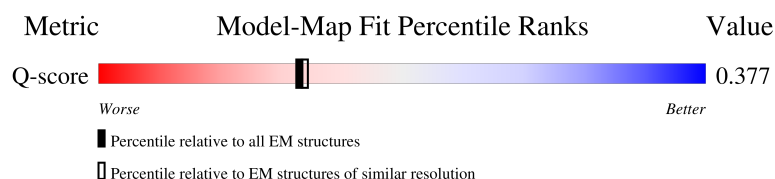
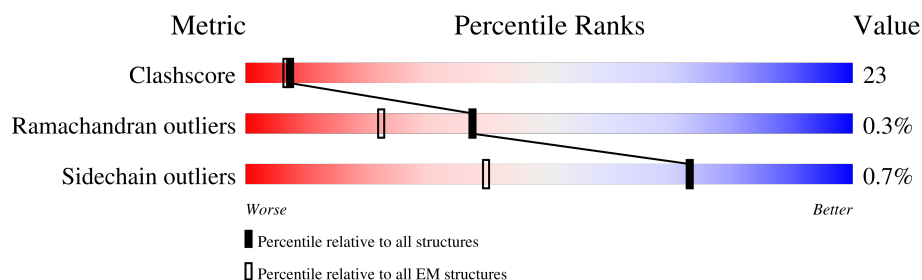
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.70 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	

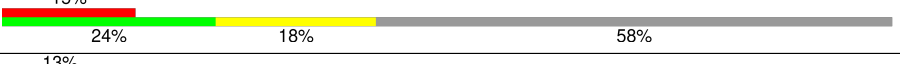
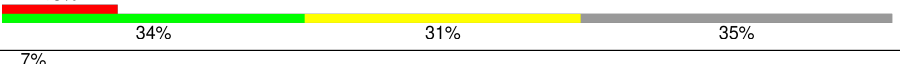
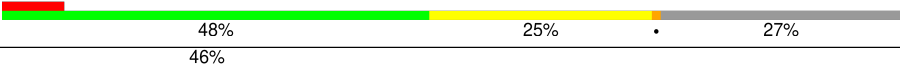
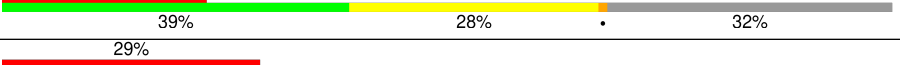
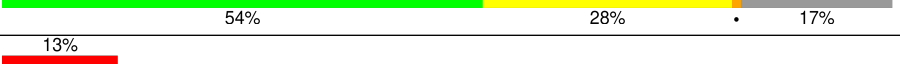
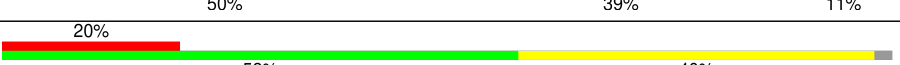
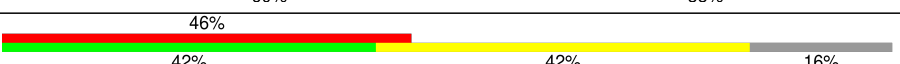
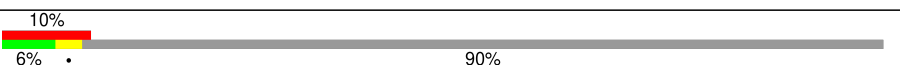
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24	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	1B	201	-	-	X	-
46	SF4	1I	201	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67180 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	87	Total	C	N	O	S	0	0
			700	479	100	116	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	418	Total	C	N	O	S	0	0
			3376	2159	577	616	24		

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
38	1m	128	Total	C	N	O		
			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

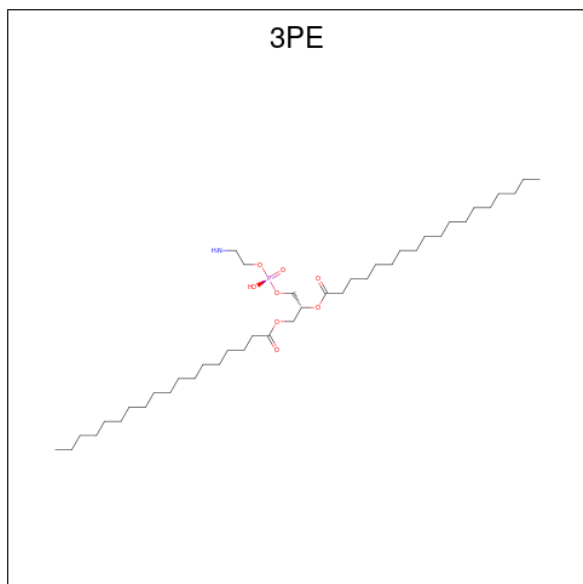
There is a discrepancy between the modelled and reference sequences:

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

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

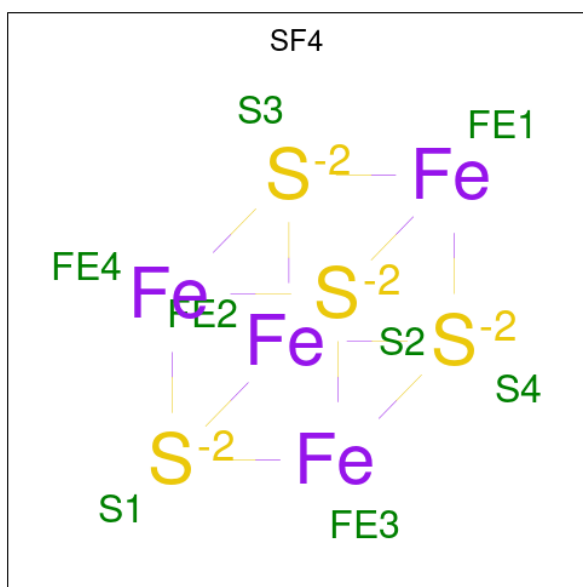
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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



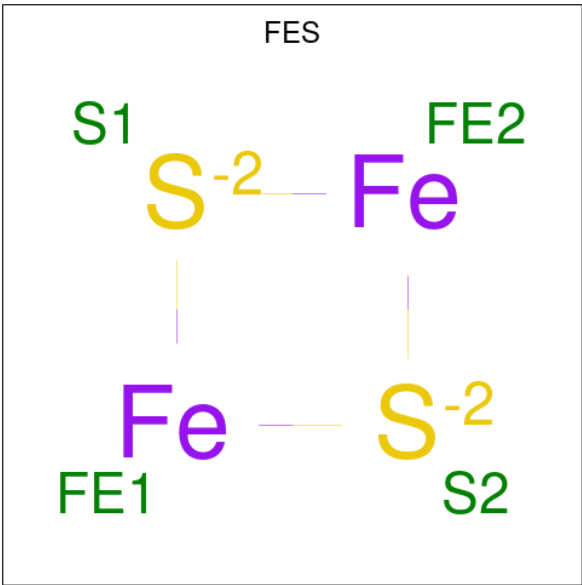
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



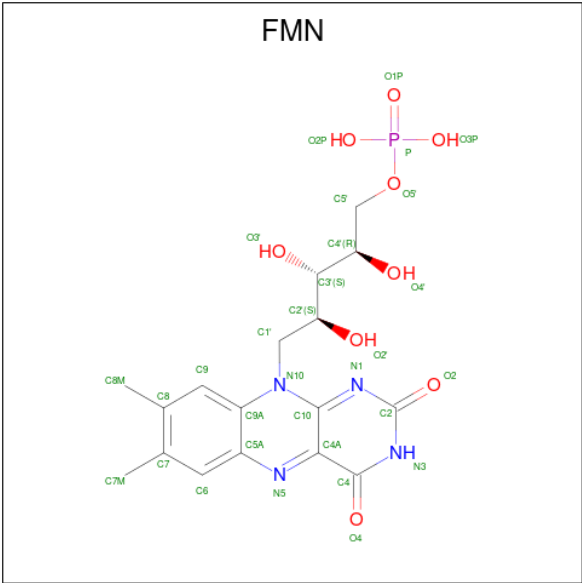
Mol	Chain	Residues	Atoms			AltConf
46	1B	1	Total	Fe	S	0
			8	4	4	
46	1F	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	

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



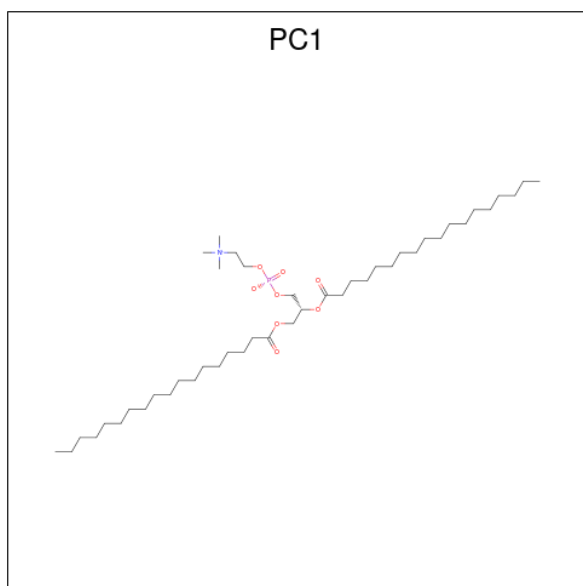
Mol	Chain	Residues	Atoms			AltConf
47	1E	1	Total	Fe	S	0
			4	2	2	
47	1G	1	Total	Fe	S	0
			4	2	2	

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



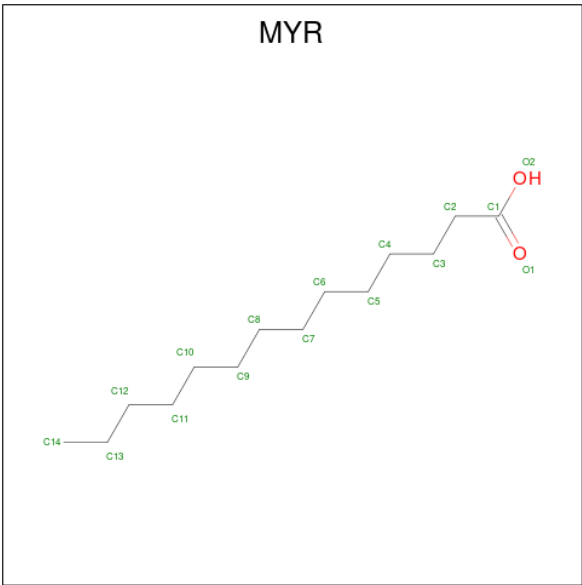
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

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



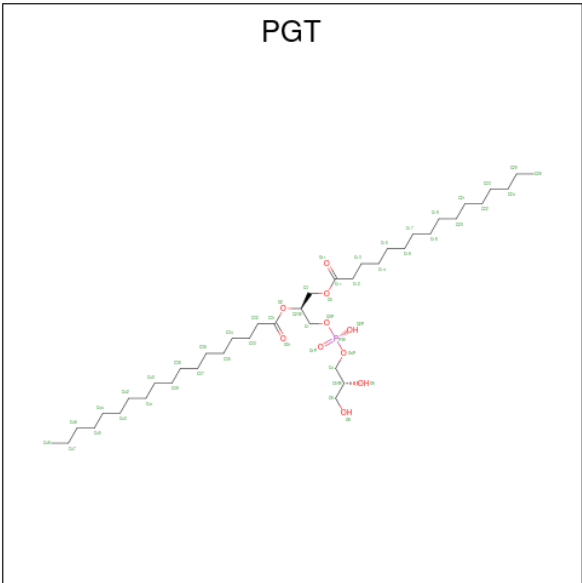
Mol	Chain	Residues	Atoms					AltConf
50	1H	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



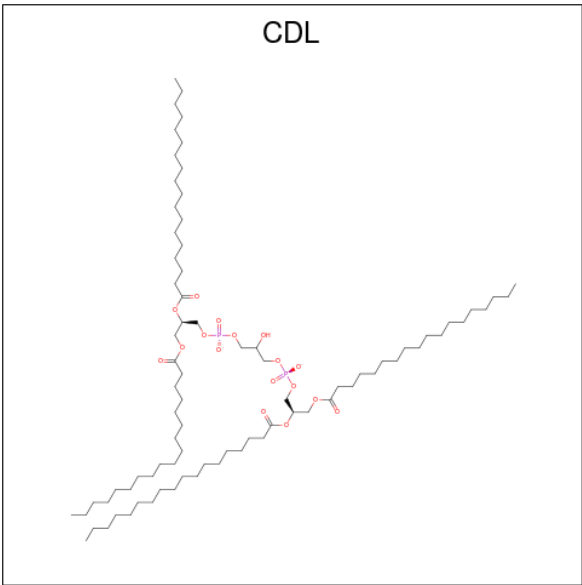
Mol	Chain	Residues	Atoms			AltConf
51	1L	1	Total	C	O	0
			15	14	1	

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



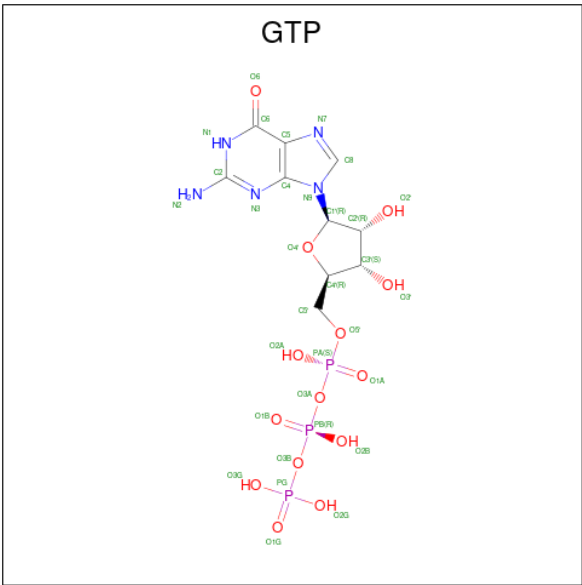
Mol	Chain	Residues	Atoms				AltConf
52	1M	1	Total	C	O	P	0
			51	40	10	1	

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



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

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

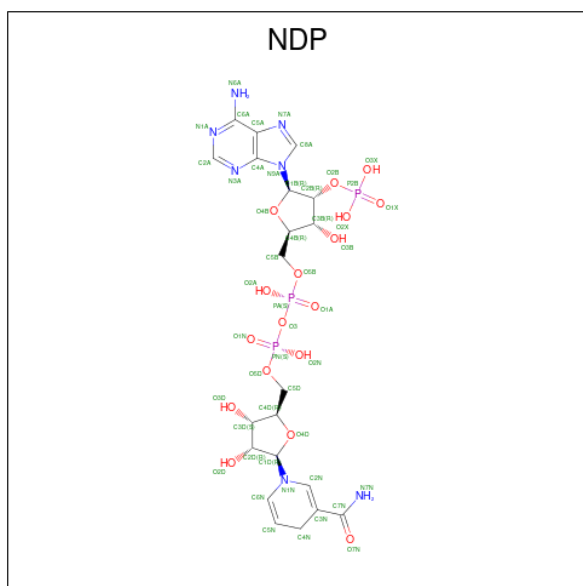


Mol	Chain	Residues	Atoms					AltConf
54	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

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

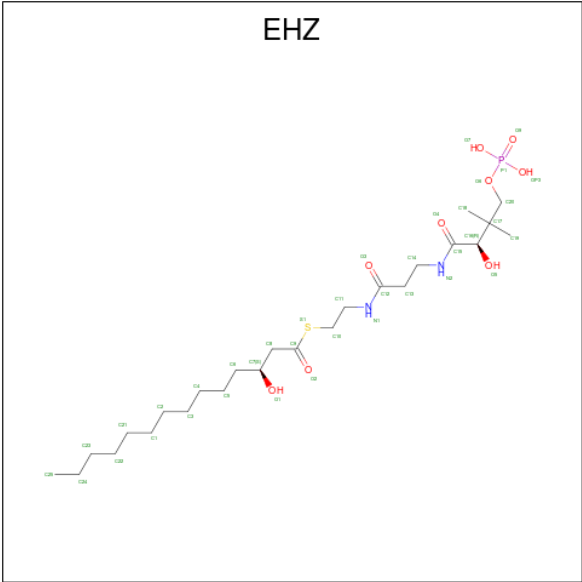


Mol	Chain	Residues	Atoms					AltConf
56	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

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

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

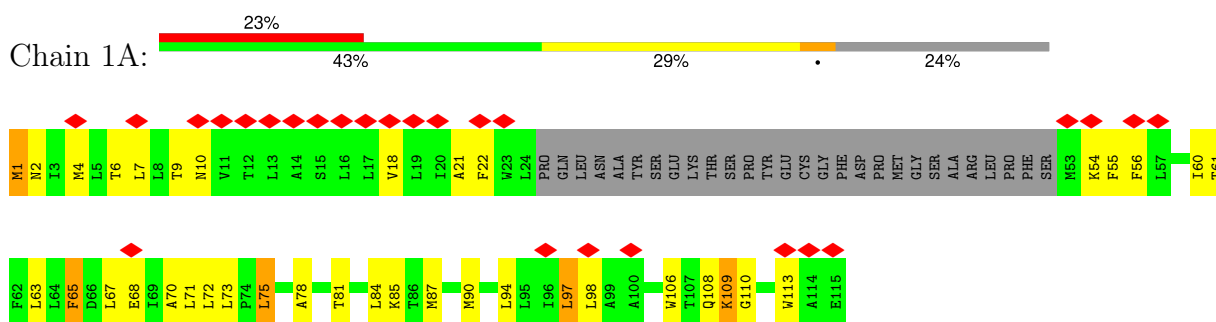


Mol	Chain	Residues	Atoms						AltConf
58	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
58	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

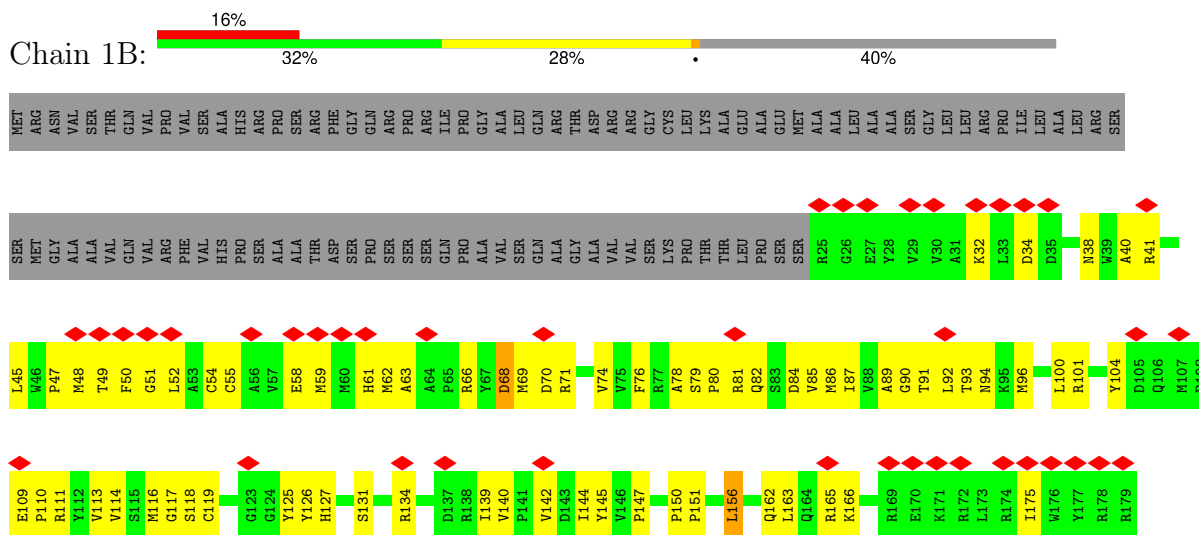
3 Residue-property plots

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

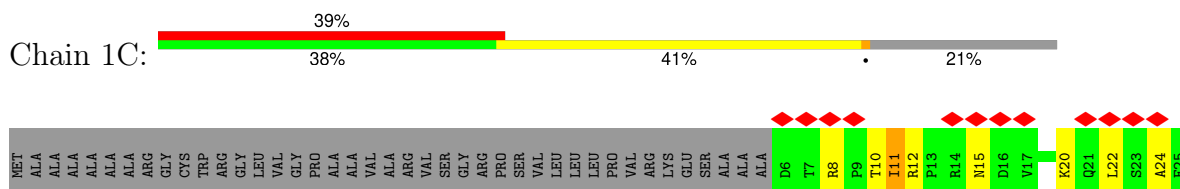
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



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

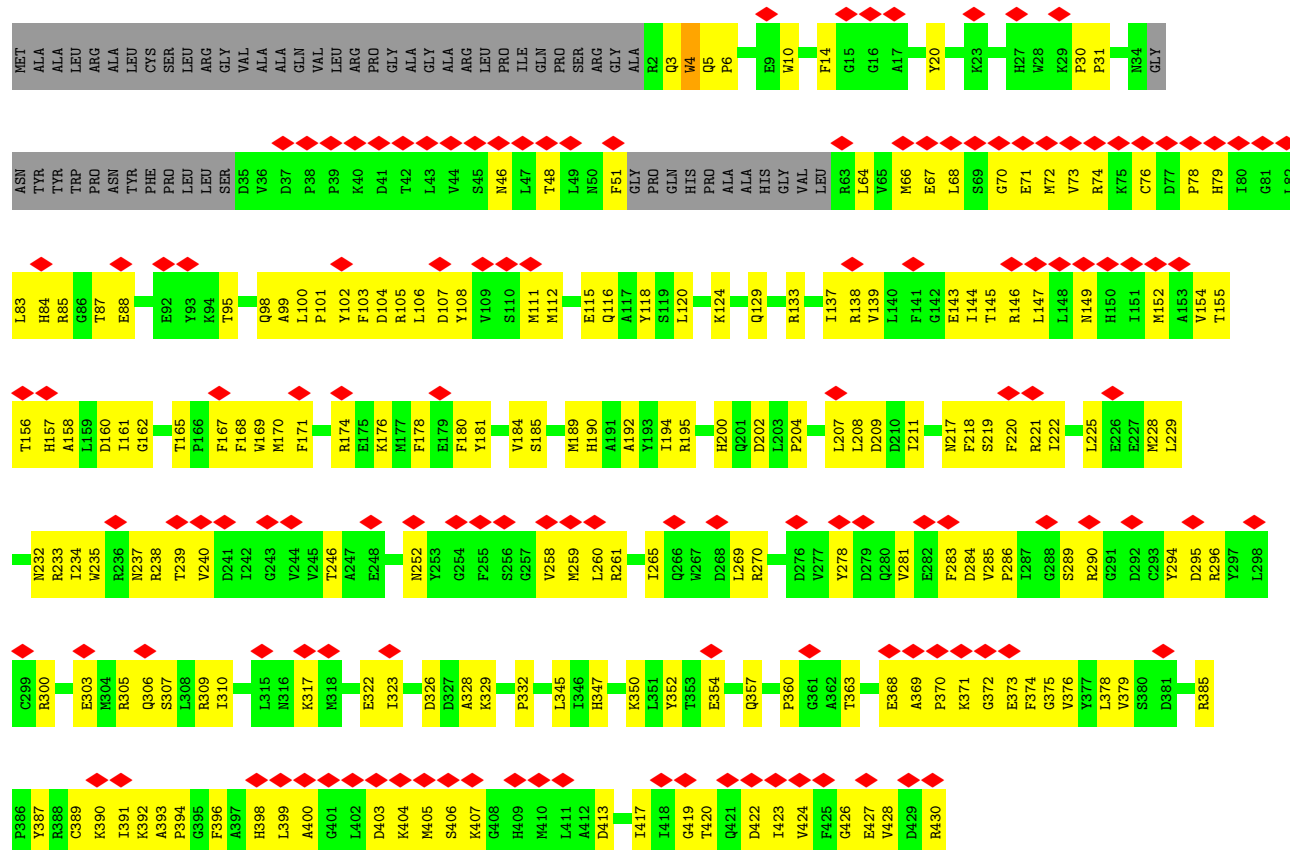


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

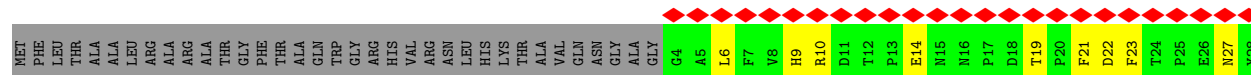
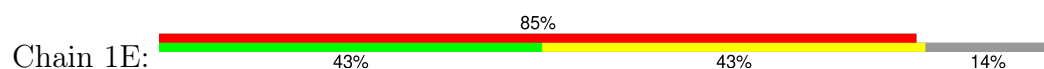




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

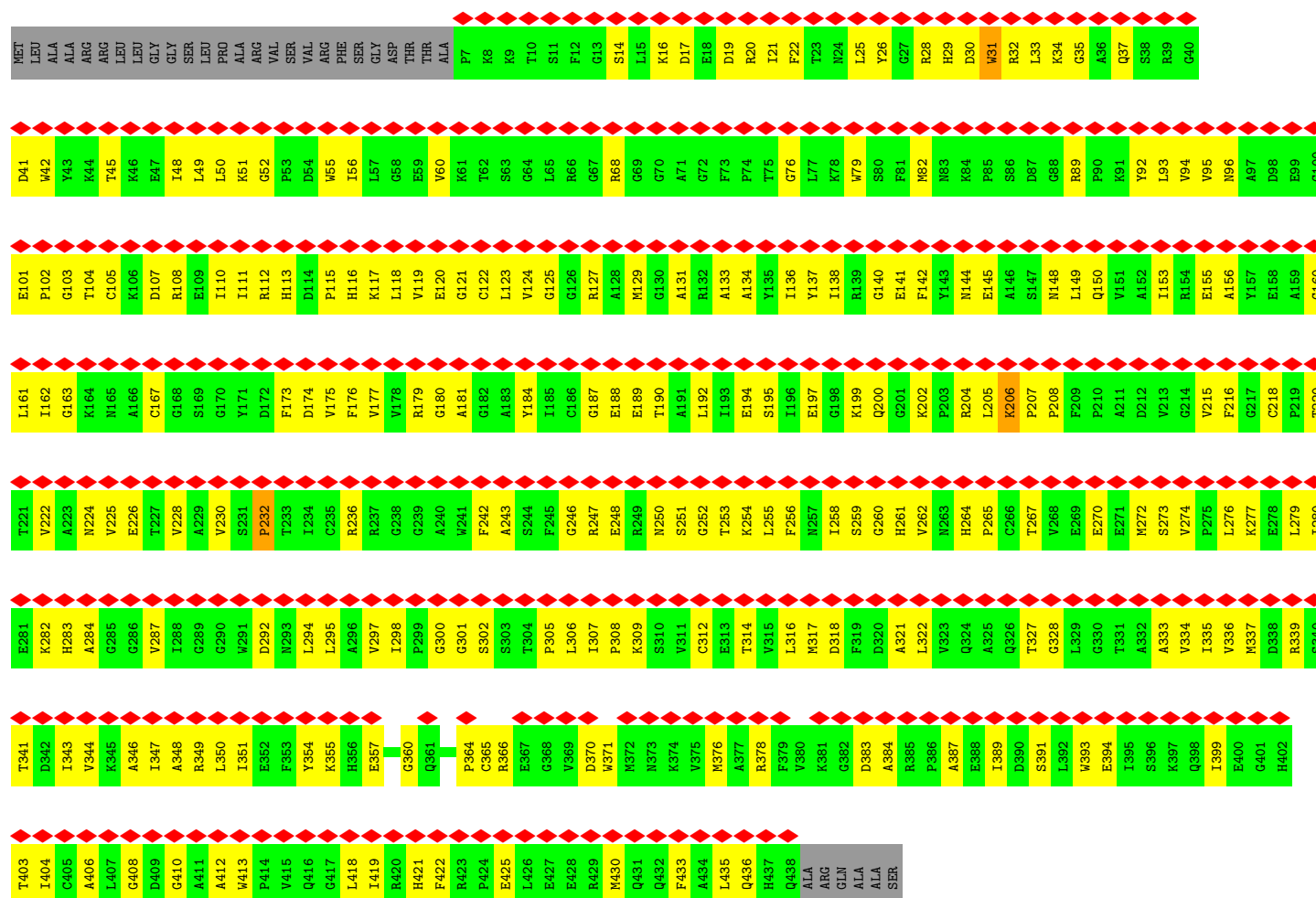
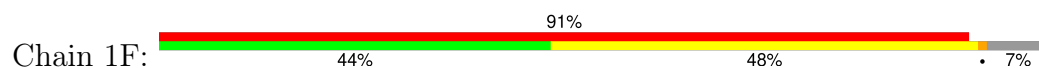


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial





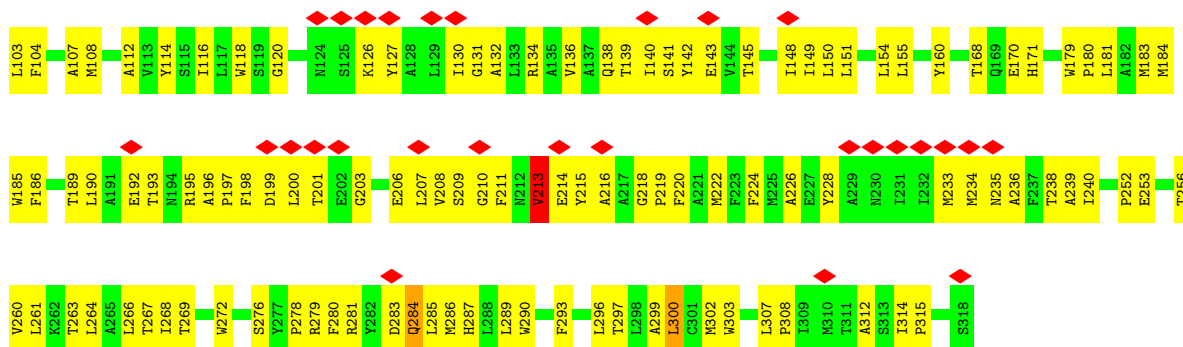
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



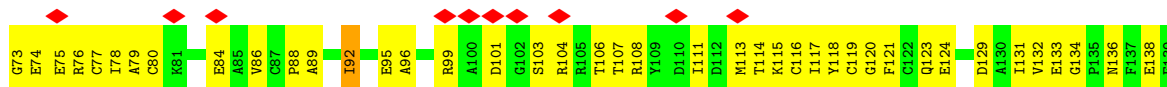
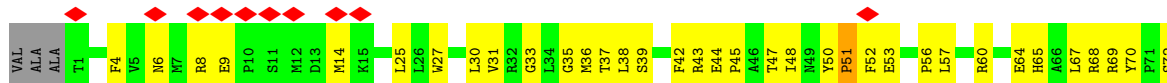
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



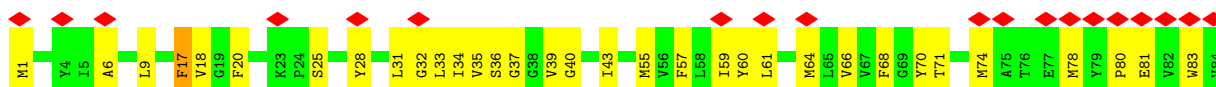




- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

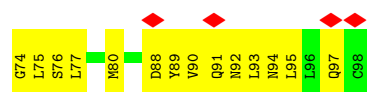


- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

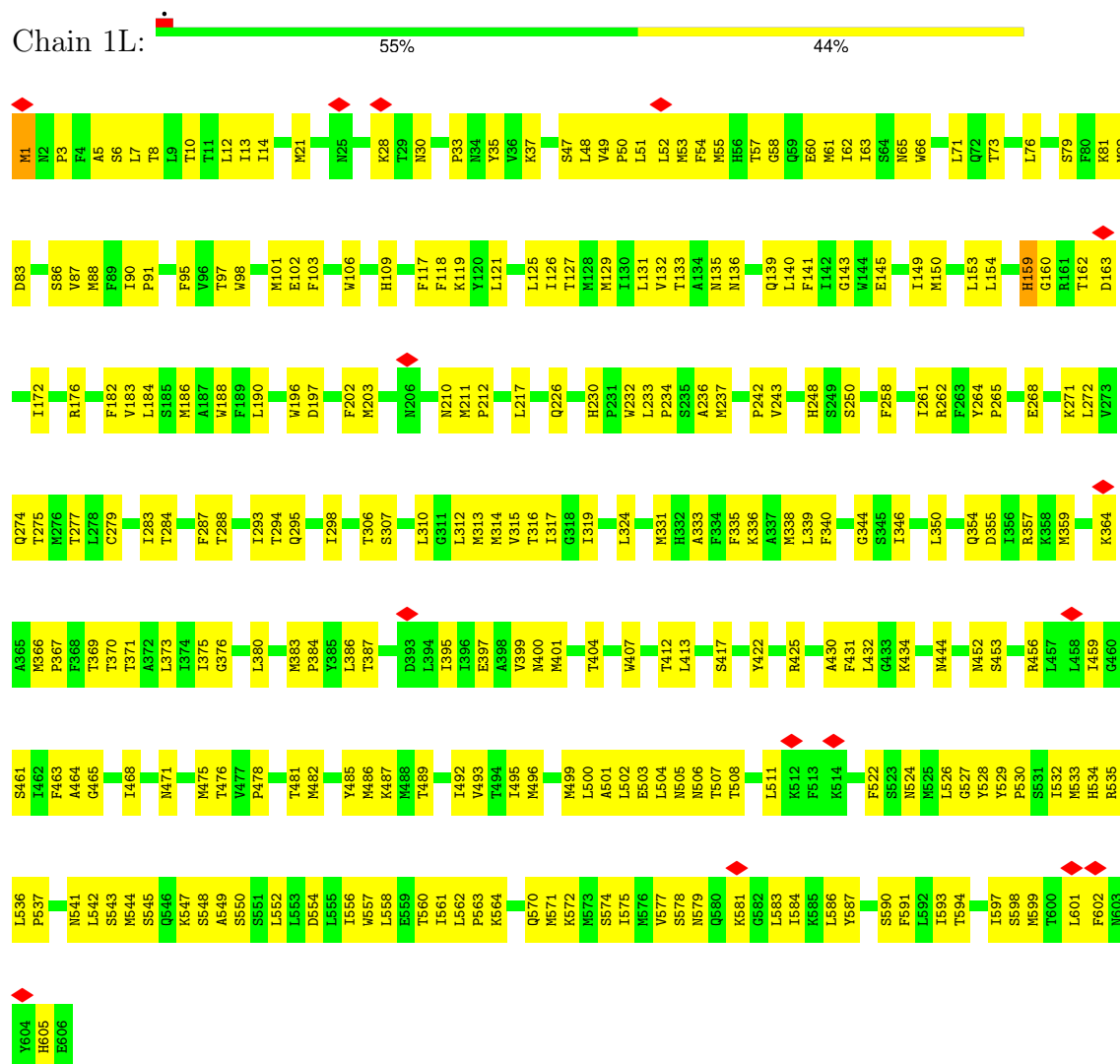


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

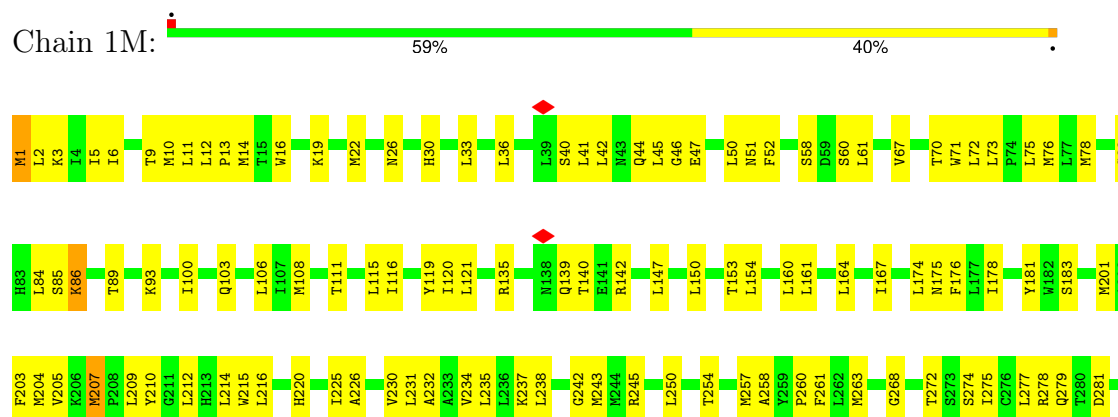


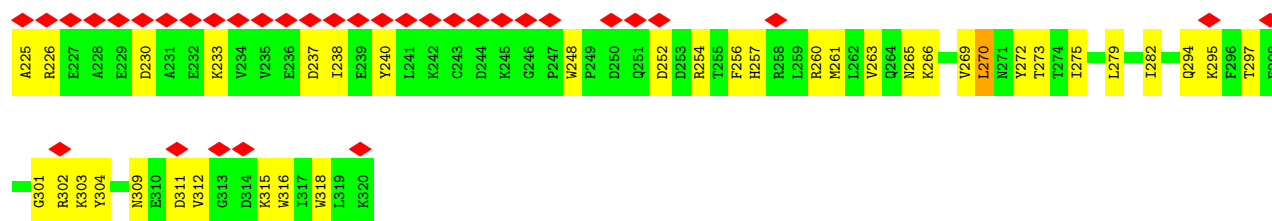


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

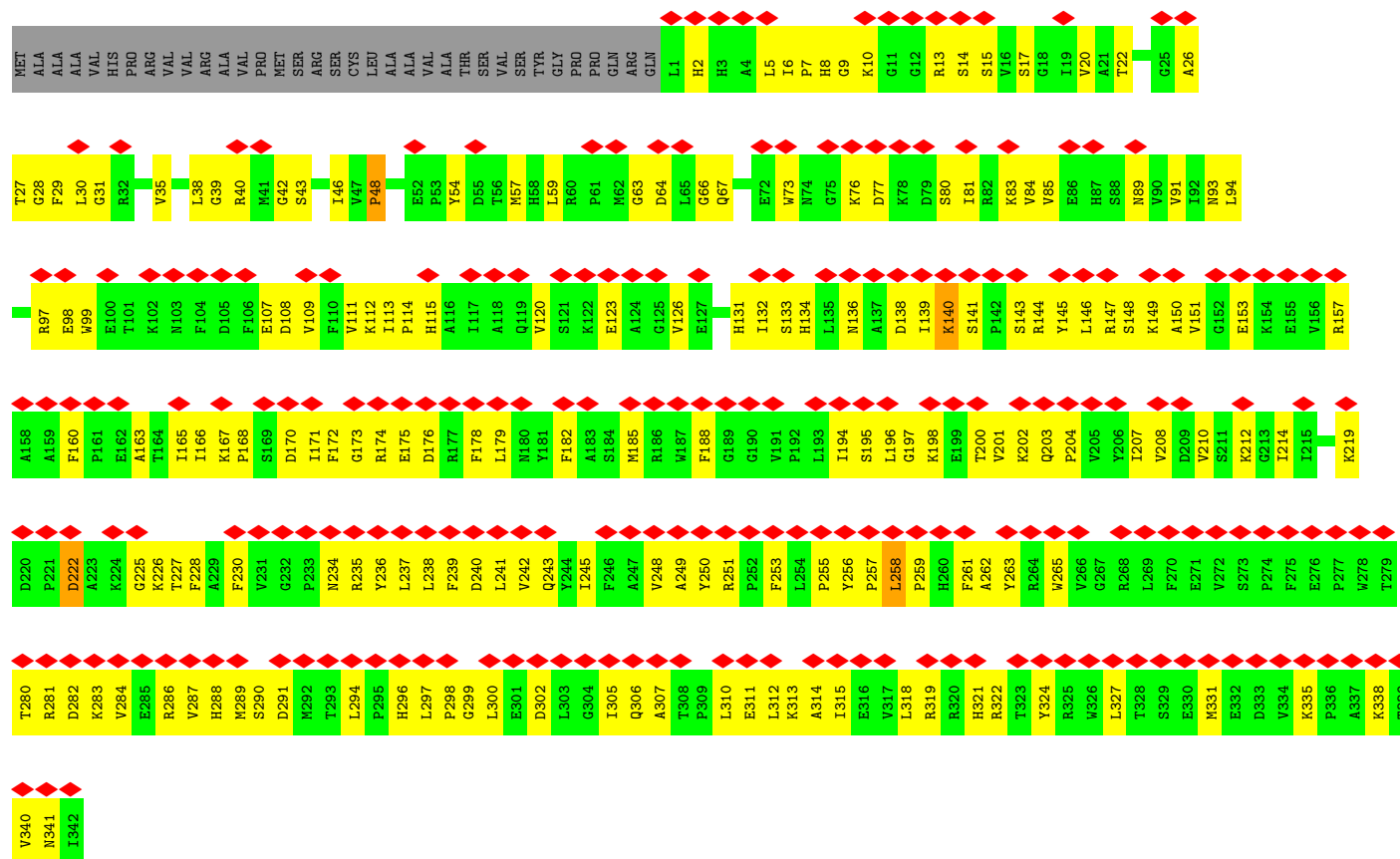
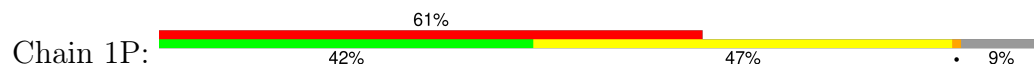


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

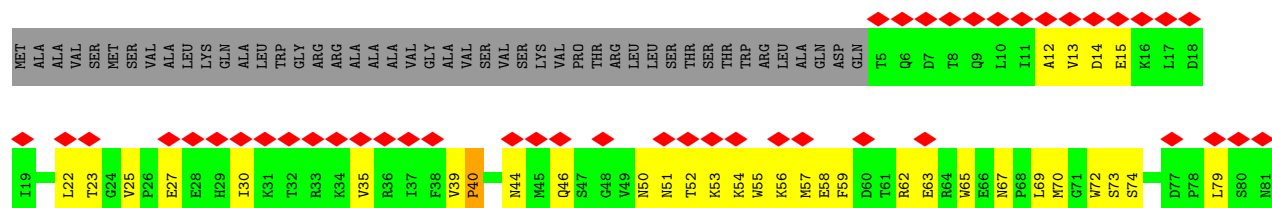
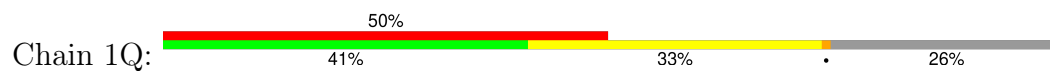


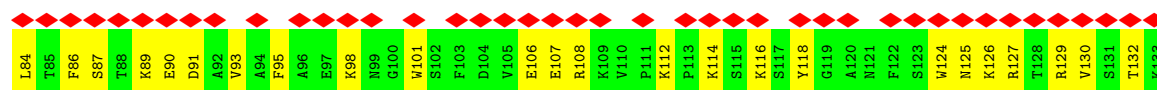


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

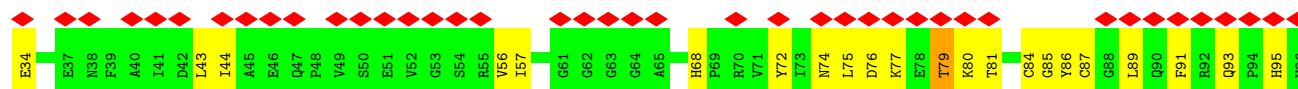
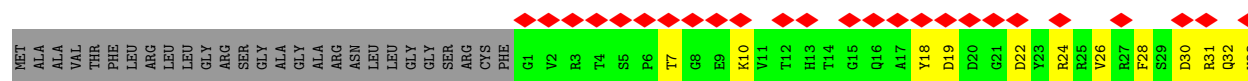


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

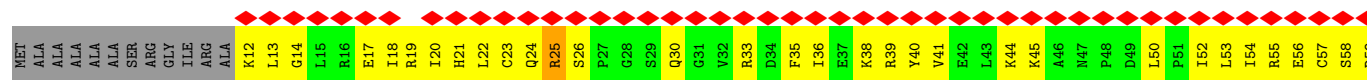
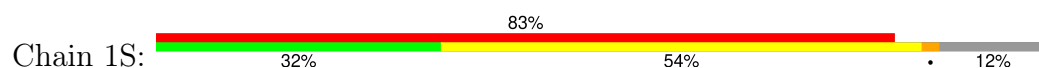




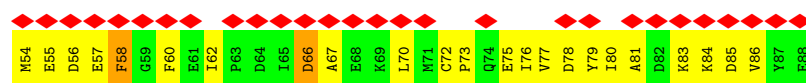
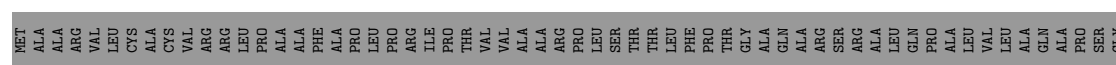
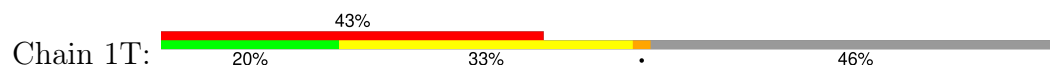
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



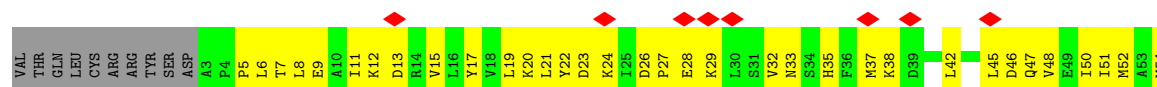
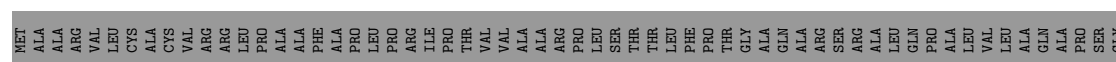
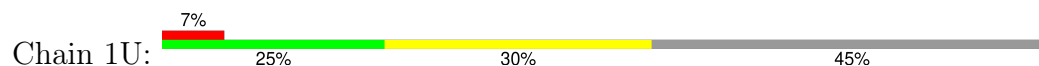
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

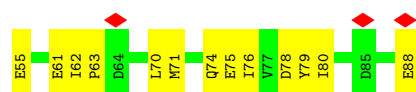


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

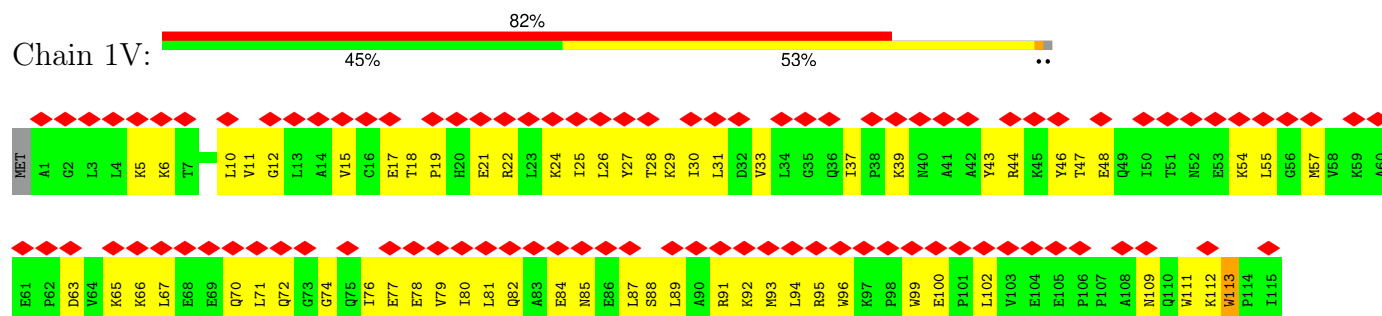


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

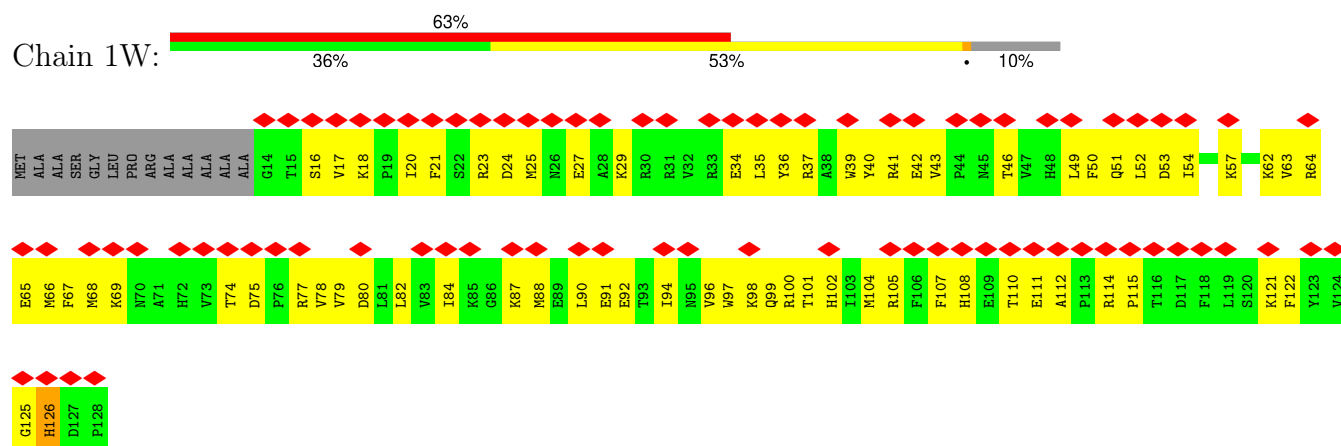




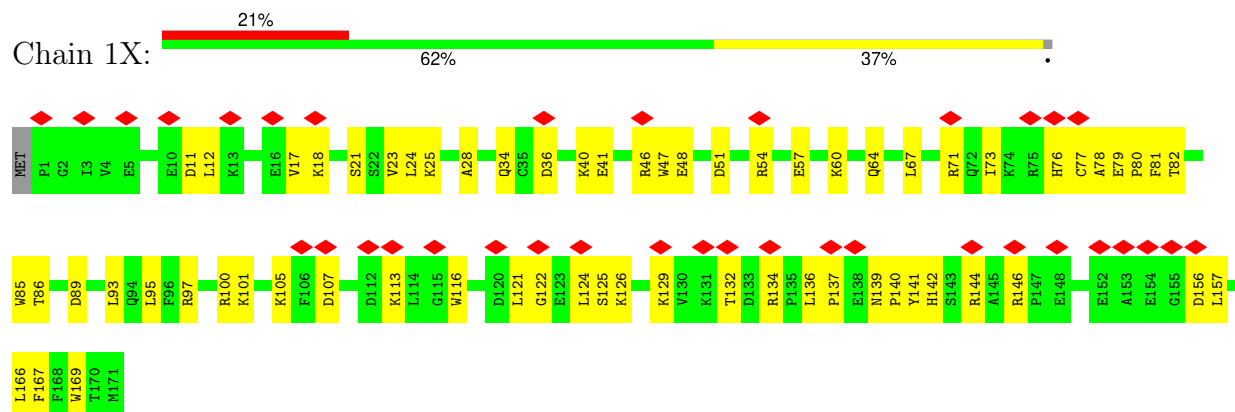
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



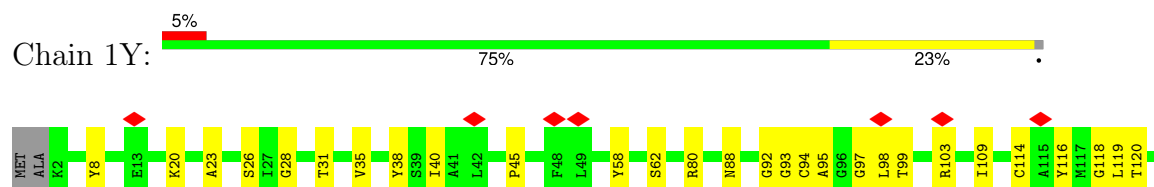
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

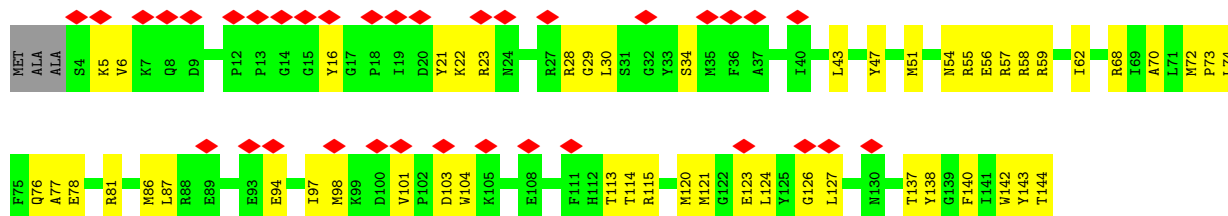


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



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



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

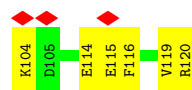


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

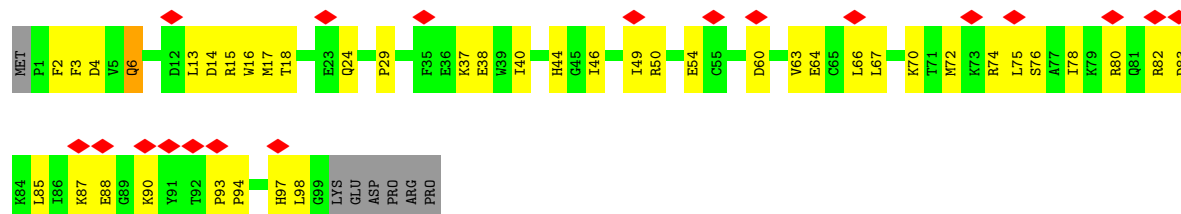


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

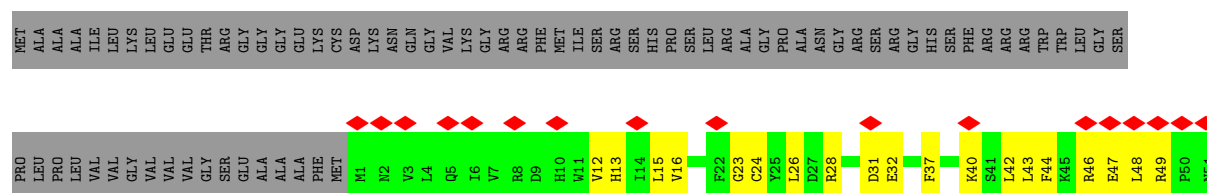




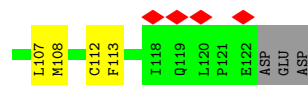
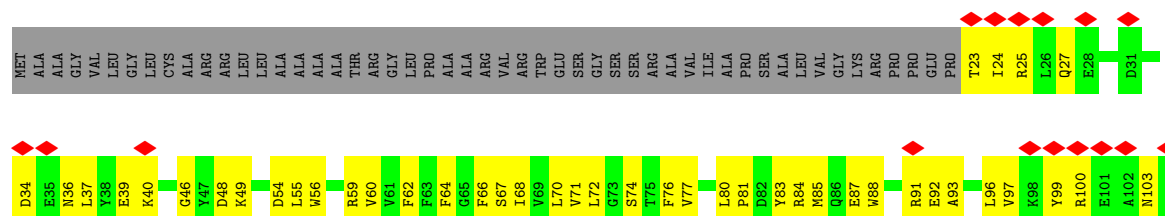
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



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

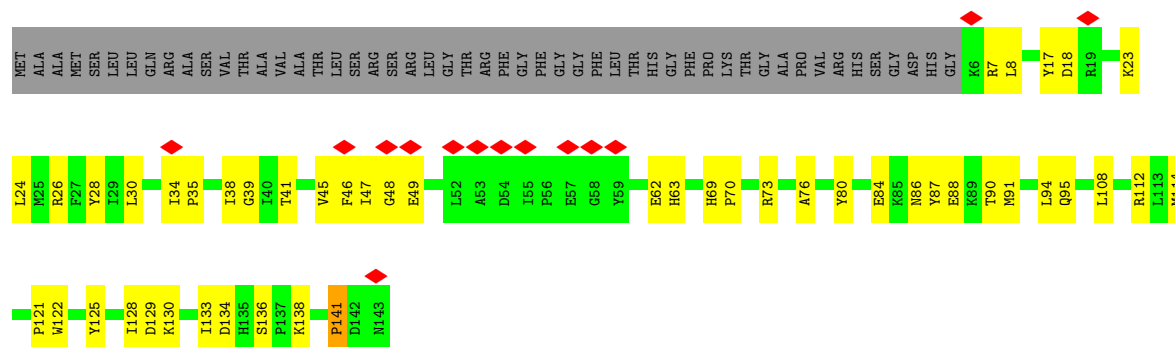


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

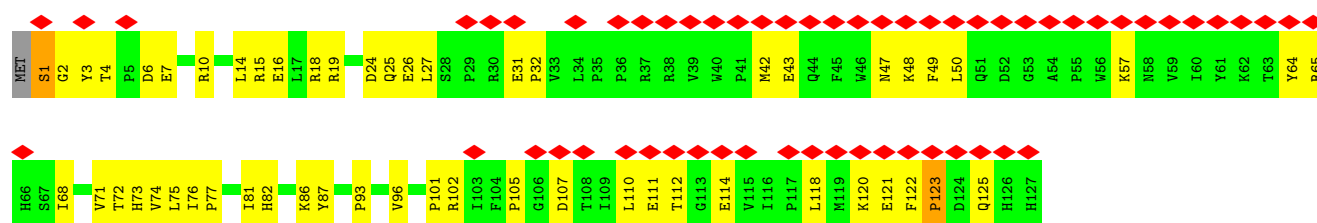


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

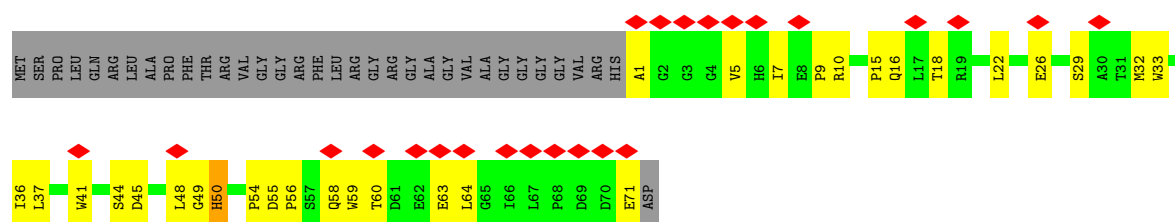




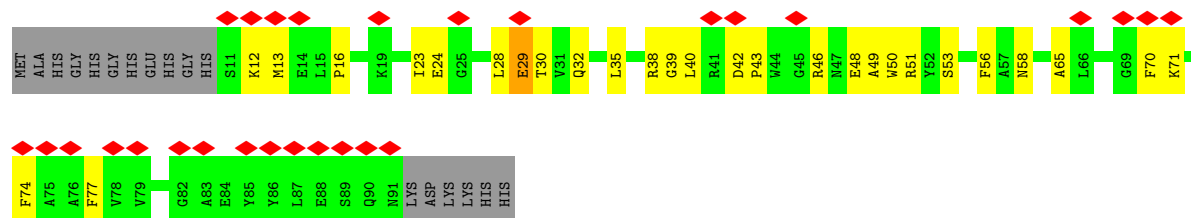
• Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



• Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

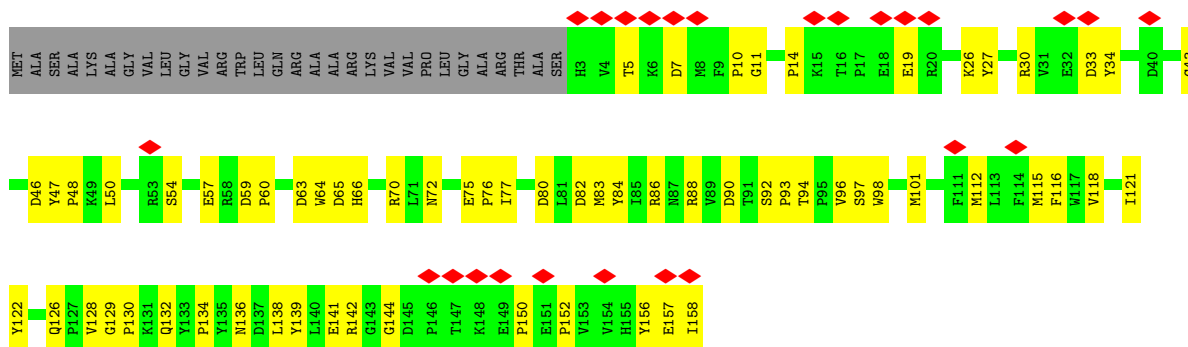


• Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3



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

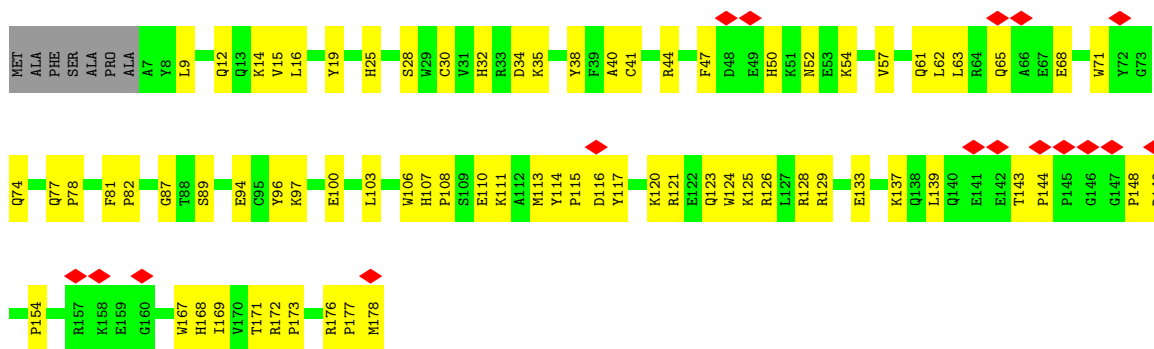




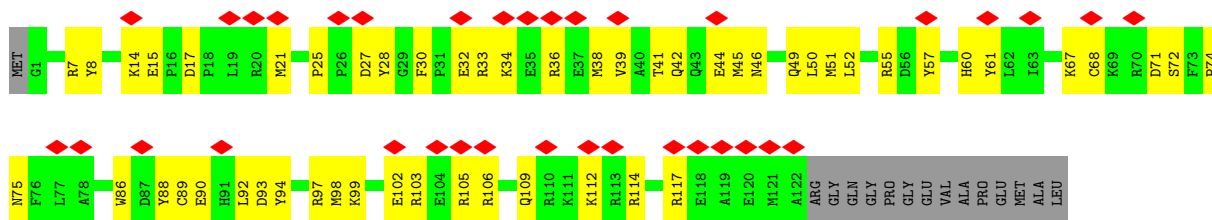
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



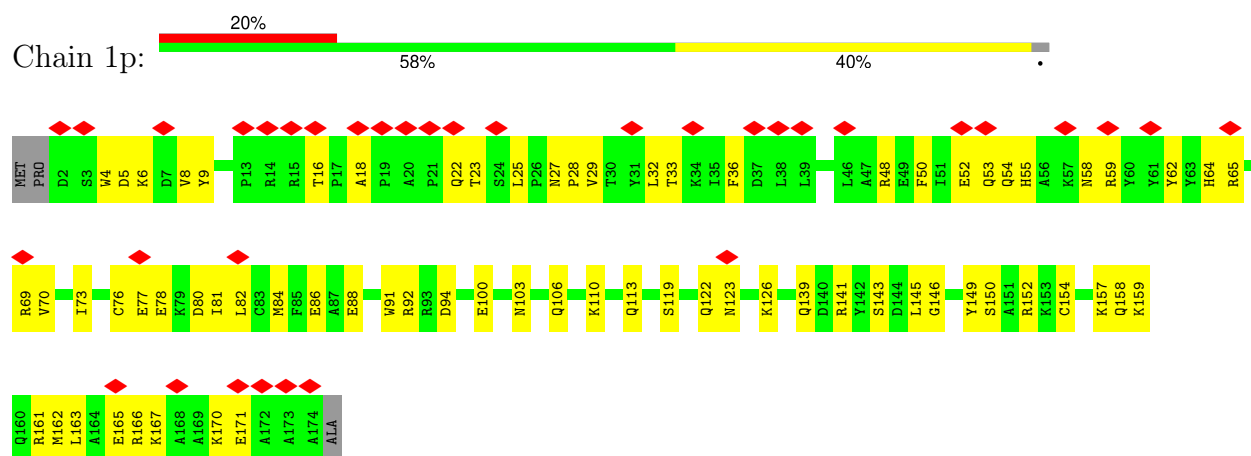
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



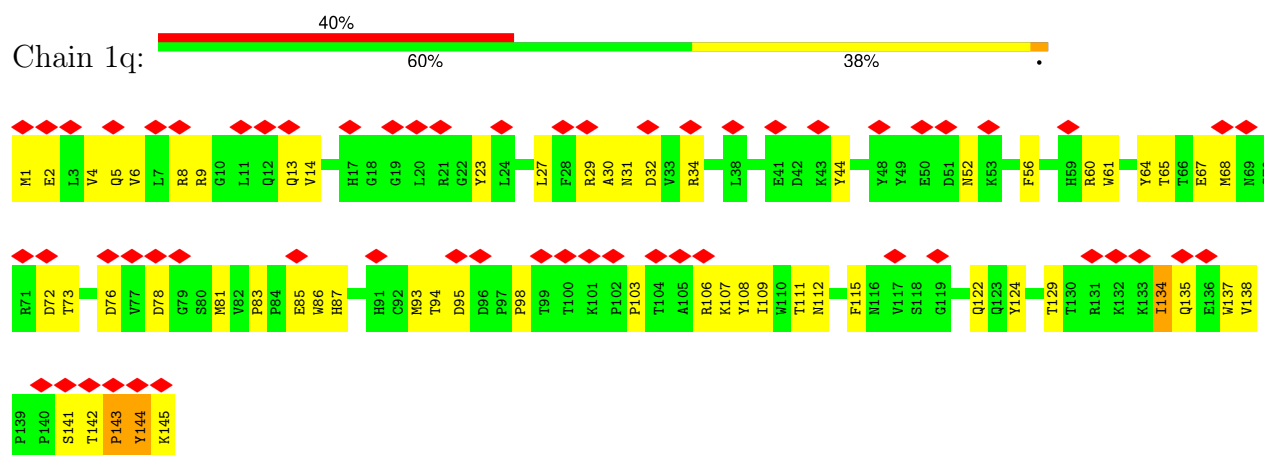
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



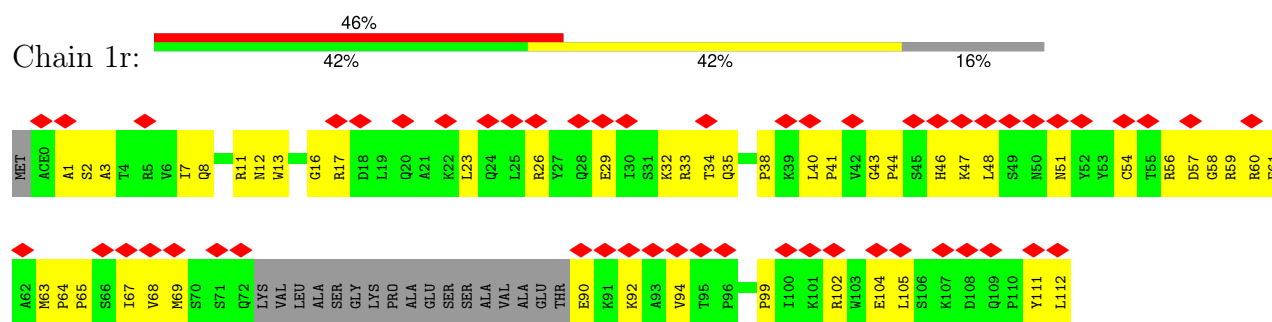
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



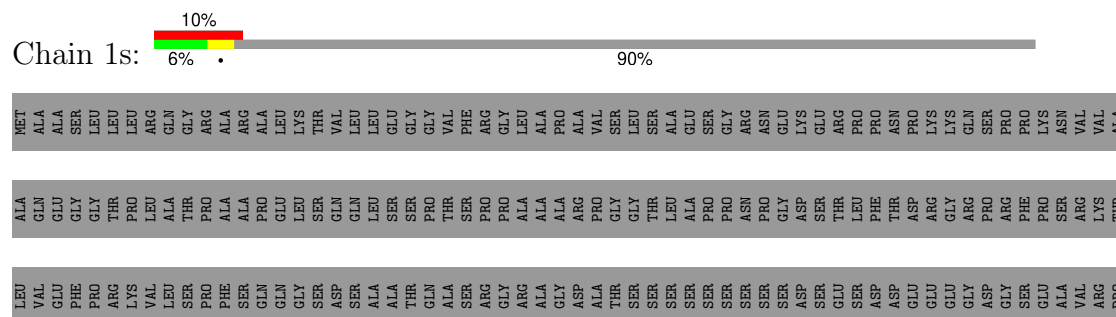
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.935	Depositor
Minimum map value	-0.432	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/705	0.42	0/963
2	1B	0.20	0/1273	0.43	0/1722
3	1C	0.17	0/1791	0.40	0/2439
4	1D	0.18	0/3464	0.39	0/4692
5	1E	0.15	0/1698	0.38	0/2311
6	1F	0.15	0/3401	0.40	1/4595 (0.0%)
7	1G	0.20	1/5451 (0.0%)	0.49	5/7387 (0.1%)
8	1H	0.19	0/2566	0.42	0/3509
9	1I	0.31	1/1443 (0.1%)	0.62	4/1952 (0.2%)
10	1J	0.17	0/1364	0.43	0/1850
11	1K	0.18	0/751	0.46	0/1018
12	1L	0.17	0/4939	0.38	0/6718
13	1M	0.18	0/3713	0.35	0/5063
14	1N	0.19	0/2765	0.41	0/3758
15	1O	0.15	0/2650	0.38	1/3588 (0.0%)
16	1P	0.17	0/2828	0.42	1/3834 (0.0%)
17	1Q	0.20	0/1070	0.50	1/1446 (0.1%)
18	1R	0.15	0/755	0.40	0/1018
19	1S	0.20	0/711	0.60	1/956 (0.1%)
20	1T	0.25	0/701	0.67	2/946 (0.2%)
20	1U	0.14	0/706	0.42	0/954
21	1V	0.18	0/946	0.49	0/1281
22	1W	0.19	0/995	0.50	0/1340
23	1X	0.13	0/1436	0.32	0/1938
24	1Y	0.15	0/1037	0.32	0/1404
25	1Z	0.17	0/1199	0.38	0/1617
26	1a	0.18	0/577	0.39	0/777
27	1b	0.15	0/664	0.40	0/912
28	1c	0.18	0/430	0.45	1/581 (0.2%)
29	1d	0.15	0/1024	0.33	0/1383
30	1e	0.15	0/836	0.34	0/1118
31	1f	0.13	0/499	0.42	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.16	0/858	0.42	0/1165
33	1h	0.25	0/1184	0.52	2/1603 (0.1%)
34	1i	0.17	0/1131	0.45	1/1541 (0.1%)
35	1j	0.14	0/627	0.45	2/858 (0.2%)
36	1k	0.15	0/668	0.36	0/903
37	1l	0.14	0/1365	0.38	0/1867
38	1m	0.14	0/1092	0.35	0/1481
39	1n	0.13	0/1549	0.30	0/2098
40	1o	0.15	0/1069	0.36	0/1430
41	1p	0.14	0/1481	0.30	0/1997
42	1q	0.23	0/1253	0.54	2/1704 (0.1%)
43	1r	0.17	0/782	0.50	0/1057
44	1s	0.15	0/394	0.35	0/533
All	All	0.18	2/67841 (0.0%)	0.42	24/91980 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	1F	0	1
7	1G	0	2
13	1M	0	1
21	1V	0	1
All	All	0	5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1I	51	PRO	CG-CD	-6.39	1.34	1.51
7	1G	389	PRO	CG-CD	-5.13	1.33	1.50

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	1I	51	PRO	N-CD-CG	-12.35	88.98	103.80
33	1h	141	PRO	CA-N-CD	-11.05	96.53	112.00
9	1I	51	PRO	CA-N-CD	-10.46	96.86	111.50
20	1T	27	PRO	CA-N-CD	-9.81	98.26	112.00
7	1G	389	PRO	CA-N-CD	-8.75	99.75	112.00
9	1I	51	PRO	CA-CB-CG	-8.37	88.11	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1O	175	PRO	CA-N-CD	-7.94	100.89	112.00
7	1G	389	PRO	N-CD-CG	-6.87	92.89	103.20
33	1h	141	PRO	N-CD-CG	-6.85	92.93	103.20
19	1S	25	ARG	CA-CB-CG	6.50	127.11	114.10
6	1F	232	PRO	CA-N-CD	-6.45	102.97	112.00
7	1G	289	GLY	N-CA-C	6.33	128.19	113.18
35	1j	54	PRO	CA-C-N	5.96	128.95	120.49
35	1j	54	PRO	C-N-CA	5.96	128.95	120.49
16	1P	48	PRO	CA-N-CD	-5.95	103.68	112.00
42	1q	143	PRO	CA-N-CD	-5.71	104.01	112.00
7	1G	287	GLU	N-CA-C	5.67	122.87	110.80
20	1T	27	PRO	N-CD-CG	-5.62	94.76	103.20
7	1G	338	VAL	N-CA-C	-5.56	106.40	112.80
28	1c	7	PRO	CA-N-CD	-5.56	104.22	112.00
9	1I	51	PRO	CB-CG-CD	-5.35	93.10	105.40
34	1i	123	PRO	CA-N-CD	-5.25	104.65	112.00
42	1q	144	TYR	N-CA-C	5.24	117.04	110.91
17	1Q	40	PRO	CA-N-CD	-5.23	104.68	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	1F	206	LYS	Peptide
7	1G	284	ILE	Peptide
7	1G	286	ASN	Peptide
13	1M	207	MET	Peptide
21	1V	113	TRP	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	700	0	749	47	0
2	1B	1242	0	1249	84	0
3	1C	1740	0	1691	125	0
4	1D	3376	0	3316	203	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1E	1658	0	1662	105	0
6	1F	3325	0	3288	200	0
7	1G	5362	0	5387	366	0
8	1H	2504	0	2602	152	0
9	1I	1412	0	1365	116	0
10	1J	1339	0	1337	72	0
11	1K	750	0	794	55	0
12	1L	4818	0	4956	229	0
13	1M	3632	0	3836	175	0
14	1N	2712	0	2872	151	0
15	1O	2590	0	2556	106	0
16	1P	2751	0	2776	174	0
17	1Q	1047	0	1042	67	0
18	1R	741	0	704	34	0
19	1S	700	0	719	56	0
20	1T	689	0	687	61	0
20	1U	694	0	691	46	0
21	1V	927	0	972	73	0
22	1W	971	0	975	77	0
23	1X	1398	0	1378	53	0
24	1Y	1016	0	1020	24	0
25	1Z	1168	0	1161	56	0
26	1a	562	0	557	29	0
27	1b	643	0	645	32	0
28	1c	417	0	425	9	0
29	1d	996	0	990	31	0
30	1e	816	0	823	40	0
31	1f	487	0	497	22	0
32	1g	835	0	795	48	0
33	1h	1151	0	1164	55	0
34	1i	1100	0	1106	60	0
35	1j	601	0	546	29	0
36	1k	649	0	626	21	0
37	1l	1310	0	1204	76	0
38	1m	1062	0	1075	48	0
39	1n	1495	0	1434	64	0
40	1o	1045	0	1018	70	0
41	1p	1449	0	1416	69	0
42	1q	1212	0	1174	69	0
43	1r	767	0	789	63	0
44	1s	382	0	351	17	0
45	1A	47	0	71	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1L	119	0	163	18	0
45	1N	51	0	82	6	0
45	1Y	51	0	82	1	0
46	1B	8	0	0	2	0
46	1F	8	0	0	1	0
46	1G	16	0	0	1	0
46	1I	16	0	0	2	0
47	1E	4	0	0	0	0
47	1G	4	0	0	0	0
48	1F	31	0	19	4	0
49	1G	1	0	0	1	0
50	1H	54	0	88	7	0
50	1I	44	0	60	2	0
50	1J	35	0	44	2	0
50	1M	44	0	62	2	0
50	1f	46	0	69	6	0
51	1L	15	0	27	2	0
52	1M	51	0	78	8	0
53	1N	77	0	98	2	0
53	1a	61	0	66	4	0
54	1O	32	0	12	3	0
55	1O	1	0	0	0	0
56	1P	48	0	26	5	0
57	1R	1	0	0	0	0
58	1W	37	0	0	0	0
58	1n	37	0	0	0	0
All	All	67180	0	67467	3144	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 23.

All (3144) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:290:LEU:N	42:1q:142:THR:O	2.01	0.93
34:1i:76:ILE:HD12	34:1i:77:PRO:HD3	1.50	0.91
2:1B:125:TYR:HE1	9:1L:88:PRO:HB2	1.36	0.91
7:1G:288:LYS:H	42:1q:143:PRO:HD2	1.36	0.90
37:1l:134:PRO:HB3	40:1o:38:MET:HE2	1.55	0.89
7:1G:290:LEU:HD23	42:1q:141:SER:HA	1.55	0.89
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.54	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:1:SAC:HG	34:1i:2:GLY:N	1.71	0.88
2:1B:166:LYS:HE3	9:1I:142:GLU:HG2	1.55	0.87
7:1G:25:THR:HA	7:1G:72:PRO:HA	1.56	0.87
40:1o:14:LYS:HD2	40:1o:109:GLN:HG3	1.57	0.86
7:1G:289:GLY:N	42:1q:143:PRO:O	2.08	0.85
9:1I:70:TYR:HE2	18:1R:87:CYS:HA	1.41	0.85
16:1P:40:ARG:HH21	22:1W:110:THR:HG23	1.42	0.84
7:1G:640:ASN:OD1	7:1G:641:TYR:N	2.09	0.84
2:1B:79:SER:HB3	8:1H:209:SER:HB2	1.60	0.84
7:1G:290:LEU:H	42:1q:143:PRO:HA	1.43	0.84
14:1N:25:HIS:NE2	30:1e:17:MET:SD	2.51	0.83
11:1K:95:LEU:HB3	14:1N:54:GLU:HG3	1.60	0.83
15:1O:237:ASP:HA	15:1O:240:TYR:HB2	1.60	0.82
4:1D:138:ARG:HG3	4:1D:194:ILE:HD12	1.60	0.82
21:1V:74:GLY:HA2	43:1r:102:ARG:HH12	1.42	0.82
7:1G:389:PRO:HD2	7:1G:390:LEU:H	1.43	0.81
7:1G:289:GLY:H	42:1q:143:PRO:C	1.90	0.79
14:1N:230:LEU:HD11	14:1N:244:MET:HE1	1.61	0.79
17:1Q:127:ARG:HG2	44:1s:70:ARG:HH12	1.47	0.79
39:1n:62:LEU:HA	39:1n:65:GLN:HE22	1.47	0.79
14:1N:322:GLN:O	29:1d:49:ARG:NH2	2.15	0.79
8:1H:102:VAL:HG21	8:1H:154:LEU:HD21	1.64	0.79
6:1F:95:VAL:HB	6:1F:136:ILE:HG22	1.65	0.78
6:1F:399:ILE:HD11	6:1F:412:ALA:HB2	1.65	0.78
7:1G:190:MET:HE2	7:1G:190:MET:HA	1.65	0.78
12:1L:190:LEU:HD23	13:1M:383:THR:HG21	1.64	0.78
7:1G:286:ASN:O	42:1q:144:TYR:HB2	1.82	0.78
18:1R:84:CYS:HB3	18:1R:87:CYS:SG	2.23	0.78
7:1G:670:ASP:O	7:1G:672:TYR:N	2.16	0.78
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.65	0.77
6:1F:79:TRP:HA	6:1F:82:MET:HE3	1.67	0.77
16:1P:245:ILE:HG13	16:1P:318:LEU:HD11	1.65	0.77
5:1E:100:ILE:HB	5:1E:139:LEU:HA	1.64	0.77
6:1F:21:ILE:HG21	6:1F:230:VAL:HG12	1.67	0.77
6:1F:120:GLU:HB2	6:1F:232:PRO:HG3	1.65	0.77
16:1P:262:ALA:HA	16:1P:265:TRP:HD1	1.50	0.77
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.66	0.77
7:1G:325:ALA:HA	7:1G:328:LEU:HD12	1.66	0.77
7:1G:537:LEU:HD22	7:1G:538:PRO:HD2	1.67	0.77
2:1B:34:ASP:OD1	2:1B:38:ASN:ND2	2.17	0.76
45:1L:702:3PE:H242	37:1l:88:ARG:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:81:THR:OG1	18:1R:91:PHE:O	2.03	0.76
6:1F:355:LYS:HD2	6:1F:370:ASP:HA	1.67	0.76
23:1X:18:LYS:HA	26:1a:54:ILE:HD11	1.66	0.76
6:1F:190:THR:HB	6:1F:204:ARG:HB2	1.67	0.76
40:1o:109:GLN:OE1	40:1o:109:GLN:N	2.19	0.76
12:1L:508:THR:O	39:1n:35:LYS:NZ	2.18	0.76
5:1E:30:ARG:HG2	44:1s:52:LEU:HB3	1.68	0.76
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	1.68	0.76
2:1B:66:ARG:HH22	43:1r:26:ARG:HH22	1.32	0.75
7:1G:288:LYS:HG3	42:1q:142:THR:HB	1.68	0.75
15:1O:200:GLN:O	15:1O:204:ASN:ND2	2.19	0.75
14:1N:128:LEU:HD11	14:1N:213:LEU:HD13	1.68	0.75
4:1D:158:ALA:HB2	4:1D:229:LEU:HD11	1.67	0.75
19:1S:62:PRO:HG2	19:1S:79:ASN:HA	1.66	0.75
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.20	0.75
12:1L:597:ILE:HD12	12:1L:601:LEU:HB3	1.67	0.75
6:1F:387:ALA:HB1	43:1r:48:LEU:HD21	1.67	0.75
21:1V:66:LYS:O	21:1V:70:GLN:NE2	2.20	0.75
30:1e:40:ILE:HD11	33:1h:128:ILE:HB	1.67	0.75
19:1S:14:GLY:HA2	19:1S:97:LYS:HB2	1.68	0.74
38:1m:44:ARG:HH12	38:1m:48:LEU:HG	1.52	0.74
4:1D:161:ILE:HG23	8:1H:278:PRO:HB3	1.69	0.74
7:1G:652:VAL:HG22	7:1G:653:ASN:H	1.53	0.74
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	1.70	0.74
16:1P:138:ASP:HB2	16:1P:141:SER:HB3	1.68	0.74
4:1D:107:ASP:HB3	4:1D:427:GLU:HB2	1.69	0.74
7:1G:228:ILE:HG13	7:1G:581:GLN:HB3	1.68	0.74
4:1D:66:MET:HE3	4:1D:76:CYS:HB3	1.70	0.74
2:1B:113:VAL:HG13	2:1B:142:VAL:HA	1.69	0.73
4:1D:413:ASP:OD1	8:1H:281:ARG:NH1	2.21	0.73
6:1F:384:ALA:HB3	6:1F:430:MET:HE2	1.70	0.73
3:1C:50:ILE:HD11	3:1C:107:VAL:HG12	1.70	0.73
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.70	0.73
38:1m:116:GLN:NE2	38:1m:117:GLU:OE2	2.20	0.73
26:1a:23:THR:O	26:1a:27:HIS:ND1	2.21	0.73
3:1C:30:ALA:HA	3:1C:37:VAL:HG21	1.70	0.73
6:1F:347:ILE:HA	6:1F:350:LEU:HB2	1.71	0.73
12:1L:556:ILE:HD11	38:1m:75:ILE:HG12	1.70	0.73
13:1M:135:ARG:NH1	14:1N:304:MET:SD	2.61	0.73
10:1J:18:VAL:HG11	10:1J:96:GLY:HA3	1.70	0.73
10:1J:146:LEU:HA	11:1K:58:MET:HE1	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:84:ILE:HA	22:1W:87:LYS:HB3	1.71	0.73
5:1E:131:THR:HG21	5:1E:135:LYS:HD2	1.71	0.72
6:1F:105:CYS:HB3	6:1F:108:ARG:HH21	1.54	0.72
33:1h:62:GLU:OE1	33:1h:63:HIS:N	2.22	0.72
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.70	0.72
12:1L:578:SER:HB2	14:1N:172:GLN:HE21	1.53	0.72
56:1P:501:NDP:H8A	56:1P:501:NDP:H51A	1.71	0.72
32:1g:23:THR:O	32:1g:25:ARG:N	2.17	0.72
20:1T:36:PHE:HA	20:1T:40:LEU:HB2	1.72	0.72
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.70	0.72
3:1C:48:LEU:HB3	3:1C:105:ILE:HG22	1.72	0.72
15:1O:315:LYS:HD2	15:1O:316:TRP:H	1.54	0.72
34:1i:105:PRO:O	40:1o:67:LYS:NZ	2.22	0.72
10:1J:152:TRP:HE1	14:1N:19:LEU:HD21	1.55	0.71
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.71	0.71
17:1Q:22:LEU:HD23	22:1W:78:VAL:HG23	1.71	0.71
16:1P:134:HIS:H	16:1P:149:LYS:HE3	1.54	0.71
20:1T:54:MET:HE3	20:1T:76:ILE:HG21	1.70	0.71
12:1L:106:TRP:O	12:1L:109:HIS:ND1	2.23	0.71
13:1M:41:LEU:O	13:1M:44:GLN:NE2	2.23	0.71
52:1M:501:PGT:H362	14:1N:280:THR:HG21	1.73	0.71
15:1O:233:LYS:HD3	21:1V:91:ARG:NH2	2.06	0.71
24:1Y:94:CYS:O	24:1Y:98:LEU:N	2.14	0.71
27:1b:60:GLY:O	27:1b:61:ASN:ND2	2.23	0.71
8:1H:215:TYR:HB3	8:1H:220:PHE:HB2	1.73	0.71
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.71	0.71
12:1L:283:ILE:HD13	37:1l:112:MET:HG2	1.72	0.71
16:1P:20:VAL:HB	16:1P:89:ASN:H	1.54	0.71
38:1m:117:GLU:OE2	38:1m:117:GLU:N	2.18	0.71
15:1O:15:THR:HA	15:1O:18:LEU:HD12	1.70	0.71
21:1V:57:MET:HE2	21:1V:70:GLN:HB3	1.70	0.71
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.72	0.71
15:1O:26:THR:HB	15:1O:169:VAL:HG12	1.73	0.71
16:1P:300:LEU:HD22	16:1P:307:ALA:HB2	1.72	0.71
6:1F:250:ASN:HD22	6:1F:318:ASP:HB2	1.56	0.71
14:1N:211:MET:SD	14:1N:333:SER:OG	2.49	0.71
7:1G:504:ASP:OD1	19:1S:55:ARG:NH1	2.24	0.70
10:1J:171:ILE:HD11	11:1K:76:SER:HB2	1.73	0.70
21:1V:82:GLN:N	21:1V:82:GLN:OE1	2.24	0.70
37:1l:156:TYR:HB3	40:1o:33:ARG:HG2	1.71	0.70
42:1q:73:THR:HG21	42:1q:81:MET:HE1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:314:MET:HA	12:1L:317:ILE:HG22	1.74	0.70
15:1O:18:LEU:HD11	15:1O:256:PHE:HE2	1.57	0.70
32:1g:62:PHE:O	33:1h:28:TYR:OH	2.07	0.70
20:1T:83:LYS:HZ2	20:1T:84:LYS:HB3	1.56	0.70
2:1B:52:LEU:HD21	2:1B:96:MET:HG2	1.73	0.70
37:1l:136:ASN:HB3	37:1l:152:PRO:HA	1.73	0.70
14:1N:18:MET:HA	14:1N:18:MET:HE2	1.74	0.70
20:1U:70:LEU:HD12	20:1U:76:ILE:HD12	1.74	0.70
7:1G:107:ILE:HA	9:1I:104:ARG:HH21	1.55	0.70
12:1L:545:SER:HG	13:1M:274:SER:HG	1.39	0.70
7:1G:288:LYS:N	42:1q:143:PRO:O	2.25	0.69
20:1U:6:LEU:HD13	20:1U:11:ILE:HD11	1.74	0.69
5:1E:10:ARG:HH12	18:1R:77:LYS:HG2	1.56	0.69
21:1V:30:ILE:HG22	21:1V:87:LEU:HB2	1.72	0.69
3:1C:40:VAL:HG12	3:1C:50:ILE:HG22	1.75	0.69
9:1I:9:GLU:OE1	9:1I:9:GLU:N	2.23	0.69
13:1M:164:LEU:HA	13:1M:167:ILE:HD12	1.75	0.69
7:1G:43:HIS:HB3	7:1G:46:LEU:HB3	1.75	0.69
22:1W:54:ILE:HG21	22:1W:107:PHE:HE1	1.57	0.69
4:1D:238:ARG:HG2	8:1H:284:GLN:HE22	1.57	0.69
7:1G:257:ASP:HB3	7:1G:369:ALA:HB2	1.74	0.69
12:1L:533:MET:HA	12:1L:533:MET:HE3	1.75	0.69
13:1M:150:LEU:HD13	14:1N:294:MET:HE1	1.73	0.69
13:1M:307:TRP:NE1	38:1m:127:SER:OG	2.25	0.69
14:1N:85:THR:HG22	14:1N:87:THR:HG23	1.74	0.69
5:1E:165:THR:HG23	5:1E:167:LYS:H	1.58	0.69
8:1H:140:ILE:HG21	10:1J:66:VAL:HG11	1.74	0.69
22:1W:62:LYS:HA	22:1W:65:GLU:HG3	1.75	0.69
22:1W:62:LYS:NZ	22:1W:65:GLU:OE2	2.25	0.69
8:1H:276:SER:HB2	9:1I:37:THR:HG21	1.75	0.69
3:1C:86:ARG:HH22	21:1V:113:TRP:HB2	1.56	0.68
7:1G:378:LEU:HD21	7:1G:439:PHE:HZ	1.57	0.68
21:1V:78:GLU:OE2	21:1V:78:GLU:N	2.25	0.68
40:1o:52:LEU:HD13	40:1o:55:ARG:HD2	1.75	0.68
7:1G:289:GLY:HA2	42:1q:145:LYS:C	2.18	0.68
14:1N:237:MET:HB2	14:1N:240:ILE:HG12	1.75	0.68
20:1T:47:GLN:HA	20:1T:50:ILE:HG12	1.75	0.68
53:1a:101:CDL:HB22	43:1r:3:ALA:HA	1.75	0.68
9:1I:150:ASN:ND2	42:1q:124:TYR:OH	2.26	0.68
12:1L:10:THR:O	12:1L:13:ILE:N	2.26	0.68
12:1L:593:ILE:O	12:1L:597:ILE:HG22	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:73:PRO:HD3	27:1b:52:TYR:HE2	1.59	0.68
5:1E:145:LEU:HD22	5:1E:155:GLN:HB2	1.75	0.68
7:1G:106:PRO:HB3	9:1I:80:CYS:HB2	1.76	0.68
20:1T:11:ILE:HD11	20:1T:84:LYS:HE3	1.76	0.68
7:1G:307:LEU:HD11	7:1G:338:VAL:HG21	1.76	0.68
7:1G:327:ALA:HB2	7:1G:596:ASP:HB3	1.76	0.68
8:1H:183:MET:HB3	50:1H:401:PC1:H2F2	1.76	0.68
4:1D:390:LYS:NZ	4:1D:391:ILE:O	2.26	0.68
4:1D:394:PRO:O	4:1D:398:HIS:ND1	2.25	0.68
32:1g:100:ARG:HG2	32:1g:107:LEU:HA	1.76	0.68
38:1m:21:GLU:OE1	38:1m:21:GLU:N	2.26	0.68
4:1D:307:SER:HA	4:1D:310:ILE:HD12	1.77	0.67
24:1Y:93:GLY:HA3	24:1Y:118:GLY:HA2	1.74	0.67
9:1I:64:GLU:OE2	9:1I:149:TYR:OH	2.12	0.67
15:1O:148:CYS:HA	15:1O:279:LEU:HD21	1.75	0.67
6:1F:224:ASN:ND2	48:1F:501:FMN:O2	2.27	0.67
16:1P:29:PHE:CE1	16:1P:176:ASP:HA	2.29	0.67
3:1C:190:LEU:O	17:1Q:74:SER:OG	2.11	0.67
30:1e:94:PRO:HD2	30:1e:97:HIS:CD2	2.29	0.67
35:1j:59:TRP:O	40:1o:106:ARG:NH2	2.27	0.67
40:1o:102:GLU:O	40:1o:106:ARG:N	2.27	0.67
2:1B:63:ALA:HA	2:1B:69:MET:HB2	1.76	0.67
4:1D:306:GLN:OE1	4:1D:309:ARG:NH2	2.26	0.67
1:1A:68:GLU:OE1	1:1A:68:GLU:N	2.19	0.67
7:1G:198:ASN:ND2	7:1G:263:ILE:O	2.24	0.67
12:1L:532:ILE:HD11	37:1l:101:MET:HB3	1.75	0.66
24:1Y:109:ILE:HD12	24:1Y:109:ILE:H	1.60	0.66
35:1j:45:ASP:HB2	35:1j:50:HIS:HB2	1.77	0.66
14:1N:9:LEU:HD22	14:1N:42:PRO:HG3	1.77	0.66
6:1F:137:TYR:HD2	6:1F:192:LEU:HG	1.60	0.66
7:1G:358:LEU:HD23	7:1G:645:ALA:HB2	1.77	0.66
17:1Q:15:GLU:HG3	22:1W:75:ASP:HB2	1.75	0.66
29:1d:34:MET:HG3	29:1d:72:GLY:HA3	1.77	0.66
3:1C:111:THR:HG21	3:1C:117:ILE:HD11	1.75	0.66
8:1H:222:MET:SD	8:1H:222:MET:N	2.68	0.66
14:1N:22:ILE:O	30:1e:6:GLN:NE2	2.29	0.66
15:1O:233:LYS:HD3	21:1V:91:ARG:HH21	1.59	0.66
37:1l:7:ASP:O	37:1l:26:LYS:NZ	2.27	0.66
37:1l:141:GLU:HA	41:1p:122:GLN:HB3	1.77	0.66
6:1F:68:ARG:NH2	6:1F:253:THR:O	2.29	0.66
12:1L:83:ASP:OD2	12:1L:262:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:134:GLN:O	14:1N:135:LYS:HD3	1.95	0.66
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.14	0.66
34:1i:110:LEU:HB3	41:1p:18:ALA:HB2	1.78	0.66
22:1W:18:LYS:O	22:1W:77:ARG:NH1	2.24	0.66
2:1B:55:CYS:HB3	2:1B:89:ALA:HB1	1.76	0.66
15:1O:168:VAL:HG11	15:1O:238:ILE:HD12	1.78	0.66
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.14	0.65
5:1E:6:LEU:O	5:1E:92:ARG:NH1	2.29	0.65
17:1Q:58:GLU:OE1	17:1Q:58:GLU:N	2.28	0.65
43:1r:32:LYS:O	43:1r:35:GLN:NE2	2.26	0.65
7:1G:366:THR:OG1	7:1G:491:ASN:ND2	2.28	0.65
14:1N:147:GLN:HB2	33:1h:125:TYR:CZ	2.31	0.65
43:1r:63:MET:SD	43:1r:64:PRO:HD2	2.37	0.65
8:1H:26:LYS:HG2	26:1a:5:ILE:HG12	1.77	0.65
9:1I:45:PRO:HB2	9:1I:47:THR:HG23	1.77	0.65
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.29	0.65
19:1S:30:GLN:OE1	19:1S:33:ARG:NH1	2.29	0.65
4:1D:165:THR:HA	8:1H:32:GLN:HB3	1.79	0.65
6:1F:184:TYR:HB3	6:1F:357:GLU:HG2	1.77	0.65
12:1L:357:ARG:NH1	39:1n:28:SER:OG	2.30	0.65
3:1C:119:SER:OG	3:1C:144:ASN:O	2.14	0.65
6:1F:14:SER:H	6:1F:282:LYS:HE3	1.61	0.65
7:1G:594:ARG:HD2	22:1W:126:HIS:HB3	1.78	0.65
8:1H:195:ARG:HD3	8:1H:196:ALA:H	1.59	0.65
9:1I:8:ARG:HH22	43:1r:111:TYR:HB2	1.61	0.65
16:1P:312:LEU:HD22	16:1P:313:LYS:HD3	1.79	0.65
34:1i:27:LEU:HB2	34:1i:31:GLU:HB2	1.77	0.65
20:1T:72:CYS:H	20:1T:75:GLU:HB2	1.61	0.65
35:1j:5:VAL:HG23	35:1j:7:ILE:H	1.60	0.65
36:1k:35:LEU:HB2	36:1k:40:LEU:HB2	1.79	0.65
25:1Z:127:LEU:HD13	30:1e:97:HIS:CE1	2.32	0.65
3:1C:166:PHE:HE1	3:1C:170:GLY:HA2	1.62	0.65
13:1M:272:THR:HA	13:1M:275:ILE:HD12	1.79	0.65
23:1X:89:ASP:OD1	26:1a:37:ARG:NH2	2.30	0.65
34:1i:76:ILE:HD12	34:1i:77:PRO:CD	2.23	0.65
10:1J:113:VAL:HG23	10:1J:119:PHE:HB2	1.79	0.65
11:1K:5:TYR:HE1	11:1K:46:LEU:HB3	1.61	0.65
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.78	0.65
4:1D:115:GLU:HB3	4:1D:194:ILE:HB	1.79	0.64
5:1E:105:THR:HA	6:1F:349:ARG:HG3	1.77	0.64
5:1E:124:LEU:HD13	5:1E:126:ILE:HG12	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:28:TYR:HA	10:1J:31:LEU:HD12	1.79	0.64
13:1M:44:GLN:HG3	13:1M:60:SER:HA	1.77	0.64
21:1V:27:TYR:HE2	21:1V:54:LYS:HB3	1.60	0.64
3:1C:131:GLU:OE2	3:1C:145:HIS:NE2	2.30	0.64
50:1M:502:PC1:H2B1	32:1g:70:LEU:HD12	1.78	0.64
17:1Q:70:MET:HG2	17:1Q:70:MET:O	1.97	0.64
20:1T:36:PHE:HB2	20:1T:37:MET:HE3	1.78	0.64
24:1Y:114:CYS:O	24:1Y:118:GLY:N	2.30	0.64
3:1C:61:LEU:HB3	3:1C:123:VAL:HG21	1.78	0.64
4:1D:20:TYR:OH	14:1N:295:ARG:NH2	2.31	0.64
13:1M:14:MET:HE1	13:1M:30:HIS:ND1	2.13	0.64
20:1T:45:LEU:HD11	22:1W:36:TYR:CE2	2.32	0.64
3:1C:199:LEU:HD13	4:1D:385:ARG:HD3	1.80	0.64
4:1D:238:ARG:NH1	8:1H:279:ARG:O	2.28	0.64
5:1E:69:VAL:HA	5:1E:72:ILE:HG22	1.79	0.64
7:1G:290:LEU:H	42:1q:143:PRO:CA	2.11	0.64
7:1G:379:LEU:HB2	7:1G:408:LEU:HD13	1.79	0.64
27:1b:78:GLU:OE1	27:1b:78:GLU:N	2.28	0.64
3:1C:127:ALA:O	3:1C:130:TYR:N	2.29	0.64
6:1F:49:LEU:O	6:1F:127:ARG:NE	2.26	0.64
8:1H:138:GLN:HA	8:1H:286:MET:HE1	1.79	0.64
9:1I:64:GLU:O	9:1I:134:GLY:N	2.30	0.64
12:1L:250:SER:HB2	12:1L:333:ALA:HA	1.80	0.64
13:1M:433:GLU:O	13:1M:437:MET:HG3	1.98	0.64
16:1P:182:PHE:HB2	16:1P:245:ILE:HD13	1.78	0.64
34:1i:71:VAL:HA	34:1i:75:LEU:HD12	1.78	0.64
7:1G:192:MET:N	7:1G:192:MET:SD	2.68	0.64
7:1G:284:ILE:O	7:1G:292:THR:OG1	2.10	0.64
7:1G:365:ASN:HB2	7:1G:488:LYS:HD2	1.80	0.64
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.31	0.64
15:1O:182:ARG:HG3	15:1O:185:LYS:HD2	1.80	0.64
6:1F:360:GLY:HA2	6:1F:366:ARG:HB2	1.79	0.64
7:1G:284:ILE:HG22	7:1G:285:ARG:H	1.63	0.64
7:1G:290:LEU:N	42:1q:143:PRO:HA	2.11	0.64
9:1I:172:ASP:OD2	9:1I:176:ARG:NH2	2.30	0.64
12:1L:599:MET:O	12:1L:605:HIS:ND1	2.30	0.64
16:1P:319:ARG:NH1	16:1P:327:LEU:O	2.30	0.64
3:1C:94:TYR:HB2	3:1C:107:VAL:HG22	1.79	0.64
5:1E:37:ASN:O	44:1s:65:GLN:NE2	2.30	0.64
16:1P:228:PHE:HA	16:1P:298:PRO:HG2	1.78	0.64
25:1Z:121:MET:HE1	25:1Z:137:THR:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:96:MET:HE2	2:1B:96:MET:HA	1.80	0.64
4:1D:157:HIS:HD2	4:1D:419:GLY:HA3	1.62	0.64
7:1G:382:THR:HB	7:1G:454:GLY:HA3	1.80	0.64
3:1C:132:ARG:HH21	3:1C:151:ILE:HG21	1.63	0.64
12:1L:7:LEU:HD11	12:1L:49:VAL:HB	1.80	0.64
12:1L:364:LYS:NZ	36:1k:58:ASN:O	2.31	0.64
15:1O:199:LEU:O	15:1O:202:ILE:HG13	1.98	0.64
7:1G:136:ALA:O	18:1R:74:ASN:ND2	2.31	0.63
7:1G:470:VAL:HA	7:1G:473:ILE:HG12	1.79	0.63
13:1M:36:LEU:HD21	50:1f:101:PC1:H371	1.79	0.63
7:1G:227:SER:O	7:1G:253:ARG:NH2	2.31	0.63
13:1M:72:LEU:HD23	13:1M:75:LEU:HD12	1.80	0.63
32:1g:85:MET:H	32:1g:85:MET:HE2	1.63	0.63
42:1q:27:LEU:O	42:1q:31:ASN:ND2	2.32	0.63
8:1H:203:GLY:O	8:1H:208:VAL:N	2.31	0.63
9:1I:89:ALA:O	9:1I:115:LYS:NZ	2.26	0.63
9:1I:133:GLU:N	9:1I:133:GLU:OE1	2.32	0.63
15:1O:76:ASN:OD1	15:1O:95:ARG:NE	2.32	0.63
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	1.80	0.63
1:1A:84:LEU:HD21	27:1b:45:ASN:HD22	1.62	0.63
15:1O:141:GLN:NE2	15:1O:201:ASP:OD2	2.24	0.63
34:1i:65:ARG:HH11	34:1i:65:ARG:HG2	1.63	0.63
7:1G:381:GLY:O	7:1G:456:SER:OG	2.16	0.63
52:1M:501:PGT:O4P	52:1M:501:PGT:O6	2.15	0.63
7:1G:46:LEU:HD11	7:1G:161:ARG:HB2	1.80	0.63
21:1V:66:LYS:C	21:1V:70:GLN:HE21	2.06	0.63
37:1l:80:ASP:HB3	37:1l:83:MET:SD	2.39	0.63
5:1E:72:ILE:HG23	5:1E:73:LEU:HD22	1.80	0.63
5:1E:106:THR:OG1	6:1F:346:ALA:O	2.16	0.63
15:1O:130:SER:O	15:1O:133:VAL:HG22	1.98	0.63
31:1f:53:GLU:HG2	31:1f:54:VAL:HG23	1.80	0.63
37:1l:129:GLY:HA2	40:1o:21:MET:HE1	1.81	0.63
1:1A:7:LEU:HD23	8:1H:84:THR:HG21	1.81	0.63
4:1D:169:TRP:CH2	9:1I:36:MET:HE1	2.34	0.63
14:1N:120:GLN:HA	14:1N:176:ARG:HE	1.63	0.63
14:1N:318:GLU:OE1	29:1d:50:ARG:NH1	2.31	0.63
20:1U:22:TYR:OH	20:1U:46:ASP:OD2	2.16	0.63
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	1.80	0.63
11:1K:91:GLN:OE1	11:1K:91:GLN:N	2.23	0.62
12:1L:486:MET:O	12:1L:489:THR:OG1	2.17	0.62
13:1M:108:MET:HB3	13:1M:121:LEU:HD13	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:339:MET:HG3	29:1d:34:MET:HE3	1.81	0.62
20:1T:52:MET:HE1	22:1W:37:ARG:HA	1.81	0.62
7:1G:138:GLU:HB3	18:1R:77:LYS:HG3	1.81	0.62
7:1G:444:LYS:HA	7:1G:477:ILE:HD13	1.81	0.62
20:1T:66:ASP:OD1	20:1T:66:ASP:N	2.30	0.62
5:1E:194:GLU:OE1	6:1F:26:TYR:OH	2.16	0.62
25:1Z:21:TYR:O	25:1Z:21:TYR:HD2	1.81	0.62
38:1m:122:GLN:HB2	38:1m:125:ASN:HB3	1.81	0.62
9:1I:113:MET:HE1	9:1I:118:TYR:CE2	2.34	0.62
16:1P:98:GLU:O	16:1P:145:TYR:OH	2.15	0.62
21:1V:74:GLY:HA2	43:1r:102:ARG:NH1	2.14	0.62
5:1E:35:VAL:HG23	5:1E:43:LYS:HB2	1.81	0.62
20:1U:45:LEU:HD21	39:1n:44:ARG:HD2	1.81	0.62
23:1X:134:ARG:O	27:1b:57:ARG:NH2	2.32	0.62
43:1r:1:ALA:O	43:1r:2:SER:N	2.33	0.62
3:1C:97:LEU:HD23	3:1C:104:GLN:HG3	1.79	0.62
4:1D:228:MET:O	4:1D:232:ASN:ND2	2.31	0.62
7:1G:266:LYS:NZ	7:1G:671:PHE:O	2.32	0.62
14:1N:36:ASN:OD1	14:1N:134:GLN:NE2	2.32	0.62
18:1R:79:THR:OG1	18:1R:80:LYS:N	2.18	0.62
30:1e:80:ARG:NH1	30:1e:83:ASP:OD2	2.32	0.62
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.14	0.62
3:1C:131:GLU:HA	3:1C:134:ILE:HG22	1.81	0.62
3:1C:193:GLU:OE1	3:1C:193:GLU:N	2.22	0.62
3:1C:204:GLU:HA	17:1Q:50:ASN:ND2	2.13	0.62
15:1O:133:VAL:HG21	15:1O:206:TYR:CE1	2.34	0.62
7:1G:288:LYS:H	42:1q:143:PRO:CD	2.11	0.62
12:1L:210:ASN:HB3	12:1L:211:MET:HE2	1.82	0.62
16:1P:46:ILE:HD13	18:1R:26:VAL:HG21	1.80	0.62
3:1C:185:ALA:HB2	22:1W:105:ARG:HE	1.64	0.62
6:1F:298:ILE:HB	6:1F:335:ILE:HB	1.82	0.62
6:1F:410:GLY:HA2	6:1F:413:TRP:CZ3	2.34	0.62
13:1M:235:LEU:HA	13:1M:238:LEU:HB3	1.82	0.62
29:1d:104:LYS:NZ	41:1p:78:GLU:OE2	2.33	0.62
5:1E:31:ILE:HG22	5:1E:50:VAL:HG23	1.82	0.62
6:1F:258:ILE:HD11	6:1F:262:VAL:HG21	1.82	0.62
15:1O:230:ASP:OD2	15:1O:233:LYS:N	2.32	0.62
17:1Q:91:ASP:OD1	17:1Q:91:ASP:N	2.33	0.62
37:1l:50:LEU:HD11	37:1l:76:PRO:HB2	1.82	0.62
3:1C:58:ILE:HD11	3:1C:118:GLU:HB2	1.81	0.61
5:1E:145:LEU:O	5:1E:160:TYR:OH	2.17	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:243:ALA:HA	6:1F:251:SER:HB2	1.81	0.61
10:1J:125:TRP:HB2	25:1Z:137:THR:HG21	1.81	0.61
15:1O:170:VAL:HG13	15:1O:223:TYR:HD2	1.64	0.61
19:1S:72:GLN:HG2	19:1S:74:LYS:HE2	1.81	0.61
39:1n:123:GLN:OE1	39:1n:126:ARG:NH2	2.33	0.61
2:1B:125:TYR:CE1	9:1I:88:PRO:HB2	2.26	0.61
4:1D:239:THR:O	4:1D:294:TYR:N	2.32	0.61
10:1J:55:MET:HE1	10:1J:59:ILE:HD13	1.80	0.61
14:1N:66:ALA:HB2	14:1N:104:MET:HG2	1.82	0.61
7:1G:460:ARG:NE	7:1G:462:ASP:OD1	2.33	0.61
7:1G:503:LEU:HD12	7:1G:509:PRO:HB3	1.81	0.61
8:1H:183:MET:HE3	50:1H:401:PC1:H372	1.81	0.61
12:1L:407:TRP:NE1	37:1l:112:MET:SD	2.72	0.61
18:1R:93:GLN:HG3	18:1R:95:HIS:H	1.64	0.61
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.33	0.61
8:1H:207:LEU:HD23	8:1H:210:GLY:HA2	1.82	0.61
9:1I:136:ASN:HD22	9:1I:161:TRP:HZ2	1.47	0.61
26:1a:39:ALA:HA	26:1a:44:GLN:HB2	1.82	0.61
14:1N:170:LEU:HD21	14:1N:291:TYR:HB3	1.82	0.61
16:1P:22:THR:HG23	16:1P:46:ILE:HB	1.82	0.61
16:1P:143:SER:OG	16:1P:282:ASP:OD1	2.17	0.61
29:1d:119:VAL:HG21	41:1p:146:GLY:HA2	1.82	0.61
37:1l:63:ASP:O	38:1m:43:LYS:NZ	2.33	0.61
4:1D:111:MET:N	4:1D:111:MET:SD	2.73	0.61
7:1G:155:GLN:NE2	7:1G:181:MET:O	2.34	0.61
12:1L:340:PHE:O	12:1L:344:GLY:N	2.33	0.61
16:1P:263:TYR:HD1	16:1P:284:VAL:HB	1.66	0.61
29:1d:46:ASN:HD21	29:1d:61:GLN:HE21	1.49	0.61
38:1m:16:THR:HG23	38:1m:17:LEU:HD12	1.82	0.61
42:1q:60:ARG:NH2	42:1q:95:ASP:OD1	2.33	0.61
6:1F:162:ILE:HB	6:1F:174:ASP:HA	1.82	0.61
13:1M:22:MET:O	13:1M:26:ASN:ND2	2.33	0.61
16:1P:208:VAL:HG22	16:1P:212:LYS:HE2	1.82	0.61
16:1P:263:TYR:CD1	16:1P:284:VAL:HB	2.36	0.61
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.82	0.61
6:1F:301:GLY:H	6:1F:333:ALA:HB3	1.65	0.61
7:1G:213:TYR:O	7:1G:216:THR:OG1	2.18	0.61
7:1G:672:TYR:HB3	7:1G:684:MET:SD	2.41	0.61
9:1I:44:GLU:OE1	9:1I:44:GLU:N	2.34	0.61
20:1T:18:VAL:HG21	20:1T:57:GLU:HG2	1.83	0.61
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:337:MET:HE1	6:1F:343:ILE:HA	1.81	0.61
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	1.81	0.61
16:1P:258:LEU:HD12	16:1P:263:TYR:CD2	2.35	0.61
19:1S:81:PHE:CE1	19:1S:85:GLN:HG2	2.35	0.61
4:1D:87:THR:OG1	4:1D:88:GLU:OE1	2.19	0.61
7:1G:314:ASP:HB2	7:1G:520:LYS:HB2	1.83	0.61
7:1G:481:SER:O	7:1G:484:THR:OG1	2.15	0.61
12:1L:434:LYS:NZ	36:1k:56:PHE:O	2.31	0.61
19:1S:57:CYS:SG	19:1S:58:SER:N	2.74	0.61
3:1C:199:LEU:HD23	4:1D:354:GLU:HA	1.82	0.60
4:1D:322:GLU:HG2	43:1r:43:GLY:HA2	1.83	0.60
12:1L:159:HIS:HE1	13:1M:349:GLN:HB3	1.64	0.60
16:1P:258:LEU:HD12	16:1P:263:TYR:HD2	1.66	0.60
17:1Q:40:PRO:HD3	17:1Q:56:LYS:HD2	1.83	0.60
3:1C:113:GLU:OE1	3:1C:113:GLU:N	2.30	0.60
4:1D:270:ARG:HG2	4:1D:278:TYR:CE2	2.37	0.60
7:1G:272:ASP:HB2	7:1G:681:SER:HB2	1.83	0.60
10:1J:64:MET:HE1	11:1K:68:ALA:HA	1.82	0.60
16:1P:107:GLU:OE1	16:1P:112:LYS:NZ	2.34	0.60
19:1S:38:LYS:O	19:1S:38:LYS:NZ	2.32	0.60
19:1S:44:LYS:NZ	19:1S:50:LEU:O	2.34	0.60
3:1C:117:ILE:O	3:1C:143:ALA:N	2.30	0.60
8:1H:284:GLN:HA	8:1H:287:HIS:HB3	1.83	0.60
13:1M:60:SER:HB3	13:1M:457:PRO:HA	1.83	0.60
13:1M:447:LEU:HD21	13:1M:454:ILE:HD13	1.84	0.60
17:1Q:127:ARG:HD3	44:1s:70:ARG:HH22	1.66	0.60
23:1X:47:TRP:CH2	33:1h:141:PRO:HD3	2.36	0.60
1:1A:10:ASN:ND2	8:1H:10:ILE:HD11	2.17	0.60
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.84	0.60
5:1E:111:ARG:NH1	6:1F:260:GLY:O	2.33	0.60
7:1G:282:PRO:O	7:1G:294:THR:OG1	2.15	0.60
7:1G:437:HIS:NE2	7:1G:439:PHE:HB3	2.16	0.60
12:1L:574:SER:OG	14:1N:167:TRP:O	2.17	0.60
13:1M:153:THR:HA	13:1M:205:VAL:HG11	1.83	0.60
38:1m:54:ASN:OD1	39:1n:129:ARG:NH2	2.33	0.60
4:1D:246:THR:HA	21:1V:11:VAL:HG13	1.82	0.60
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.82	0.60
21:1V:43:TYR:HB2	21:1V:99:TRP:HZ2	1.65	0.60
40:1o:61:TYR:CD2	40:1o:89:CYS:HB2	2.36	0.60
2:1B:165:ARG:NH1	42:1q:78:ASP:OD1	2.34	0.60
5:1E:27:ASN:HA	5:1E:30:ARG:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:587:TYR:O	12:1L:590:SER:OG	2.19	0.60
13:1M:115:LEU:HB3	13:1M:164:LEU:HD23	1.83	0.60
34:1i:18:ARG:NH1	39:1n:172:ARG:O	2.34	0.60
1:1A:9:THR:HG21	8:1H:6:ILE:HG21	1.83	0.60
7:1G:347:GLU:OE1	7:1G:459:GLN:NE2	2.35	0.60
12:1L:97:THR:HG21	12:1L:125:LEU:HD11	1.84	0.60
14:1N:62:THR:HG21	14:1N:114:TRP:CD1	2.37	0.60
17:1Q:15:GLU:HG2	22:1W:74:THR:HG23	1.83	0.60
32:1g:66:PHE:HA	32:1g:70:LEU:HB3	1.83	0.60
4:1D:169:TRP:NE1	8:1H:32:GLN:HA	2.17	0.60
5:1E:100:ILE:HA	5:1E:156:ILE:HG22	1.83	0.60
7:1G:169:VAL:HG21	7:1G:191:PHE:HE1	1.66	0.60
13:1M:237:LYS:HE3	13:1M:319:HIS:HD1	1.67	0.60
7:1G:283:MET:HB3	7:1G:291:LEU:HD12	1.83	0.60
7:1G:295:THR:OG1	7:1G:297:GLU:OE1	2.20	0.60
7:1G:348:VAL:N	7:1G:459:GLN:OE1	2.34	0.60
9:1I:123:GLN:NE2	9:1I:132:VAL:HG12	2.17	0.60
17:1Q:90:GLU:OE1	17:1Q:90:GLU:N	2.25	0.60
19:1S:26:SER:O	19:1S:33:ARG:NH2	2.35	0.60
27:1b:27:LEU:HB3	27:1b:31:LEU:HD11	1.83	0.60
1:1A:21:ALA:HB1	8:1H:218:GLY:HA2	1.83	0.60
6:1F:276:LEU:HD23	6:1F:317:MET:HG2	1.83	0.60
13:1M:47:GLU:HB3	41:1p:92:ARG:HE	1.67	0.60
20:1U:21:LEU:O	36:1k:46:ARG:NH2	2.35	0.60
21:1V:27:TYR:HB3	21:1V:55:LEU:HD22	1.83	0.60
21:1V:37:ILE:O	21:1V:44:ARG:NH1	2.35	0.60
24:1Y:80:ARG:NH1	24:1Y:88:ASN:OD1	2.35	0.60
44:1s:63:MET:HE3	44:1s:64:PRO:HD3	1.84	0.60
5:1E:27:ASN:OD1	5:1E:30:ARG:NH1	2.33	0.59
12:1L:324:LEU:HG	12:1L:476:THR:HG21	1.84	0.59
13:1M:106:LEU:HD13	13:1M:234:VAL:HG11	1.84	0.59
18:1R:57:ILE:HG12	18:1R:75:LEU:HD12	1.84	0.59
33:1h:17:TYR:HE1	39:1n:107:HIS:HB2	1.67	0.59
7:1G:6:SER:OG	7:1G:7:ASN:N	2.35	0.59
9:1I:99:ARG:NH2	9:1I:101:ASP:OD2	2.34	0.59
13:1M:257:MET:HE3	13:1M:260:PRO:HG2	1.82	0.59
16:1P:168:PRO:HA	16:1P:230:PHE:HB2	1.83	0.59
36:1k:23:ILE:HG12	36:1k:32:GLN:HG3	1.82	0.59
1:1A:10:ASN:HD22	8:1H:10:ILE:HD11	1.68	0.59
3:1C:116:PRO:HB2	3:1C:143:ALA:HB2	1.85	0.59
4:1D:332:PRO:HB3	4:1D:352:TYR:HE1	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:10:GLU:O	7:1G:75:LYS:NZ	2.32	0.59
12:1L:425:ARG:NH2	45:1L:704:3PE:O13	2.35	0.59
16:1P:230:PHE:HD2	16:1P:300:LEU:HD12	1.67	0.59
20:1T:22:TYR:HD2	20:1T:23:ASP:H	1.51	0.59
25:1Z:56:GLU:HA	25:1Z:59:ARG:HD3	1.82	0.59
37:1l:34:TYR:OH	37:1l:46:ASP:O	2.19	0.59
41:1p:88:GLU:OE2	41:1p:150:SER:OG	2.18	0.59
6:1F:95:VAL:HG22	6:1F:228:VAL:HG21	1.84	0.59
6:1F:309:LYS:HA	6:1F:312:CYS:HB2	1.84	0.59
9:1I:113:MET:HB2	9:1I:147:LEU:O	2.03	0.59
12:1L:14:ILE:H	12:1L:14:ILE:HD12	1.67	0.59
14:1N:5:ILE:HA	14:1N:8:THR:HG22	1.84	0.59
20:1U:48:VAL:HG21	39:1n:16:LEU:HB3	1.84	0.59
34:1i:71:VAL:O	34:1i:76:ILE:HG13	2.02	0.59
34:1i:107:ASP:H	40:1o:67:LYS:HZ1	1.50	0.59
39:1n:167:TRP:O	39:1n:171:THR:OG1	2.16	0.59
5:1E:22:ASP:OD1	5:1E:23:PHE:N	2.35	0.59
6:1F:137:TYR:CE1	6:1F:180:GLY:HA2	2.37	0.59
20:1T:40:LEU:HB3	20:1T:42:LEU:HG	1.84	0.59
2:1B:81:ARG:HD2	8:1H:61:LEU:HD21	1.85	0.59
4:1D:295:ASP:OD1	9:1I:6:ASN:ND2	2.33	0.59
6:1F:365:CYS:HB2	46:1F:502:SF4:S2	2.43	0.59
12:1L:310:LEU:HA	12:1L:313:MET:HG3	1.84	0.59
32:1g:112:CYS:SG	32:1g:113:PHE:N	2.76	0.59
34:1i:102:ARG:HB2	40:1o:49:GLN:HG2	1.84	0.59
1:1A:106:TRP:NE1	45:1A:201:3PE:O12	2.24	0.59
6:1F:199:LYS:HE3	17:1Q:132:THR:HA	1.84	0.59
10:1J:125:TRP:HH2	25:1Z:126:GLY:HA2	1.67	0.59
45:1L:703:3PE:O14	24:1Y:58:TYR:OH	2.15	0.59
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.83	0.59
13:1M:338:HIS:NE2	32:1g:34:ASP:OD2	2.35	0.59
14:1N:344:SER:HB2	29:1d:82:MET:HB3	1.84	0.59
31:1f:42:LEU:HD23	31:1f:42:LEU:H	1.67	0.59
1:1A:54:LYS:NZ	4:1D:71:GLU:OE1	2.23	0.59
4:1D:111:MET:HE3	4:1D:189:MET:HG3	1.85	0.59
4:1D:300:ARG:NH2	4:1D:422:ASP:OD2	2.35	0.59
4:1D:305:ARG:NH1	25:1Z:22:LYS:O	2.36	0.59
10:1J:68:PHE:HZ	11:1K:30:LEU:HB3	1.67	0.59
14:1N:319:HIS:HD2	14:1N:321:LYS:H	1.50	0.59
25:1Z:138:TYR:HB3	25:1Z:142:TRP:CD1	2.38	0.59
3:1C:158:GLU:OE2	3:1C:158:GLU:N	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:285:ARG:HH11	7:1G:291:LEU:HD22	1.67	0.59
8:1H:207:LEU:O	8:1H:209:SER:N	2.35	0.59
12:1L:132:VAL:HG23	12:1L:258:PHE:CZ	2.38	0.59
3:1C:127:ALA:HA	3:1C:130:TYR:HD1	1.68	0.59
4:1D:220:PHE:HD2	43:1r:17:ARG:HH21	1.49	0.59
7:1G:632:ARG:NH2	19:1S:59:ASP:OD1	2.34	0.59
8:1H:168:THR:OG1	25:1Z:57:ARG:NH1	2.35	0.59
12:1L:81:LYS:C	12:1L:82:MET:HE2	2.28	0.59
23:1X:126:LYS:HD2	27:1b:66:PRO:HG3	1.85	0.59
25:1Z:28:ARG:NH2	43:1r:13:TRP:O	2.31	0.59
29:1d:10:PRO:HG3	30:1e:4:ASP:HB3	1.84	0.59
4:1D:289:SER:OG	4:1D:290:ARG:N	2.26	0.58
42:1q:2:GLU:HA	42:1q:5:GLN:HE22	1.68	0.58
3:1C:50:ILE:HD13	3:1C:52:ILE:HG23	1.84	0.58
12:1L:359:MET:N	12:1L:359:MET:SD	2.76	0.58
12:1L:482:MET:HB3	12:1L:486:MET:SD	2.43	0.58
7:1G:433:ALA:O	7:1G:476:ASN:ND2	2.37	0.58
7:1G:693:GLU:N	7:1G:693:GLU:OE2	2.35	0.58
12:1L:526:LEU:HD23	12:1L:530:PRO:HG2	1.86	0.58
20:1T:31:SER:N	20:1T:34:SER:OG	2.36	0.58
20:1T:34:SER:H	20:1T:73:PRO:HD2	1.69	0.58
6:1F:264:HIS:ND1	6:1F:284:ALA:O	2.31	0.58
7:1G:283:MET:HG3	7:1G:291:LEU:HB3	1.85	0.58
7:1G:673:MET:HA	7:1G:673:MET:HE3	1.85	0.58
12:1L:12:LEU:HD11	12:1L:129:MET:HB2	1.85	0.58
12:1L:132:VAL:O	12:1L:262:ARG:NH2	2.25	0.58
12:1L:295:GLN:O	12:1L:425:ARG:NH1	2.37	0.58
16:1P:236:TYR:HB3	16:1P:240:ASP:HB3	1.83	0.58
23:1X:95:LEU:HD13	23:1X:97:ARG:HG3	1.85	0.58
4:1D:66:MET:HE2	4:1D:73:VAL:HG21	1.84	0.58
7:1G:108:CYS:O	7:1G:218:ARG:NH1	2.22	0.58
9:1I:76:ARG:NH1	9:1I:129:ASP:OD1	2.34	0.58
12:1L:346:ILE:HD11	12:1L:359:MET:HG2	1.85	0.58
17:1Q:55:TRP:O	17:1Q:86:PHE:N	2.35	0.58
23:1X:11:ASP:N	23:1X:11:ASP:OD1	2.33	0.58
25:1Z:59:ARG:NH2	27:1b:81:LYS:O	2.37	0.58
2:1B:109:GLU:OE2	2:1B:111:ARG:NE	2.37	0.58
3:1C:32:ILE:HG22	3:1C:33:LEU:HD12	1.85	0.58
4:1D:51:PHE:HB3	4:1D:64:LEU:HB3	1.86	0.58
16:1P:200:THR:O	16:1P:238:LEU:N	2.37	0.58
16:1P:236:TYR:HB2	16:1P:241:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:51:ILE:HB	20:1T:62:ILE:HD11	1.85	0.58
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.03	0.58
6:1F:259:SER:N	6:1F:334:VAL:O	2.31	0.58
11:1K:2:PRO:HD3	30:1e:72:MET:HE1	1.84	0.58
13:1M:204:MET:HA	13:1M:207:MET:HB2	1.85	0.58
34:1i:4:THR:OG1	34:1i:6:ASP:OD1	2.16	0.58
7:1G:667:THR:HG22	7:1G:668:ILE:H	1.68	0.58
12:1L:293:ILE:HD12	12:1L:294:THR:HG23	1.86	0.58
20:1T:14:ARG:HA	20:1T:17:TYR:CD1	2.39	0.58
37:1l:59:ASP:O	37:1l:64:TRP:NE1	2.34	0.58
38:1m:52:ASP:OD1	38:1m:54:ASN:ND2	2.34	0.58
1:1A:110:GLY:HA2	10:1J:169:MET:HE2	1.86	0.58
3:1C:116:PRO:HG3	22:1W:20:ILE:HG23	1.86	0.58
7:1G:283:MET:HB3	7:1G:560:ILE:HB	1.85	0.58
8:1H:29:GLY:O	8:1H:34:ARG:N	2.37	0.58
13:1M:70:THR:HA	13:1M:103:GLN:HE21	1.68	0.58
7:1G:632:ARG:HB3	7:1G:635:ASP:HB2	1.85	0.58
13:1M:261:PHE:HB2	13:1M:302:MET:HE1	1.86	0.58
14:1N:292:PHE:HA	14:1N:295:ARG:HB3	1.84	0.58
16:1P:153:GLU:OE1	16:1P:165:ILE:HG12	2.03	0.58
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.37	0.58
33:1h:114:MET:HG2	33:1h:122:TRP:CD1	2.38	0.58
4:1D:200:HIS:NE2	9:1I:124:GLU:OE2	2.37	0.57
4:1D:430:ARG:HH11	4:1D:430:ARG:H	1.50	0.57
7:1G:549:HIS:HB2	7:1G:676:SER:HB2	1.85	0.57
8:1H:65:THR:HA	16:1P:324:TYR:HB3	1.86	0.57
8:1H:235:ASN:CG	8:1H:266:LEU:HB3	2.29	0.57
8:1H:269:THR:HA	8:1H:272:TRP:HB3	1.86	0.57
9:1I:119:CYS:HB2	9:1I:121:PHE:H	1.68	0.57
20:1T:11:ILE:HG23	20:1T:80:ILE:HG22	1.85	0.57
22:1W:34:GLU:HA	22:1W:37:ARG:HG2	1.86	0.57
22:1W:99:GLN:H	22:1W:102:HIS:HD2	1.52	0.57
36:1k:49:ALA:O	36:1k:53:SER:OG	2.18	0.57
37:1l:94:THR:HG22	37:1l:96:VAL:H	1.69	0.57
2:1B:61:HIS:HA	4:1D:171:PHE:HZ	1.69	0.57
2:1B:81:ARG:HG3	8:1H:216:ALA:HB2	1.87	0.57
4:1D:238:ARG:HD2	8:1H:281:ARG:HG2	1.85	0.57
7:1G:138:GLU:N	7:1G:138:GLU:OE1	2.35	0.57
12:1L:417:SER:HB2	12:1L:493:VAL:HB	1.85	0.57
12:1L:502:LEU:O	12:1L:506:ASN:ND2	2.37	0.57
17:1Q:13:VAL:HG12	17:1Q:15:GLU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:8:LEU:HD12	20:1U:9:GLU:OE1	2.03	0.57
21:1V:44:ARG:O	21:1V:48:GLU:HG3	2.04	0.57
50:1f:101:PC1:H3A1	32:1g:72:LEU:HD11	1.84	0.57
4:1D:157:HIS:CD2	4:1D:419:GLY:HA3	2.40	0.57
5:1E:154:VAL:HG12	5:1E:161:TYR:HB2	1.85	0.57
14:1N:320:THR:OG1	15:1O:265:ASN:ND2	2.37	0.57
15:1O:311:ASP:OD1	15:1O:312:VAL:N	2.36	0.57
17:1Q:89:LYS:O	17:1Q:93:VAL:HG12	2.04	0.57
21:1V:85:ASN:O	21:1V:89:LEU:N	2.35	0.57
4:1D:405:MET:HE3	4:1D:417:ILE:HD12	1.85	0.57
13:1M:13:PRO:HB3	45:1N:401:3PE:H2C1	1.86	0.57
13:1M:216:LEU:HD13	13:1M:220:HIS:NE2	2.20	0.57
52:1M:501:PGT:H131	52:1M:501:PGT:H361	1.85	0.57
20:1T:34:SER:HB2	20:1T:73:PRO:HG2	1.86	0.57
22:1W:87:LYS:O	22:1W:87:LYS:HD3	2.04	0.57
33:1h:130:LYS:O	33:1h:133:ILE:HG13	2.04	0.57
37:1l:65:ASP:HB3	38:1m:46:TYR:HE2	1.69	0.57
5:1E:48:LEU:HB3	5:1E:49:PRO:HD3	1.86	0.57
7:1G:704:CYS:SG	9:1I:103:SER:HA	2.44	0.57
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.36	0.57
32:1g:66:PHE:HB2	33:1h:28:TYR:CE2	2.39	0.57
36:1k:12:LYS:HA	36:1k:12:LYS:HE3	1.86	0.57
7:1G:362:TYR:OH	7:1G:504:ASP:OD1	2.19	0.57
9:1I:72:SER:O	42:1q:107:LYS:NZ	2.36	0.57
50:1I:203:PC1:H11	25:1Z:29:GLY:HA3	1.86	0.57
15:1O:78:SER:O	15:1O:92:ASN:ND2	2.36	0.57
42:1q:5:GLN:HA	42:1q:8:ARG:HB3	1.86	0.57
4:1D:303:GLU:O	4:1D:307:SER:OG	2.21	0.57
7:1G:60:GLU:HG2	7:1G:61:LYS:HG3	1.85	0.57
8:1H:35:LYS:HB2	9:1I:47:THR:HG21	1.84	0.57
9:1I:164:GLU:OE2	42:1q:87:HIS:ND1	2.36	0.57
14:1N:103:ALA:O	14:1N:107:GLY:N	2.35	0.57
3:1C:95:ASN:HD21	3:1C:106:ARG:HH11	1.52	0.57
3:1C:202:PRO:HG3	17:1Q:46:GLN:OE1	2.05	0.57
9:1I:39:SER:OG	9:1I:43:ARG:NH2	2.38	0.57
9:1I:70:TYR:CD1	9:1I:76:ARG:HG2	2.40	0.57
12:1L:102:GLU:HB2	12:1L:453:SER:HB3	1.87	0.57
14:1N:5:ILE:H	14:1N:5:ILE:HD12	1.70	0.57
33:1h:7:ARG:CZ	34:1i:27:LEU:HG	2.34	0.57
39:1n:19:TYR:HB2	39:1n:47:PHE:HE2	1.69	0.57
40:1o:61:TYR:CE2	40:1o:89:CYS:HB2	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:102:LEU:HD21	14:1N:141:VAL:HB	1.87	0.57
15:1O:47:GLY:O	15:1O:120:GLN:NE2	2.38	0.57
22:1W:37:ARG:O	22:1W:41:ARG:NH1	2.37	0.57
27:1b:14:LYS:HA	27:1b:14:LYS:HE3	1.86	0.57
35:1j:55:ASP:OD2	35:1j:58:GLN:N	2.35	0.57
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.85	0.57
39:1n:176:ARG:HG3	39:1n:178:MET:SD	2.45	0.57
9:1I:74:GLU:HG2	18:1R:44:ILE:HD13	1.86	0.57
9:1I:153:LYS:HD2	9:1I:157:ASN:HD21	1.68	0.57
12:1L:407:TRP:CD2	37:1I:115:MET:HE2	2.39	0.57
15:1O:270:LEU:O	15:1O:273:THR:OG1	2.20	0.57
16:1P:311:GLU:OE2	16:1P:311:GLU:N	2.27	0.57
29:1d:34:MET:HE2	29:1d:34:MET:HA	1.87	0.57
32:1g:113:PHE:O	41:1p:158:GLN:NE2	2.33	0.57
40:1o:68:CYS:O	40:1o:72:SER:OG	2.19	0.57
8:1H:77:LEU:HD13	8:1H:118:TRP:HZ3	1.70	0.56
8:1H:215:TYR:CE2	8:1H:219:PRO:HB2	2.40	0.56
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	1.85	0.56
32:1g:23:THR:C	32:1g:25:ARG:H	2.11	0.56
33:1h:114:MET:HG2	33:1h:122:TRP:NE1	2.20	0.56
6:1F:184:TYR:CE2	48:1F:501:FMN:H6	2.40	0.56
6:1F:205:LEU:HB2	17:1Q:118:TYR:CZ	2.40	0.56
7:1G:367:THR:OG1	7:1G:577:GLU:OE1	2.19	0.56
16:1P:29:PHE:HZ	16:1P:173:GLY:HA3	1.69	0.56
24:1Y:40:ILE:HD12	24:1Y:45:PRO:HG3	1.87	0.56
44:1s:71:GLN:HE21	44:1s:75:HIS:HD2	1.51	0.56
3:1C:32:ILE:HD11	21:1V:46:TYR:HD2	1.70	0.56
4:1D:281:VAL:HG21	4:1D:310:ILE:HG23	1.87	0.56
4:1D:326:ASP:OD1	7:1G:127:ARG:NH2	2.38	0.56
4:1D:375:GLY:O	4:1D:392:LYS:N	2.30	0.56
7:1G:107:ILE:HD13	9:1I:78:ILE:HG23	1.86	0.56
7:1G:538:PRO:HB2	7:1G:541:CYS:SG	2.44	0.56
7:1G:599:ILE:HG22	22:1W:122:PHE:HE1	1.71	0.56
13:1M:424:ASN:OD1	38:1m:55:ARG:NH1	2.38	0.56
17:1Q:30:ILE:HD12	17:1Q:101:TRP:CD1	2.40	0.56
20:1U:35:HIS:HE2	20:1U:71:MET:HE3	1.71	0.56
35:1j:10:ARG:NH1	35:1j:16:GLN:OE1	2.38	0.56
39:1n:71:TRP:O	39:1n:74:GLN:NE2	2.36	0.56
43:1r:29:GLU:N	43:1r:29:GLU:OE2	2.38	0.56
5:1E:148:CYS:HA	5:1E:153:MET:HE2	1.87	0.56
7:1G:165:GLU:HA	7:1G:396:ARG:HH21	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:389:PRO:HD2	7:1G:390:LEU:N	2.08	0.56
20:1U:35:HIS:NE2	20:1U:71:MET:HE3	2.21	0.56
21:1V:67:LEU:HA	21:1V:70:GLN:HG2	1.87	0.56
5:1E:82:GLU:OE2	7:1G:174:THR:N	2.37	0.56
11:1K:42:ILE:O	11:1K:45:THR:OG1	2.23	0.56
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.38	0.56
16:1P:147:ARG:O	16:1P:151:VAL:HG22	2.05	0.56
19:1S:61:GLN:HB2	19:1S:79:ASN:HD22	1.70	0.56
30:1e:66:LEU:HD12	30:1e:67:LEU:HD22	1.88	0.56
41:1p:139:GLN:HA	41:1p:143:SER:HB3	1.86	0.56
6:1F:16:LYS:HB2	6:1F:19:ASP:HB2	1.87	0.56
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.88	0.56
15:1O:207:LYS:HA	15:1O:211:LEU:HD23	1.86	0.56
16:1P:198:LYS:HE3	16:1P:239:PHE:CD2	2.41	0.56
20:1U:20:LYS:HE3	20:1U:27:PRO:HB3	1.87	0.56
42:1q:111:THR:OG1	42:1q:112:ASN:OD1	2.21	0.56
44:1s:71:GLN:HE21	44:1s:75:HIS:CD2	2.23	0.56
8:1H:134:ARG:HH22	8:1H:207:LEU:HD21	1.69	0.56
9:1I:70:TYR:CE2	18:1R:87:CYS:HA	2.32	0.56
21:1V:54:LYS:HD2	21:1V:71:LEU:HB3	1.88	0.56
4:1D:259:MET:HE1	4:1D:296:ARG:CZ	2.35	0.56
7:1G:249:ARG:HH11	7:1G:251:LEU:HD21	1.69	0.56
15:1O:192:MET:N	15:1O:192:MET:SD	2.78	0.56
41:1p:4:TRP:O	41:1p:6:LYS:NZ	2.38	0.56
1:1A:108:GLN:O	1:1A:110:GLY:N	2.39	0.56
4:1D:145:THR:HG1	4:1D:181:TYR:HH	1.54	0.56
6:1F:140:GLY:HA2	6:1F:179:ARG:HG3	1.87	0.56
6:1F:295:LEU:HD22	6:1F:339:ARG:HG3	1.88	0.56
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.88	0.56
13:1M:44:GLN:HB2	32:1g:83:TYR:HE1	1.71	0.56
15:1O:260:ARG:HA	15:1O:263:VAL:HG22	1.87	0.56
16:1P:97:ARG:H	16:1P:109:VAL:HG21	1.70	0.56
34:1i:14:LEU:HD13	39:1n:169:ILE:HG21	1.88	0.56
34:1i:77:PRO:O	34:1i:81:ILE:HG12	2.06	0.56
6:1F:194:GLU:OE2	6:1F:202:LYS:N	2.35	0.56
7:1G:243:ARG:HD2	7:1G:244:THR:HB	1.88	0.56
7:1G:257:ASP:OD1	7:1G:257:ASP:N	2.39	0.56
13:1M:50:LEU:N	13:1M:58:SER:O	2.38	0.56
21:1V:18:THR:O	21:1V:18:THR:OG1	2.24	0.56
21:1V:76:ILE:HA	21:1V:79:VAL:HG22	1.88	0.56
22:1W:49:LEU:O	22:1W:51:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:99:ALA:HA	4:1D:102:TYR:HD2	1.70	0.55
4:1D:237:ASN:HA	4:1D:240:VAL:HG12	1.88	0.55
6:1F:197:GLU:OE2	6:1F:204:ARG:NH2	2.39	0.55
8:1H:233:MET:O	8:1H:236:ALA:N	2.39	0.55
13:1M:176:PHE:HE2	13:1M:245:ARG:HB3	1.71	0.55
19:1S:17:GLU:HB3	19:1S:67:ARG:HG2	1.89	0.55
20:1T:80:ILE:O	20:1T:83:LYS:HE3	2.05	0.55
27:1b:23:ALA:O	27:1b:27:LEU:HD12	2.06	0.55
30:1e:6:GLN:OE1	30:1e:15:ARG:NH1	2.39	0.55
9:1I:14:MET:HE1	27:1b:9:LYS:HG2	1.88	0.55
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.05	0.55
16:1P:250:TYR:HE2	16:1P:322:ARG:HD2	1.71	0.55
20:1T:14:ARG:HA	20:1T:17:TYR:HD1	1.72	0.55
3:1C:38:GLN:NE2	3:1C:110:TYR:OH	2.40	0.55
6:1F:272:MET:SD	6:1F:273:SER:OG	2.58	0.55
10:1J:172:THR:HA	11:1K:80:MET:HE2	1.87	0.55
12:1L:359:MET:HB2	12:1L:430:ALA:HA	1.88	0.55
12:1L:501:ALA:O	12:1L:505:ASN:ND2	2.38	0.55
12:1L:535:ARG:NH2	37:1I:92:SER:OG	2.39	0.55
15:1O:24:VAL:HB	15:1O:166:PRO:HA	1.89	0.55
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.89	0.55
21:1V:22:ARG:HH12	21:1V:26:LEU:HB2	1.70	0.55
28:1c:27:LEU:HD11	29:1d:70:PHE:CG	2.42	0.55
5:1E:76:PRO:HG3	7:1G:170:ASP:OD2	2.06	0.55
5:1E:129:GLY:N	5:1E:139:LEU:O	2.21	0.55
12:1L:561:ILE:HG23	12:1L:562:LEU:H	1.72	0.55
16:1P:176:ASP:CG	16:1P:179:LEU:H	2.15	0.55
16:1P:201:VAL:N	16:1P:290:SER:OG	2.38	0.55
16:1P:250:TYR:OH	16:1P:322:ARG:NH1	2.40	0.55
17:1Q:59:PHE:HD2	17:1Q:79:LEU:HB3	1.70	0.55
22:1W:68:MET:N	22:1W:68:MET:SD	2.79	0.55
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	1.87	0.55
40:1o:117:ARG:O	40:1o:117:ARG:NH1	2.30	0.55
1:1A:90:MET:HE3	10:1J:151:THR:HA	1.89	0.55
14:1N:72:MET:HA	14:1N:75:ILE:HB	1.88	0.55
17:1Q:59:PHE:CD2	17:1Q:79:LEU:HB3	2.42	0.55
20:1T:45:LEU:HD11	22:1W:36:TYR:CZ	2.41	0.55
1:1A:113:TRP:HH2	8:1H:287:HIS:HB2	1.72	0.55
7:1G:501:ALA:HB2	7:1G:574:VAL:HB	1.87	0.55
7:1G:624:GLU:OE1	7:1G:628:PRO:HA	2.07	0.55
7:1G:672:TYR:O	7:1G:678:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:577:VAL:HA	45:1L:703:3PE:H331	1.87	0.55
17:1Q:35:VAL:HG22	17:1Q:59:PHE:CE1	2.41	0.55
25:1Z:97:ILE:HG23	25:1Z:98:MET:SD	2.47	0.55
34:1i:101:PRO:HG2	41:1p:16:THR:HG22	1.89	0.55
42:1q:29:ARG:NH1	42:1q:64:TYR:O	2.40	0.55
7:1G:359:ARG:CZ	7:1G:359:ARG:HA	2.36	0.55
7:1G:611:LEU:HD13	7:1G:612:PRO:HD2	1.86	0.55
8:1H:179:TRP:NE1	25:1Z:43:LEU:HG	2.21	0.55
12:1L:524:ASN:OD1	39:1n:77:GLN:HG3	2.06	0.55
14:1N:44:LEU:HG	14:1N:122:ILE:HG21	1.88	0.55
32:1g:64:PHE:HA	32:1g:68:ILE:HB	1.88	0.55
3:1C:86:ARG:NH2	21:1V:113:TRP:HB2	2.20	0.55
8:1H:150:LEU:O	8:1H:154:LEU:HD12	2.07	0.55
9:1I:92:ILE:HG12	9:1I:111:ILE:HG12	1.89	0.55
16:1P:283:LYS:HA	16:1P:286:ARG:HG2	1.89	0.55
31:1f:28:ARG:HH12	50:1f:101:PC1:H112	1.72	0.55
33:1h:34:ILE:O	33:1h:38:ILE:HG12	2.07	0.55
1:1A:67:LEU:HD12	11:1K:65:VAL:HG22	1.88	0.55
3:1C:90:PHE:HE1	3:1C:113:GLU:HG3	1.72	0.55
7:1G:118:ASP:OD2	17:1Q:46:GLN:NE2	2.40	0.55
7:1G:306:MET:N	7:1G:306:MET:SD	2.80	0.55
12:1L:76:LEU:HD21	12:1L:196:TRP:HE3	1.71	0.55
13:1M:355:MET:HA	13:1M:355:MET:HE3	1.88	0.55
16:1P:294:LEU:HB2	16:1P:296:HIS:CE1	2.41	0.55
37:1l:98:TRP:O	37:1l:101:MET:HB2	2.07	0.55
43:1r:47:LYS:N	43:1r:47:LYS:HD3	2.22	0.55
1:1A:54:LYS:NZ	4:1D:71:GLU:HB3	2.22	0.55
4:1D:158:ALA:HA	4:1D:161:ILE:HG22	1.88	0.55
4:1D:283:PHE:HA	4:1D:309:ARG:NH2	2.22	0.55
4:1D:284:ASP:OD2	4:1D:309:ARG:NH2	2.35	0.55
13:1M:355:MET:HE1	13:1M:437:MET:SD	2.47	0.55
17:1Q:56:LYS:HE2	17:1Q:58:GLU:OE2	2.06	0.55
19:1S:39:ARG:HH22	19:1S:86:VAL:HG13	1.72	0.55
20:1U:52:MET:HA	20:1U:55:GLU:HB2	1.89	0.55
2:1B:81:ARG:HD3	8:1H:214:GLU:HG3	1.88	0.54
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.40	0.54
4:1D:204:PRO:HG2	4:1D:207:LEU:HB2	1.89	0.54
6:1F:138:ILE:O	6:1F:180:GLY:N	2.37	0.54
6:1F:163:GLY:N	6:1F:173:PHE:O	2.39	0.54
7:1G:359:ARG:HG3	19:1S:56:GLU:HB3	1.89	0.54
11:1K:71:ALA:O	11:1K:75:LEU:HD12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:597:ILE:CD1	12:1L:601:LEU:HB3	2.36	0.54
13:1M:285:LEU:HD13	13:1M:342:MET:HE1	1.88	0.54
14:1N:312:LYS:HD2	15:1O:75:GLY:H	1.72	0.54
15:1O:32:CYS:N	54:1O:401:GTP:O1A	2.31	0.54
15:1O:214:MET:HA	15:1O:217:LYS:HD3	1.87	0.54
19:1S:13:LEU:HD22	19:1S:72:GLN:OE1	2.06	0.54
33:1h:134:ASP:OD1	33:1h:136:SER:OG	2.24	0.54
6:1F:160:GLY:O	6:1F:167:CYS:N	2.39	0.54
7:1G:504:ASP:O	19:1S:55:ARG:NH1	2.40	0.54
8:1H:283:ASP:OD1	8:1H:283:ASP:N	2.39	0.54
14:1N:120:GLN:HB2	14:1N:177:LYS:HD3	1.88	0.54
16:1P:145:TYR:O	16:1P:149:LYS:HG2	2.07	0.54
19:1S:18:ILE:HG23	19:1S:52:ILE:HG23	1.90	0.54
20:1T:83:LYS:HD2	20:1T:84:LYS:N	2.23	0.54
23:1X:41:GLU:N	23:1X:41:GLU:OE1	2.41	0.54
29:1d:99:GLU:OE1	29:1d:99:GLU:N	2.40	0.54
39:1n:30:CYS:O	39:1n:32:HIS:N	2.38	0.54
3:1C:137:MET:HB3	3:1C:162:PHE:CG	2.42	0.54
7:1G:126:ASP:OD2	7:1G:127:ARG:NH2	2.40	0.54
7:1G:255:HIS:CD2	7:1G:255:HIS:O	2.61	0.54
14:1N:73:ALA:HB1	14:1N:98:MET:HB2	1.88	0.54
22:1W:62:LYS:HD3	22:1W:107:PHE:CE2	2.42	0.54
32:1g:66:PHE:O	32:1g:71:VAL:N	2.40	0.54
1:1A:22:PHE:HA	8:1H:60:PRO:HG2	1.89	0.54
2:1B:111:ARG:N	16:1P:54:TYR:OH	2.28	0.54
4:1D:219:SER:HA	4:1D:222:ILE:HG12	1.88	0.54
4:1D:390:LYS:HE2	4:1D:430:ARG:HD2	1.88	0.54
5:1E:89:MET:SD	5:1E:89:MET:N	2.65	0.54
6:1F:137:TYR:HE2	6:1F:195:SER:HB2	1.72	0.54
7:1G:276:ARG:HA	42:1q:135:GLN:HB2	1.89	0.54
8:1H:209:SER:HB3	8:1H:213:VAL:HA	1.89	0.54
12:1L:584:ILE:HD11	14:1N:58:LYS:HG2	1.89	0.54
13:1M:258:ALA:HA	13:1M:302:MET:HE3	1.89	0.54
14:1N:7:THR:HG21	53:1N:402:CDL:H352	1.89	0.54
20:1T:47:GLN:NE2	20:1T:67:ALA:O	2.40	0.54
21:1V:21:GLU:O	21:1V:25:ILE:HG12	2.06	0.54
50:1f:101:PC1:H282	50:1f:101:PC1:H351	1.89	0.54
40:1o:7:ARG:NH2	40:1o:15:GLU:O	2.39	0.54
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.89	0.54
11:1K:2:PRO:HG2	11:1K:5:TYR:CD2	2.42	0.54
12:1L:258:PHE:HA	12:1L:261:ILE:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:113:TRP:CG	21:1V:113:TRP:O	2.61	0.54
44:1s:71:GLN:NE2	44:1s:75:HIS:HD2	2.04	0.54
2:1B:90:GLY:HA2	46:1B:201:SF4:S2	2.47	0.54
4:1D:379:VAL:HG13	4:1D:387:TYR:HB3	1.89	0.54
7:1G:286:ASN:C	42:1q:143:PRO:HB2	2.33	0.54
14:1N:267:ILE:HD12	14:1N:279:PRO:HB3	1.88	0.54
16:1P:281:ARG:O	16:1P:284:VAL:HG22	2.08	0.54
29:1d:17:GLU:N	29:1d:17:GLU:OE2	2.41	0.54
35:1j:56:PRO:HA	35:1j:59:TRP:CE3	2.42	0.54
2:1B:126:TYR:HE1	4:1D:85:ARG:NE	2.06	0.54
4:1D:371:LYS:HZ3	4:1D:424:VAL:HG21	1.73	0.54
6:1F:280:ILE:HD12	6:1F:280:ILE:H	1.72	0.54
7:1G:375:ASP:OD2	7:1G:448:LYS:N	2.40	0.54
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.07	0.54
12:1L:126:ILE:HD12	12:1L:127:THR:N	2.22	0.54
3:1C:132:ARG:HD2	3:1C:149:ARG:H	1.72	0.54
6:1F:82:MET:HG3	6:1F:129:MET:HB3	1.89	0.54
6:1F:156:ALA:HA	6:1F:161:LEU:HD12	1.89	0.54
9:1I:113:MET:HE3	9:1I:113:MET:O	2.07	0.54
12:1L:54:PHE:O	12:1L:58:GLY:N	2.41	0.54
15:1O:46:LEU:HB2	15:1O:48:LEU:HD11	1.89	0.54
16:1P:139:ILE:HG13	16:1P:150:ALA:HB3	1.89	0.54
20:1U:35:HIS:CE1	20:1U:38:LYS:HD3	2.43	0.54
20:1U:74:GLN:NE2	20:1U:78:ASP:OD2	2.41	0.54
33:1h:47:ILE:HA	41:1p:58:ASN:HD21	1.72	0.54
41:1p:162:MET:HA	41:1p:165:GLU:HG2	1.89	0.54
2:1B:125:TYR:CD1	9:1I:117:ILE:HD13	2.43	0.54
5:1E:99:HIS:HA	5:1E:138:THR:OG1	2.07	0.54
6:1F:307:ILE:HA	6:1F:421:HIS:ND1	2.23	0.54
7:1G:314:ASP:O	7:1G:520:LYS:N	2.41	0.54
7:1G:378:LEU:HD21	7:1G:439:PHE:CZ	2.41	0.54
7:1G:591:GLY:HA2	16:1P:6:ILE:HG21	1.90	0.54
12:1L:136:ASN:OD1	12:1L:139:GLN:N	2.38	0.54
13:1M:309:PHE:HB2	13:1M:458:LEU:HD12	1.90	0.54
14:1N:251:MET:HB3	14:1N:293:TYR:CE2	2.43	0.54
15:1O:134:PHE:O	15:1O:138:MET:HG3	2.08	0.54
16:1P:315:ILE:H	16:1P:331:MET:HE1	1.72	0.54
21:1V:91:ARG:NH1	21:1V:91:ARG:HB2	2.23	0.54
39:1n:9:LEU:O	39:1n:14:LYS:NZ	2.36	0.54
1:1A:63:LEU:HD22	11:1K:72:ALA:HB2	1.90	0.54
5:1E:103:CYS:HB3	5:1E:153:MET:SD	2.48	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:58:GLU:HG2	7:1G:85:LYS:HB3	1.90	0.54
7:1G:628:PRO:HD3	19:1S:21:HIS:CE1	2.43	0.54
14:1N:320:THR:HG21	15:1O:265:ASN:HA	1.90	0.54
16:1P:144:ARG:H	16:1P:144:ARG:HD2	1.73	0.54
22:1W:51:GLN:HB2	22:1W:100:ARG:HH21	1.73	0.54
37:1I:72:ASN:ND2	37:1I:75:GLU:OE2	2.39	0.54
38:1m:2:PHE:CD2	38:1m:3:PRO:HD2	2.41	0.54
3:1C:28:TYR:O	3:1C:32:ILE:HG12	2.08	0.53
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.24	0.53
14:1N:192:ALA:HB1	14:1N:270:MET:HE1	1.90	0.53
23:1X:51:ASP:OD2	23:1X:54:ARG:N	2.39	0.53
40:1o:27:ASP:N	40:1o:27:ASP:OD1	2.39	0.53
2:1B:62:MET:HE2	2:1B:156:LEU:HD11	1.90	0.53
2:1B:84:ASP:OD2	8:1H:54:LYS:NZ	2.18	0.53
3:1C:22:LEU:HD12	3:1C:48:LEU:HB2	1.90	0.53
4:1D:404:LYS:HA	4:1D:407:LYS:HE2	1.89	0.53
7:1G:546:GLN:HG3	7:1G:599:ILE:HD11	1.90	0.53
13:1M:5:ILE:O	13:1M:9:THR:HG23	2.07	0.53
16:1P:306:GLN:NE2	16:1P:307:ALA:O	2.42	0.53
17:1Q:62:ARG:HG3	17:1Q:63:GLU:H	1.73	0.53
25:1Z:21:TYR:O	25:1Z:21:TYR:CD2	2.61	0.53
26:1a:22:ALA:O	26:1a:26:ILE:HD12	2.09	0.53
34:1i:10:ARG:NH2	39:1n:154:PRO:O	2.36	0.53
5:1E:159:ASN:OD1	5:1E:184:PRO:HB3	2.08	0.53
6:1F:125:GLY:O	6:1F:129:MET:HG2	2.08	0.53
8:1H:51:ASP:OD1	8:1H:52:ALA:N	2.42	0.53
9:1I:138:GLU:OE1	9:1I:138:GLU:N	2.42	0.53
13:1M:325:MET:HG3	13:1M:440:HIS:HB3	1.90	0.53
20:1U:35:HIS:CE1	20:1U:71:MET:HE3	2.43	0.53
4:1D:116:GLN:HE22	4:1D:138:ARG:HG2	1.72	0.53
5:1E:156:ILE:HD11	5:1E:161:TYR:CE2	2.44	0.53
6:1F:136:ILE:HD11	6:1F:177:VAL:HA	1.89	0.53
6:1F:137:TYR:HE1	6:1F:180:GLY:HA2	1.74	0.53
7:1G:308:GLN:NE2	7:1G:607:ALA:O	2.42	0.53
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.90	0.53
15:1O:175:PRO:HD2	15:1O:175:PRO:O	2.08	0.53
15:1O:175:PRO:HD2	15:1O:178:GLU:HB3	1.89	0.53
1:1A:61:THR:O	1:1A:65:PHE:HB2	2.09	0.53
7:1G:94:MET:HE3	7:1G:120:SER:HA	1.89	0.53
7:1G:278:ARG:NH1	7:1G:279:LEU:O	2.42	0.53
7:1G:331:LEU:HD12	7:1G:525:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:264:LEU:HD12	26:1a:13:ALA:HB2	1.90	0.53
13:1M:42:LEU:HD21	13:1M:67:VAL:HG11	1.91	0.53
14:1N:109:SER:O	14:1N:111:PHE:N	2.41	0.53
19:1S:23:CYS:HB2	19:1S:60:VAL:H	1.73	0.53
23:1X:121:LEU:HD13	25:1Z:62:ILE:HD11	1.91	0.53
43:1r:57:ASP:O	43:1r:61:GLU:HG2	2.07	0.53
3:1C:118:GLU:CD	3:1C:118:GLU:H	2.15	0.53
3:1C:155:TYR:OH	4:1D:79:HIS:ND1	2.41	0.53
4:1D:228:MET:HB3	9:1I:36:MET:HE2	1.91	0.53
6:1F:272:MET:SD	6:1F:273:SER:N	2.82	0.53
7:1G:359:ARG:NH1	7:1G:362:TYR:OH	2.40	0.53
7:1G:432:ILE:HD11	7:1G:437:HIS:HD2	1.73	0.53
9:1I:75:GLU:OE2	9:1I:151:LYS:NZ	2.33	0.53
12:1L:1:FME:HE1	34:1i:86:LYS:HA	1.91	0.53
12:1L:591:PHE:CZ	14:1N:111:PHE:HA	2.44	0.53
13:1M:119:TYR:CZ	13:1M:161:LEU:HB2	2.44	0.53
14:1N:339:MET:HE2	14:1N:339:MET:HA	1.90	0.53
16:1P:166:ILE:HD12	16:1P:230:PHE:CE1	2.44	0.53
23:1X:17:VAL:HG21	25:1Z:74:LEU:HD21	1.91	0.53
25:1Z:72:MET:HE2	27:1b:52:TYR:HD2	1.73	0.53
32:1g:77:VAL:HA	32:1g:80:LEU:HG	1.90	0.53
34:1i:50:LEU:HD13	34:1i:57:LYS:HG3	1.90	0.53
35:1j:71:GLU:O	40:1o:114:ARG:NH1	2.41	0.53
38:1m:69:TYR:CZ	38:1m:74:ASN:HB2	2.44	0.53
42:1q:85:GLU:OE2	42:1q:85:GLU:N	2.27	0.53
2:1B:101:ARG:NH1	2:1B:139:ILE:O	2.40	0.53
3:1C:40:VAL:HG22	43:1r:69:MET:HE3	1.91	0.53
4:1D:100:LEU:HD12	4:1D:118:TYR:HD2	1.73	0.53
4:1D:378:LEU:HD23	4:1D:378:LEU:H	1.74	0.53
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.89	0.53
52:1M:501:PGT:H242	14:1N:284:MET:HG3	1.91	0.53
14:1N:97:MET:HA	14:1N:97:MET:HE2	1.91	0.53
19:1S:78:LEU:HA	19:1S:81:PHE:CD2	2.43	0.53
27:1b:27:LEU:O	27:1b:31:LEU:HD12	2.09	0.53
36:1k:71:LYS:H	36:1k:71:LYS:HD3	1.74	0.53
5:1E:99:HIS:O	5:1E:157:ASN:N	2.40	0.53
7:1G:256:GLU:O	7:1G:394:ARG:NH1	2.42	0.53
7:1G:380:VAL:HG21	7:1G:429:LEU:HD11	1.91	0.53
9:1I:69:ARG:HD3	42:1q:108:TYR:CD1	2.44	0.53
12:1L:370:THR:HA	12:1L:431:PHE:CE2	2.44	0.53
13:1M:279:GLN:OE1	13:1M:284:SER:OG	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:112:HIS:HB2	14:1N:184:ILE:HD13	1.90	0.53
14:1N:272:LYS:HE3	33:1h:108:LEU:HD21	1.90	0.53
16:1P:166:ILE:HG23	16:1P:230:PHE:CE1	2.44	0.53
21:1V:92:LYS:HA	21:1V:95:ARG:HH21	1.74	0.53
33:1h:94:LEU:HD12	41:1p:81:ILE:HG12	1.91	0.53
1:1A:113:TRP:CZ2	8:1H:286:MET:HB3	2.44	0.53
4:1D:195:ARG:HG3	4:1D:200:HIS:HB2	1.90	0.53
4:1D:234:ILE:HG21	8:1H:280:PHE:CE1	2.43	0.53
7:1G:588:THR:HG22	22:1W:126:HIS:NE2	2.23	0.53
12:1L:312:LEU:O	12:1L:316:THR:HG23	2.09	0.53
13:1M:160:LEU:HG	13:1M:164:LEU:HD11	1.91	0.53
20:1U:26:ASP:OD1	20:1U:29:LYS:HD2	2.09	0.53
21:1V:111:TRP:O	21:1V:112:LYS:HG2	2.09	0.53
23:1X:142:HIS:ND1	25:1Z:114:THR:OG1	2.37	0.53
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.08	0.53
38:1m:14:PRO:HB2	38:1m:16:THR:HG22	1.90	0.53
43:1r:104:GLU:N	43:1r:104:GLU:OE2	2.40	0.53
8:1H:220:PHE:CZ	8:1H:224:PHE:HD2	2.27	0.53
11:1K:94:ASN:HD22	12:1L:583:LEU:HD21	1.74	0.53
14:1N:230:LEU:HD23	14:1N:296:LEU:HD11	1.90	0.53
22:1W:84:ILE:O	22:1W:88:MET:N	2.42	0.53
23:1X:129:LYS:HD3	27:1b:65:VAL:HG13	1.90	0.53
40:1o:36:ARG:NH2	40:1o:93:ASP:OD1	2.42	0.53
1:1A:6:THR:HG21	8:1H:87:VAL:HG11	1.91	0.52
4:1D:155:THR:HB	4:1D:167:PHE:CB	2.39	0.52
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.91	0.52
7:1G:24:THR:HG23	7:1G:28:GLN:HB3	1.91	0.52
7:1G:357:ASP:N	7:1G:357:ASP:OD1	2.42	0.52
7:1G:572:THR:OG1	7:1G:633:TYR:OH	2.22	0.52
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.44	0.52
25:1Z:120:MET:O	25:1Z:123:GLU:HG2	2.09	0.52
30:1e:14:ASP:O	30:1e:18:THR:OG1	2.26	0.52
41:1p:5:ASP:HB3	41:1p:8:VAL:HB	1.91	0.52
3:1C:203:TRP:CG	7:1G:119:GLN:HE22	2.27	0.52
4:1D:352:TYR:CD2	9:1I:86:VAL:HG21	2.44	0.52
5:1E:54:ALA:O	5:1E:58:ASN:ND2	2.42	0.52
6:1F:29:HIS:NE2	44:1s:35:ASN:OD1	2.42	0.52
6:1F:137:TYR:CD2	6:1F:192:LEU:HG	2.43	0.52
7:1G:551:ASP:OD2	7:1G:679:ARG:NE	2.38	0.52
11:1K:89:TYR:O	11:1K:92:ASN:ND2	2.42	0.52
13:1M:204:MET:HE3	13:1M:209:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:206:LEU:HD12	14:1N:346:LEU:HD21	1.91	0.52
17:1Q:12:ALA:HA	22:1W:16:SER:HA	1.90	0.52
37:1l:132:GLN:HB2	40:1o:57:TYR:CE1	2.44	0.52
39:1n:116:ASP:OD1	39:1n:117:TYR:N	2.43	0.52
42:1q:115:PHE:HD1	42:1q:115:PHE:H	1.55	0.52
13:1M:26:ASN:OD1	31:1f:13:HIS:NE2	2.42	0.52
13:1M:82:SER:OG	13:1M:432:ARG:NH2	2.42	0.52
16:1P:141:SER:O	16:1P:147:ARG:NH2	2.43	0.52
31:1f:49:ARG:HB2	31:1f:52:GLU:OE1	2.09	0.52
35:1j:9:PRO:HD2	36:1k:13:MET:HE1	1.91	0.52
40:1o:55:ARG:NH2	41:1p:119:SER:HB2	2.25	0.52
1:1A:60:ILE:H	1:1A:60:ILE:HD12	1.73	0.52
6:1F:215:VAL:HG22	6:1F:220:THR:OG1	2.09	0.52
6:1F:259:SER:HA	6:1F:265:PRO:HB3	1.91	0.52
6:1F:274:VAL:O	6:1F:317:MET:HG3	2.08	0.52
11:1K:25:HIS:HD2	11:1K:27:MET:HB2	1.75	0.52
12:1L:159:HIS:NE2	13:1M:416:ARG:HA	2.25	0.52
12:1L:274:GLN:O	12:1L:277:THR:OG1	2.23	0.52
14:1N:28:LEU:HA	14:1N:31:ILE:HB	1.91	0.52
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.90	0.52
32:1g:80:LEU:HD22	32:1g:81:PRO:HD2	1.90	0.52
43:1r:92:LYS:HE2	43:1r:92:LYS:N	2.25	0.52
3:1C:39:GLN:O	3:1C:51:PHE:N	2.38	0.52
8:1H:130:ILE:HD12	8:1H:131:GLY:N	2.25	0.52
10:1J:25:SER:N	10:1J:81:GLU:OE1	2.39	0.52
10:1J:119:PHE:CD1	11:1K:6:MET:HB2	2.44	0.52
12:1L:197:ASP:HB2	41:1p:110:LYS:HE2	1.92	0.52
12:1L:557:TRP:HA	12:1L:560:THR:HG22	1.91	0.52
13:1M:116:ILE:HG12	13:1M:174:LEU:HD12	1.90	0.52
13:1M:326:LEU:HA	13:1M:329:LEU:HD13	1.92	0.52
16:1P:280:THR:O	16:1P:284:VAL:HG13	2.09	0.52
35:1j:41:TRP:HB2	36:1k:77:PHE:HZ	1.75	0.52
2:1B:54:CYS:CA	4:1D:108:TYR:HB2	2.40	0.52
7:1G:190:MET:HE3	7:1G:695:ILE:HD13	1.92	0.52
7:1G:252:PRO:HG2	17:1Q:44:ASN:HD22	1.73	0.52
11:1K:26:LEU:HD23	11:1K:88:ASP:HB2	1.90	0.52
12:1L:10:THR:O	12:1L:13:ILE:HG22	2.10	0.52
12:1L:306:THR:O	12:1L:310:LEU:N	2.32	0.52
16:1P:136:ASN:O	16:1P:146:LEU:HB3	2.09	0.52
2:1B:54:CYS:SG	4:1D:190:HIS:NE2	2.75	0.52
3:1C:10:THR:O	4:1D:129:GLN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:71:GLU:HG2	4:1D:72:MET:HB2	1.91	0.52
4:1D:428:VAL:O	4:1D:430:ARG:NH1	2.43	0.52
5:1E:95:VAL:O	5:1E:135:LYS:NZ	2.41	0.52
6:1F:246:GLY:HA3	6:1F:251:SER:HA	1.92	0.52
7:1G:255:HIS:NE2	7:1G:258:ILE:HD13	2.23	0.52
7:1G:460:ARG:NH1	7:1G:659:ASP:O	2.43	0.52
8:1H:195:ARG:HD3	8:1H:196:ALA:N	2.25	0.52
8:1H:263:THR:O	8:1H:267:THR:OG1	2.28	0.52
12:1L:542:LEU:HD11	37:1l:88:ARG:HD2	1.91	0.52
13:1M:139:GLN:O	13:1M:142:ARG:NH1	2.43	0.52
13:1M:201:MET:HG2	52:1M:501:PGT:H441	1.91	0.52
15:1O:13:ARG:O	15:1O:17:LYS:NZ	2.30	0.52
37:1l:33:ASP:OD1	37:1l:33:ASP:N	2.37	0.52
37:1l:54:SER:N	37:1l:57:GLU:OE1	2.43	0.52
43:1r:46:HIS:C	43:1r:47:LYS:HD3	2.35	0.52
6:1F:189:GLU:HA	6:1F:222:VAL:HG11	1.90	0.52
6:1F:207:PRO:HA	6:1F:208:PRO:C	2.35	0.52
7:1G:37:ILE:H	7:1G:37:ILE:HD12	1.73	0.52
7:1G:165:GLU:O	7:1G:167:ALA:N	2.43	0.52
7:1G:289:GLY:N	42:1q:143:PRO:C	2.64	0.52
7:1G:313:ASN:O	7:1G:517:ASN:ND2	2.42	0.52
10:1J:60:TYR:CD2	10:1J:64:MET:HG3	2.45	0.52
12:1L:452:ASN:HB3	12:1L:456:ARG:HH12	1.74	0.52
21:1V:87:LEU:HD23	21:1V:91:ARG:HH12	1.74	0.52
2:1B:86:MET:HE1	2:1B:104:TYR:HB2	1.92	0.52
4:1D:369:ALA:HB2	4:1D:374:PHE:HB2	1.91	0.52
5:1E:121:GLN:NE2	5:1E:126:ILE:O	2.40	0.52
7:1G:172:LEU:HB3	7:1G:185:THR:HG23	1.92	0.52
7:1G:494:HIS:CE1	7:1G:499:GLN:HG3	2.45	0.52
10:1J:126:VAL:HB	25:1Z:120:MET:HE2	1.91	0.52
15:1O:138:MET:HB3	15:1O:143:PHE:HB2	1.91	0.52
15:1O:201:ASP:HA	15:1O:204:ASN:HD21	1.75	0.52
19:1S:24:GLN:HB2	19:1S:25:ARG:NH1	2.25	0.52
22:1W:18:LYS:HA	22:1W:18:LYS:HE3	1.92	0.52
34:1i:107:ASP:N	40:1o:67:LYS:HZ1	2.08	0.52
2:1B:127:HIS:CE1	2:1B:134:ARG:HG2	2.45	0.52
6:1F:306:LEU:O	6:1F:421:HIS:ND1	2.43	0.52
7:1G:135:ARG:NH1	7:1G:179:ASN:OD1	2.43	0.52
12:1L:597:ILE:HG13	12:1L:602:PHE:CZ	2.45	0.52
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.44	0.52
13:1M:422:HIS:HB2	38:1m:59:ILE:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:27:GLU:N	17:1Q:27:GLU:OE1	2.43	0.52
23:1X:126:LYS:HD3	27:1b:74:GLY:HA3	1.92	0.52
23:1X:146:ARG:NH1	30:1e:38:GLU:OE1	2.42	0.52
34:1i:64:TYR:O	34:1i:68:ILE:HG22	2.10	0.52
43:1r:90:GLU:O	43:1r:92:LYS:NZ	2.29	0.52
2:1B:58:GLU:OE1	2:1B:61:HIS:ND1	2.43	0.51
5:1E:156:ILE:HD12	5:1E:156:ILE:O	2.10	0.51
7:1G:318:ILE:HD13	7:1G:344:CYS:SG	2.50	0.51
7:1G:455:SER:OG	7:1G:493:LEU:O	2.20	0.51
9:1I:67:LEU:HD21	9:1I:77:CYS:HB2	1.92	0.51
9:1I:119:CYS:HB3	9:1I:121:PHE:CD2	2.45	0.51
24:1Y:94:CYS:HB3	24:1Y:98:LEU:HD23	1.93	0.51
35:1j:64:LEU:HD11	40:1o:102:GLU:HG3	1.92	0.51
43:1r:8:GLN:HG2	43:1r:11:ARG:HH21	1.75	0.51
6:1F:247:ARG:HH11	6:1F:316:LEU:HD23	1.75	0.51
14:1N:150:ASN:HB3	14:1N:153:LEU:HB3	1.91	0.51
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	1.93	0.51
16:1P:168:PRO:HB2	16:1P:171:ILE:HD11	1.90	0.51
16:1P:197:GLY:HA2	16:1P:288:HIS:HE1	1.76	0.51
20:1T:81:ALA:O	20:1T:84:LYS:NZ	2.41	0.51
22:1W:54:ILE:HG21	22:1W:107:PHE:CE1	2.43	0.51
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.45	0.51
36:1k:38:ARG:N	36:1k:38:ARG:HD2	2.24	0.51
1:1A:56:PHE:CZ	1:1A:60:ILE:HD11	2.46	0.51
2:1B:126:TYR:CD1	4:1D:85:ARG:HD2	2.46	0.51
6:1F:17:ASP:HA	6:1F:20:ARG:HG3	1.91	0.51
7:1G:74:MET:HE3	7:1G:77:TRP:CZ3	2.46	0.51
9:1I:68:ARG:HH12	9:1I:76:ARG:NH1	2.09	0.51
15:1O:153:ASN:HA	15:1O:156:LYS:HB3	1.91	0.51
27:1b:56:LEU:HD11	27:1b:62:MET:HG3	1.91	0.51
41:1p:119:SER:OG	41:1p:119:SER:O	2.29	0.51
4:1D:161:ILE:HD13	4:1D:235:TRP:CE3	2.45	0.51
4:1D:403:ASP:OD1	4:1D:407:LYS:NZ	2.41	0.51
7:1G:42:TYR:HD1	7:1G:48:VAL:HG12	1.75	0.51
12:1L:83:ASP:CG	12:1L:262:ARG:HH12	2.18	0.51
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.92	0.51
14:1N:207:ILE:O	14:1N:210:THR:OG1	2.28	0.51
40:1o:57:TYR:O	40:1o:60:HIS:ND1	2.42	0.51
5:1E:100:ILE:HD11	5:1E:137:PHE:HD2	1.75	0.51
6:1F:287:VAL:HG21	6:1F:294:LEU:HD12	1.91	0.51
7:1G:110:GLN:HB3	7:1G:114:CYS:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:288:LYS:N	42:1q:143:PRO:HD2	2.16	0.51
7:1G:442:ILE:O	7:1G:446:ALA:N	2.43	0.51
9:1I:52:PHE:CZ	42:1q:30:ALA:HA	2.45	0.51
10:1J:33:LEU:O	10:1J:37:GLY:N	2.37	0.51
14:1N:1:FME:HG2	14:1N:6:TYR:HB2	1.93	0.51
14:1N:200:MET:HE1	14:1N:343:LEU:HD13	1.93	0.51
14:1N:245:MET:HE2	45:1N:401:3PE:H3A2	1.92	0.51
15:1O:141:GLN:NE2	15:1O:198:TYR:HA	2.25	0.51
16:1P:171:ILE:HB	56:1P:501:NDP:N7N	2.25	0.51
20:1T:70:LEU:HD12	20:1T:76:ILE:HG13	1.93	0.51
28:1c:37:GLU:OE1	28:1c:37:GLU:N	2.41	0.51
1:1A:70:ALA:HB2	10:1J:59:ILE:HG21	1.92	0.51
3:1C:183:VAL:O	22:1W:101:THR:OG1	2.26	0.51
3:1C:189:GLU:OE2	16:1P:14:SER:N	2.44	0.51
4:1D:48:THR:HA	4:1D:67:GLU:HA	1.92	0.51
5:1E:10:ARG:NH2	18:1R:76:ASP:O	2.44	0.51
7:1G:670:ASP:CG	7:1G:671:PHE:H	2.19	0.51
8:1H:210:GLY:O	8:1H:213:VAL:HG13	2.10	0.51
10:1J:18:VAL:HA	11:1K:14:ILE:HD13	1.92	0.51
12:1L:397:GLU:OE2	12:1L:482:MET:HG2	2.10	0.51
13:1M:297:VAL:O	13:1M:301:ILE:HG12	2.11	0.51
13:1M:300:ALA:O	13:1M:308:SER:OG	2.21	0.51
13:1M:442:LEU:N	13:1M:443:PRO:HD2	2.26	0.51
14:1N:267:ILE:O	14:1N:271:THR:OG1	2.25	0.51
32:1g:48:ASP:OD1	32:1g:49:LYS:N	2.44	0.51
3:1C:78:LEU:HG	3:1C:130:TYR:HB3	1.93	0.51
4:1D:202:ASP:HB2	4:1D:323:ILE:HD13	1.92	0.51
7:1G:59:ILE:HG13	7:1G:77:TRP:CD1	2.46	0.51
9:1I:120:GLY:HA2	9:1I:133:GLU:OE2	2.11	0.51
10:1J:110:GLU:HG2	10:1J:112:GLU:HG2	1.93	0.51
39:1n:133:GLU:OE2	39:1n:133:GLU:N	2.25	0.51
41:1p:50:PHE:O	41:1p:53:GLN:NE2	2.44	0.51
4:1D:167:PHE:O	4:1D:171:PHE:HB3	2.11	0.51
12:1L:35:TYR:OH	34:1i:73:HIS:NE2	2.31	0.51
12:1L:570:GLN:OE1	14:1N:167:TRP:NE1	2.43	0.51
19:1S:39:ARG:NH2	19:1S:86:VAL:HG13	2.26	0.51
20:1U:12:LYS:NZ	20:1U:13:ASP:OD1	2.44	0.51
28:1c:43:LYS:HD3	28:1c:48:LEU:HD22	1.93	0.51
33:1h:17:TYR:CE1	39:1n:107:HIS:HB2	2.45	0.51
3:1C:210:ARG:HH12	3:1C:212:PRO:HA	1.75	0.51
6:1F:22:PHE:HE2	6:1F:255:LEU:HD11	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:116:HIS:O	6:1F:120:GLU:HG2	2.11	0.51
6:1F:297:VAL:HG23	6:1F:336:VAL:HA	1.93	0.51
7:1G:38:PRO:HG3	7:1G:123:PHE:CD2	2.45	0.51
7:1G:546:GLN:NE2	7:1G:596:ASP:OD1	2.43	0.51
16:1P:64:ASP:HB3	16:1P:67:GLN:HG2	1.93	0.51
24:1Y:123:LEU:HA	24:1Y:126:MET:HG3	1.91	0.51
26:1a:26:ILE:HD12	26:1a:26:ILE:H	1.76	0.51
32:1g:71:VAL:O	32:1g:74:SER:OG	2.19	0.51
32:1g:93:ALA:O	32:1g:97:VAL:HG23	2.11	0.51
38:1m:49:GLN:HG3	38:1m:59:ILE:HG12	1.92	0.51
2:1B:78:ALA:HB1	8:1H:208:VAL:HG13	1.93	0.51
2:1B:81:ARG:HE	8:1H:216:ALA:N	2.09	0.51
4:1D:160:ASP:O	8:1H:279:ARG:NH1	2.41	0.51
7:1G:46:LEU:HD11	7:1G:161:ARG:CB	2.41	0.51
8:1H:296:LEU:HD13	8:1H:300:LEU:HD23	1.91	0.51
9:1I:48:ILE:HG23	9:1I:53:GLU:HB2	1.93	0.51
9:1I:73:GLY:HA2	42:1q:108:TYR:CE1	2.45	0.51
9:1I:113:MET:HE1	9:1I:118:TYR:HE2	1.75	0.51
10:1J:160:SER:O	10:1J:164:GLY:N	2.44	0.51
12:1L:1:FME:HE1	34:1i:86:LYS:HG3	1.94	0.51
12:1L:560:THR:HA	12:1L:564:LYS:HB2	1.91	0.51
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	1.91	0.51
16:1P:240:ASP:OD1	16:1P:338:LYS:HB3	2.10	0.51
22:1W:108:HIS:HB3	22:1W:111:GLU:CD	2.36	0.51
30:1e:44:HIS:ND1	33:1h:130:LYS:HD3	2.26	0.51
4:1D:83:LEU:O	4:1D:85:ARG:HG3	2.11	0.50
5:1E:149:VAL:HB	6:1F:105:CYS:HB2	1.92	0.50
6:1F:141:GLU:OE1	6:1F:141:GLU:N	2.42	0.50
7:1G:115:ASP:O	7:1G:119:GLN:HG2	2.11	0.50
7:1G:450:MET:HG2	7:1G:487:TRP:HZ2	1.76	0.50
8:1H:268:ILE:O	8:1H:272:TRP:N	2.38	0.50
10:1J:159:TRP:HE1	14:1N:12:THR:HG22	1.76	0.50
11:1K:23:ARG:HG3	11:1K:24:SER:H	1.76	0.50
13:1M:403:THR:O	13:1M:407:SER:OG	2.19	0.50
17:1Q:114:LYS:HD3	17:1Q:114:LYS:N	2.26	0.50
42:1q:67:GLU:OE2	42:1q:68:MET:N	2.43	0.50
4:1D:87:THR:OG1	4:1D:88:GLU:N	2.42	0.50
4:1D:139:VAL:HG23	4:1D:278:TYR:CE1	2.45	0.50
4:1D:157:HIS:HE1	4:1D:239:THR:HG22	1.76	0.50
8:1H:224:PHE:HE1	8:1H:228:TYR:CZ	2.29	0.50
11:1K:97:GLN:NE2	12:1L:581:LYS:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:76:ILE:O	20:1U:80:ILE:HG12	2.10	0.50
22:1W:75:ASP:HB3	22:1W:78:VAL:HG12	1.92	0.50
27:1b:17:VAL:HG13	27:1b:18:LEU:HD22	1.93	0.50
50:1f:101:PC1:H361	32:1g:76:PHE:CE2	2.47	0.50
40:1o:55:ARG:HH22	41:1p:119:SER:HB2	1.75	0.50
3:1C:129:TRP:CE3	4:1D:400:ALA:HA	2.46	0.50
3:1C:137:MET:HB3	3:1C:162:PHE:HB2	1.93	0.50
3:1C:206:PHE:HB3	43:1r:60:ARG:HD3	1.92	0.50
4:1D:143:GLU:HA	4:1D:146:ARG:HB3	1.93	0.50
4:1D:147:LEU:HD22	4:1D:218:PHE:HE2	1.76	0.50
4:1D:357:GLN:OE1	43:1r:59:ARG:NH2	2.44	0.50
5:1E:147:ALA:HB3	5:1E:153:MET:HG3	1.92	0.50
7:1G:344:CYS:HA	7:1G:508:LYS:HB2	1.93	0.50
9:1I:89:ALA:HB1	9:1I:115:LYS:HE2	1.93	0.50
16:1P:97:ARG:HD2	16:1P:99:TRP:CE2	2.46	0.50
40:1o:75:ASN:HD22	41:1p:25:LEU:HD21	1.77	0.50
3:1C:8:ARG:HD3	3:1C:11:ILE:HD11	1.93	0.50
3:1C:133:GLU:HA	3:1C:136:ASP:HB2	1.92	0.50
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.93	0.50
6:1F:433:PHE:HA	6:1F:436:GLN:HE21	1.77	0.50
7:1G:524:LEU:HB3	7:1G:545:TYR:HA	1.93	0.50
50:1H:401:PC1:H382	9:1I:25:LEU:HD12	1.93	0.50
9:1I:116:CYS:HB2	46:1I:201:SF4:S1	2.52	0.50
12:1L:132:VAL:HG13	12:1L:133:THR:HG23	1.93	0.50
45:1L:703:3PE:H371	45:1L:703:3PE:H231	1.93	0.50
13:1M:354:LEU:HD22	33:1h:18:ASP:OD1	2.11	0.50
19:1S:24:GLN:HE22	19:1S:58:SER:HB2	1.76	0.50
20:1U:37:MET:HB3	20:1U:42:LEU:HB3	1.94	0.50
21:1V:93:MET:HG2	21:1V:96:TRP:HD1	1.76	0.50
31:1f:37:PHE:HA	31:1f:40:LYS:HG3	1.94	0.50
32:1g:100:ARG:NE	32:1g:107:LEU:O	2.44	0.50
34:1i:120:LYS:HE3	34:1i:121:GLU:OE1	2.11	0.50
6:1F:122:CYS:HB3	6:1F:173:PHE:HE2	1.76	0.50
7:1G:285:ARG:HG2	7:1G:290:LEU:O	2.11	0.50
7:1G:626:VAL:HA	19:1S:19:ARG:HH21	1.77	0.50
12:1L:51:LEU:HB3	12:1L:55:MET:HE1	1.93	0.50
12:1L:319:ILE:HG21	12:1L:404:THR:HG22	1.93	0.50
13:1M:278:ARG:CZ	37:1l:83:MET:HE3	2.42	0.50
13:1M:422:HIS:HD2	38:1m:59:ILE:HB	1.77	0.50
15:1O:90:ASP:O	32:1g:27:GLN:NE2	2.35	0.50
18:1R:56:VAL:C	18:1R:57:ILE:HD13	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:19:ARG:CZ	19:1S:65:TRP:HB3	2.42	0.50
23:1X:137:PRO:HG2	23:1X:140:PRO:HG3	1.94	0.50
32:1g:85:MET:HE2	32:1g:85:MET:N	2.27	0.50
33:1h:129:ASP:OD1	33:1h:129:ASP:N	2.45	0.50
37:1l:90:ASP:OD1	37:1l:90:ASP:N	2.44	0.50
41:1p:28:PRO:O	41:1p:32:LEU:HG	2.12	0.50
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.94	0.50
5:1E:111:ARG:HB3	5:1E:152:PRO:HD3	1.93	0.50
5:1E:150:ASN:ND2	5:1E:163:ASP:OD2	2.34	0.50
6:1F:118:LEU:HD12	6:1F:225:VAL:HG13	1.93	0.50
7:1G:155:GLN:HG2	7:1G:181:MET:HG2	1.92	0.50
13:1M:351:LEU:HD11	13:1M:419:TYR:HB2	1.94	0.50
21:1V:82:GLN:HA	21:1V:85:ASN:HD21	1.75	0.50
34:1i:120:LYS:HB3	40:1o:39:VAL:HG22	1.94	0.50
39:1n:139:LEU:O	39:1n:143:THR:OG1	2.22	0.50
1:1A:4:MET:HE2	25:1Z:142:TRP:CZ3	2.46	0.50
3:1C:12:ARG:HA	4:1D:129:GLN:HB3	1.94	0.50
7:1G:296:TRP:O	7:1G:300:LEU:HD12	2.12	0.50
7:1G:319:ALA:HB3	7:1G:345:THR:HA	1.94	0.50
7:1G:440:SER:HA	7:1G:443:LEU:HD13	1.93	0.50
9:1I:149:TYR:HD2	9:1I:154:LEU:HD22	1.77	0.50
12:1L:324:LEU:HB3	12:1L:395:ILE:HD11	1.94	0.50
15:1O:86:PRO:HB2	15:1O:87:LYS:HD3	1.94	0.50
18:1R:7:THR:O	18:1R:7:THR:HG22	2.12	0.50
22:1W:64:ARG:O	22:1W:68:MET:HE2	2.11	0.50
22:1W:115:PRO:O	22:1W:121:LYS:HE3	2.12	0.50
26:1a:1:MET:HA	26:1a:1:MET:HE3	1.93	0.50
32:1g:67:SER:HA	32:1g:71:VAL:HB	1.93	0.50
40:1o:57:TYR:H	40:1o:57:TYR:HD1	1.60	0.50
5:1E:23:PHE:HB3	5:1E:27:ASN:HB2	1.94	0.50
13:1M:231:LEU:HA	13:1M:235:LEU:HG	1.92	0.50
20:1T:52:MET:HA	20:1T:55:GLU:OE1	2.11	0.50
31:1f:24:CYS:O	31:1f:28:ARG:NE	2.45	0.50
31:1f:54:VAL:HG12	31:1f:55:THR:O	2.11	0.50
32:1g:91:ARG:HG2	32:1g:91:ARG:HH11	1.77	0.50
39:1n:144:PRO:HG2	39:1n:148:PRO:HA	1.93	0.50
3:1C:50:ILE:HD12	3:1C:50:ILE:O	2.11	0.50
4:1D:161:ILE:HD11	4:1D:238:ARG:HB2	1.94	0.50
7:1G:140:LYS:H	7:1G:148:THR:HG21	1.76	0.50
10:1J:141:MET:HA	10:1J:141:MET:HE2	1.93	0.50
12:1L:160:GLY:HA3	39:1n:94:GLU:OE1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:244:MET:O	14:1N:248:LEU:HB2	2.11	0.50
16:1P:174:ARG:HB3	16:1P:175:GLU:OE2	2.11	0.50
17:1Q:65:TRP:CE2	17:1Q:74:SER:HB3	2.47	0.50
22:1W:42:GLU:OE1	22:1W:42:GLU:N	2.45	0.50
30:1e:85:LEU:HB3	30:1e:90:LYS:HB2	1.93	0.50
34:1i:71:VAL:HA	34:1i:75:LEU:HB2	1.93	0.50
37:1l:30:ARG:CZ	38:1m:34:GLU:HG3	2.42	0.50
41:1p:55:HIS:HB3	41:1p:59:ARG:HH12	1.77	0.50
2:1B:147:PRO:HD3	9:1I:140:SER:HA	1.94	0.49
3:1C:193:GLU:OE2	17:1Q:73:SER:OG	2.29	0.49
6:1F:184:TYR:HB3	6:1F:357:GLU:CG	2.42	0.49
6:1F:327:THR:OG1	6:1F:328:GLY:N	2.45	0.49
7:1G:282:PRO:HG3	7:1G:296:TRP:CD2	2.47	0.49
7:1G:460:ARG:HH21	7:1G:657:LEU:HB3	1.76	0.49
8:1H:32:GLN:OE1	8:1H:34:ARG:NE	2.44	0.49
12:1L:413:LEU:HD12	12:1L:493:VAL:HG11	1.94	0.49
15:1O:294:GLN:O	15:1O:297:THR:OG1	2.29	0.49
16:1P:258:LEU:HD11	16:1P:262:ALA:HB3	1.94	0.49
21:1V:63:ASP:HB3	21:1V:66:LYS:HE3	1.93	0.49
23:1X:18:LYS:CA	26:1a:54:ILE:HD11	2.40	0.49
23:1X:76:HIS:ND1	23:1X:113:LYS:HE2	2.27	0.49
32:1g:87:GLU:OE2	32:1g:91:ARG:NH1	2.45	0.49
37:1l:66:HIS:O	37:1l:70:ARG:N	2.43	0.49
37:1l:97:SER:HB3	38:1m:6:LYS:HG3	1.93	0.49
37:1l:115:MET:HA	37:1l:118:VAL:HG22	1.94	0.49
37:1l:157:GLU:HG2	40:1o:34:LYS:O	2.11	0.49
44:1s:38:TYR:CZ	44:1s:40:ASN:HB3	2.47	0.49
2:1B:45:LEU:N	2:1B:74:VAL:HG12	2.27	0.49
5:1E:191:PHE:HD2	6:1F:28:ARG:HH22	1.60	0.49
6:1F:264:HIS:HB2	6:1F:284:ALA:HA	1.95	0.49
7:1G:25:THR:O	7:1G:29:ALA:N	2.43	0.49
7:1G:704:CYS:HB3	18:1R:85:GLY:HA3	1.94	0.49
12:1L:598:SER:HA	12:1L:602:PHE:CD2	2.47	0.49
16:1P:300:LEU:HB3	16:1P:305:ILE:O	2.12	0.49
32:1g:56:TRP:O	32:1g:60:VAL:HG22	2.12	0.49
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.44	0.49
35:1j:32:MET:O	35:1j:36:ILE:HG12	2.12	0.49
6:1F:60:VAL:HG13	6:1F:76:GLY:HA2	1.93	0.49
6:1F:93:LEU:HD23	6:1F:94:VAL:N	2.28	0.49
9:1I:86:VAL:CG1	9:1I:121:PHE:HB3	2.42	0.49
13:1M:331:ASN:ND2	13:1M:335:GLU:OE2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:261:MET:SD	14:1N:340:THR:OG1	2.68	0.49
16:1P:108:ASP:HA	16:1P:112:LYS:HG3	1.93	0.49
23:1X:157:LEU:HG	29:1d:21:LEU:HD21	1.94	0.49
9:1I:27:TRP:HB3	9:1I:30:LEU:HB2	1.93	0.49
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.93	0.49
9:1I:101:ASP:OD1	9:1I:101:ASP:N	2.41	0.49
13:1M:150:LEU:HD11	14:1N:254:LEU:HD21	1.92	0.49
14:1N:2:ASN:HB2	15:1O:254:ARG:HD2	1.95	0.49
14:1N:112:HIS:NE2	14:1N:164:ILE:HG21	2.28	0.49
14:1N:163:LEU:HD12	14:1N:167:TRP:CZ3	2.48	0.49
15:1O:252:ASP:N	15:1O:252:ASP:OD1	2.43	0.49
16:1P:314:ALA:HB3	16:1P:331:MET:HE1	1.94	0.49
21:1V:5:LYS:HB3	21:1V:15:VAL:HG11	1.95	0.49
21:1V:10:LEU:HD12	21:1V:10:LEU:H	1.77	0.49
32:1g:88:TRP:NE1	41:1p:65:ARG:O	2.40	0.49
39:1n:133:GLU:H	39:1n:133:GLU:CD	2.15	0.49
39:1n:178:MET:SD	39:1n:178:MET:N	2.85	0.49
2:1B:126:TYR:CE1	4:1D:85:ARG:NE	2.81	0.49
4:1D:350:LYS:HD3	7:1G:117:GLN:HB3	1.95	0.49
9:1I:119:CYS:N	46:1I:201:SF4:S2	2.85	0.49
10:1J:115:ILE:HG12	10:1J:116:ILE:HG12	1.95	0.49
12:1L:339:LEU:HD21	12:1L:376:GLY:HA3	1.93	0.49
14:1N:272:LYS:HG2	33:1h:108:LEU:HD21	1.92	0.49
17:1Q:106:GLU:OE1	17:1Q:107:GLU:N	2.46	0.49
34:1i:125:GLN:HB3	40:1o:88:TYR:HE2	1.76	0.49
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.95	0.49
40:1o:46:ASN:HA	40:1o:55:ARG:HH22	1.78	0.49
2:1B:54:CYS:HA	4:1D:108:TYR:HB2	1.94	0.49
2:1B:69:MET:SD	2:1B:74:VAL:HG23	2.53	0.49
2:1B:126:TYR:HD1	4:1D:85:ARG:HD2	1.77	0.49
4:1D:3:GLN:NE2	4:1D:5:GLN:OE1	2.42	0.49
4:1D:165:THR:HB	4:1D:169:TRP:CH2	2.47	0.49
5:1E:127:LYS:HG2	5:1E:130:GLU:HG2	1.94	0.49
6:1F:101:GLU:O	6:1F:104:THR:OG1	2.26	0.49
6:1F:321:ALA:O	6:1F:322:LEU:HD22	2.12	0.49
7:1G:500:VAL:HG21	7:1G:576:THR:HA	1.94	0.49
8:1H:142:TYR:CE1	8:1H:289:LEU:HB2	2.47	0.49
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	1.95	0.49
12:1L:62:ILE:O	34:1i:96:VAL:HA	2.13	0.49
13:1M:175:ASN:HB3	13:1M:178:ILE:HG22	1.94	0.49
14:1N:238:PRO:HB2	45:1N:401:3PE:O32	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:52:LEU:HD21	22:1W:104:MET:SD	2.53	0.49
26:1a:27:HIS:HD2	26:1a:36:LYS:HB2	1.76	0.49
28:1c:27:LEU:HD11	29:1d:70:PHE:CD2	2.47	0.49
35:1j:10:ARG:HD2	35:1j:15:PRO:HA	1.94	0.49
42:1q:56:PHE:HZ	43:1r:33:ARG:HD3	1.78	0.49
4:1D:329:LYS:NZ	7:1G:125:SER:O	2.41	0.49
5:1E:78:MET:O	5:1E:82:GLU:HG2	2.13	0.49
6:1F:33:LEU:HD22	6:1F:155:GLU:HG2	1.93	0.49
7:1G:285:ARG:CZ	42:1q:144:TYR:HA	2.43	0.49
11:1K:27:MET:HE3	11:1K:27:MET:HA	1.95	0.49
12:1L:184:LEU:HD13	13:1M:393:ILE:HG21	1.94	0.49
12:1L:500:LEU:HD12	12:1L:501:ALA:N	2.27	0.49
13:1M:237:LYS:HE2	13:1M:316:MET:O	2.13	0.49
15:1O:93:SER:OG	15:1O:94:TYR:N	2.46	0.49
16:1P:235:ARG:HG2	16:1P:341:ASN:HA	1.94	0.49
16:1P:248:VAL:HG13	16:1P:318:LEU:HD13	1.94	0.49
19:1S:22:LEU:HD23	19:1S:22:LEU:H	1.77	0.49
23:1X:21:SER:HA	23:1X:24:LEU:HD23	1.94	0.49
31:1f:42:LEU:HG	41:1p:70:VAL:HG12	1.95	0.49
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.37	0.49
38:1m:82:THR:HG23	38:1m:85:THR:H	1.78	0.49
41:1p:55:HIS:HB3	41:1p:59:ARG:NH1	2.26	0.49
2:1B:45:LEU:H	2:1B:74:VAL:HG12	1.76	0.49
2:1B:162:GLN:NE2	9:1I:140:SER:OG	2.46	0.49
4:1D:101:PRO:HB3	4:1D:105:ARG:HH21	1.77	0.49
4:1D:133:ARG:O	4:1D:137:ILE:HD12	2.13	0.49
4:1D:168:PHE:HB2	8:1H:32:GLN:HB2	1.95	0.49
6:1F:45:THR:HA	6:1F:48:ILE:HG22	1.95	0.49
8:1H:63:PRO:HB2	8:1H:66:SER:HB3	1.94	0.49
9:1I:4:PHE:HB2	43:1r:111:TYR:HD1	1.78	0.49
9:1I:84:GLU:OE1	9:1I:92:ILE:HB	2.12	0.49
9:1I:153:LYS:O	9:1I:157:ASN:ND2	2.38	0.49
12:1L:463:PHE:O	12:1L:465:GLY:N	2.46	0.49
13:1M:40:SER:O	33:1h:80:TYR:OH	2.21	0.49
20:1T:14:ARG:HD3	20:1T:58:PHE:CE2	2.47	0.49
21:1V:93:MET:HG2	21:1V:96:TRP:CD1	2.48	0.49
30:1e:76:SER:O	30:1e:80:ARG:HG2	2.13	0.49
32:1g:67:SER:N	33:1h:28:TYR:OH	2.34	0.49
2:1B:71:ARG:NH2	9:1I:50:TYR:H	2.10	0.49
6:1F:56:ILE:H	6:1F:56:ILE:HD12	1.78	0.49
6:1F:307:ILE:HG22	6:1F:421:HIS:HE1	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:343:ILE:HD12	6:1F:344:VAL:N	2.28	0.49
8:1H:85:MET:HG2	8:1H:233:MET:SD	2.52	0.49
13:1M:354:LEU:HG	13:1M:358:TRP:NE1	2.27	0.49
15:1O:111:ALA:HB1	15:1O:122:VAL:HG21	1.93	0.49
30:1e:64:GLU:OE2	30:1e:70:LYS:N	2.46	0.49
39:1n:15:VAL:HG22	39:1n:63:LEU:HD21	1.95	0.49
43:1r:3:ALA:O	43:1r:8:GLN:NE2	2.44	0.49
3:1C:79:THR:HB	4:1D:390:LYS:HG2	1.95	0.49
4:1D:296:ARG:HD2	4:1D:420:THR:OG1	2.13	0.49
4:1D:423:ILE:HG23	4:1D:428:VAL:HG21	1.94	0.49
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.13	0.49
14:1N:200:MET:HE3	14:1N:269:GLU:OE1	2.13	0.49
14:1N:211:MET:SD	14:1N:211:MET:N	2.85	0.49
14:1N:226:THR:HG23	14:1N:229:SER:H	1.78	0.49
15:1O:139:TYR:HD2	15:1O:140:ARG:HH12	1.59	0.49
20:1T:84:LYS:HG3	20:1T:86:VAL:HB	1.93	0.49
31:1f:31:ASP:OD1	31:1f:32:GLU:N	2.46	0.49
33:1h:95:GLN:HB2	41:1p:82:LEU:HD11	1.94	0.49
41:1p:91:TRP:HH2	41:1p:149:TYR:HB2	1.78	0.49
7:1G:53:ARG:NH2	7:1G:56:LEU:HD21	2.28	0.48
7:1G:465:ALA:HB2	7:1G:654:GLN:HB2	1.95	0.48
8:1H:235:ASN:OD1	8:1H:267:THR:N	2.46	0.48
12:1L:313:MET:O	12:1L:316:THR:OG1	2.26	0.48
13:1M:201:MET:HE1	13:1M:261:PHE:CE1	2.48	0.48
14:1N:106:LEU:HB3	14:1N:108:LEU:HD11	1.95	0.48
15:1O:21:THR:O	15:1O:121:GLY:N	2.46	0.48
16:1P:81:ILE:O	16:1P:85:VAL:HG22	2.12	0.48
16:1P:259:PRO:HB2	16:1P:261:PHE:HD1	1.78	0.48
20:1T:18:VAL:HA	20:1T:21:LEU:HD23	1.94	0.48
33:1h:114:MET:HG2	33:1h:122:TRP:HE1	1.78	0.48
40:1o:41:THR:O	40:1o:45:MET:HE1	2.13	0.48
4:1D:178:PHE:CE2	4:1D:189:MET:HB2	2.48	0.48
4:1D:261:ARG:NH2	4:1D:368:GLU:OE1	2.44	0.48
5:1E:131:THR:HG22	5:1E:132:THR:O	2.12	0.48
6:1F:292:ASP:O	6:1F:339:ARG:NH2	2.38	0.48
7:1G:333:ASP:HB3	7:1G:611:LEU:HD11	1.95	0.48
7:1G:363:LEU:N	7:1G:492:ILE:HG12	2.29	0.48
7:1G:670:ASP:CG	7:1G:671:PHE:N	2.72	0.48
8:1H:201:THR:O	8:1H:210:GLY:HA3	2.13	0.48
9:1I:106:THR:O	9:1I:151:LYS:HE3	2.13	0.48
10:1J:146:LEU:CA	11:1K:58:MET:HE1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:11:ALA:O	11:1K:14:ILE:HG13	2.13	0.48
12:1L:86:SER:O	12:1L:90:ILE:HG12	2.13	0.48
12:1L:550:SER:HB2	13:1M:275:ILE:HG23	1.94	0.48
13:1M:388:TRP:HD1	29:1d:120:ARG:C	2.21	0.48
14:1N:108:LEU:HB3	14:1N:161:SER:HB2	1.94	0.48
21:1V:92:LYS:HA	21:1V:95:ARG:NH2	2.28	0.48
26:1a:1:MET:HB2	26:1a:3:PHE:CZ	2.48	0.48
34:1i:16:GLU:HA	34:1i:19:ARG:HB3	1.95	0.48
36:1k:29:GLU:OE1	36:1k:30:THR:N	2.45	0.48
5:1E:10:ARG:NH2	18:1R:76:ASP:OD1	2.46	0.48
6:1F:136:ILE:HD12	6:1F:136:ILE:O	2.13	0.48
7:1G:194:GLU:OE1	7:1G:194:GLU:N	2.44	0.48
7:1G:383:ASN:O	7:1G:387:GLU:HG2	2.13	0.48
9:1I:145:GLU:OE2	16:1P:66:GLY:N	2.40	0.48
11:1K:70:GLU:O	11:1K:74:GLY:N	2.45	0.48
11:1K:94:ASN:HB3	12:1L:583:LEU:HD23	1.96	0.48
12:1L:51:LEU:HD23	12:1L:87:VAL:HG22	1.95	0.48
12:1L:541:ASN:C	12:1L:541:ASN:HD22	2.21	0.48
12:1L:548:SER:O	12:1L:550:SER:N	2.46	0.48
12:1L:571:MET:HE2	12:1L:571:MET:HA	1.95	0.48
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.13	0.48
14:1N:273:ASN:OD1	24:1Y:139:LYS:N	2.39	0.48
16:1P:210:VAL:O	16:1P:214:ILE:HG12	2.13	0.48
21:1V:27:TYR:HA	21:1V:30:ILE:HG12	1.95	0.48
23:1X:132:THR:HB	27:1b:57:ARG:HH21	1.78	0.48
34:1i:42:MET:SD	34:1i:43:GLU:N	2.86	0.48
37:1l:82:ASP:O	37:1l:88:ARG:NH1	2.38	0.48
1:1A:94:LEU:HD21	10:1J:154:VAL:HG22	1.95	0.48
5:1E:98:TYR:CE2	5:1E:176:LEU:HD22	2.48	0.48
7:1G:357:ASP:O	19:1S:54:ILE:N	2.43	0.48
8:1H:86:TRP:CD1	8:1H:233:MET:HE3	2.49	0.48
16:1P:17:SER:OG	16:1P:42:GLY:O	2.25	0.48
16:1P:318:LEU:HG	16:1P:321:HIS:HD2	1.77	0.48
18:1R:10:LYS:O	18:1R:33:LYS:NZ	2.34	0.48
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.13	0.48
20:1U:42:LEU:HD11	20:1U:47:GLN:HB2	1.94	0.48
23:1X:156:ASP:N	23:1X:156:ASP:OD1	2.44	0.48
33:1h:7:ARG:NH2	34:1i:27:LEU:HG	2.28	0.48
2:1B:41:ARG:HA	8:1H:54:LYS:HE2	1.96	0.48
3:1C:40:VAL:HG23	43:1r:68:VAL:HG23	1.94	0.48
6:1F:314:THR:O	6:1F:314:THR:OG1	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:378:ARG:NE	6:1F:383:ASP:O	2.45	0.48
7:1G:279:LEU:HD21	7:1G:550:GLY:HA3	1.95	0.48
13:1M:71:TRP:CH2	13:1M:439:LEU:HG	2.49	0.48
13:1M:367:LEU:HD21	13:1M:408:LEU:HG	1.94	0.48
16:1P:203:GLN:HE21	16:1P:235:ARG:NE	2.11	0.48
19:1S:24:GLN:O	19:1S:33:ARG:NE	2.47	0.48
23:1X:141:TYR:HA	25:1Z:115:ARG:HD3	1.94	0.48
13:1M:295:ALA:HA	13:1M:298:ILE:HD12	1.96	0.48
16:1P:144:ARG:HD2	16:1P:144:ARG:N	2.29	0.48
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.79	0.48
22:1W:111:GLU:N	22:1W:111:GLU:OE1	2.47	0.48
28:1c:39:VAL:O	28:1c:43:LYS:HG2	2.13	0.48
3:1C:71:GLN:HE21	3:1C:100:ARG:HB3	1.78	0.48
3:1C:85:THR:OG1	17:1Q:86:PHE:HA	2.14	0.48
4:1D:4:TRP:CD1	13:1M:140:THR:HA	2.49	0.48
4:1D:352:TYR:O	9:1I:86:VAL:HG23	2.14	0.48
5:1E:109:MET:HA	5:1E:113:SER:H	1.78	0.48
6:1F:42:TRP:N	6:1F:120:GLU:OE1	2.47	0.48
7:1G:409:ILE:HD13	7:1G:429:LEU:HD21	1.96	0.48
7:1G:545:TYR:HB3	7:1G:560:ILE:HD13	1.94	0.48
9:1I:141:THR:OG1	9:1I:142:GLU:N	2.46	0.48
12:1L:401:MET:HG3	12:1L:482:MET:HG3	1.95	0.48
45:1L:702:3PE:H112	45:1L:702:3PE:H11	1.94	0.48
13:1M:220:HIS:CE1	13:1M:232:ALA:HB2	2.49	0.48
15:1O:22:SER:OG	15:1O:119:GLY:O	2.28	0.48
15:1O:78:SER:N	15:1O:92:ASN:OD1	2.43	0.48
19:1S:20:ILE:HA	19:1S:64:LEU:HA	1.95	0.48
20:1T:17:TYR:O	20:1T:20:LYS:HG3	2.14	0.48
21:1V:82:GLN:HA	21:1V:85:ASN:ND2	2.28	0.48
33:1h:23:LYS:HG2	33:1h:26:ARG:HH22	1.77	0.48
3:1C:43:SER:HA	43:1r:65:PRO:HB3	1.95	0.48
6:1F:247:ARG:HD3	6:1F:273:SER:HB3	1.95	0.48
6:1F:270:GLU:OE1	6:1F:283:HIS:NE2	2.40	0.48
7:1G:611:LEU:HD12	7:1G:613:TYR:CZ	2.49	0.48
14:1N:172:GLN:OE1	14:1N:177:LYS:NZ	2.26	0.48
14:1N:182:SER:O	14:1N:186:HIS:ND1	2.44	0.48
15:1O:167:HIS:HE2	15:1O:248:TRP:HB3	1.79	0.48
16:1P:35:VAL:O	16:1P:39:GLY:N	2.33	0.48
20:1U:47:GLN:NE2	20:1U:70:LEU:O	2.47	0.48
22:1W:80:ASP:O	22:1W:84:ILE:HG23	2.14	0.48
25:1Z:77:ALA:HB1	25:1Z:81:ARG:HH22	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:6:GLN:HG2	30:1e:13:LEU:HB2	1.96	0.48
34:1i:122:PHE:CE2	40:1o:61:TYR:CE1	3.02	0.48
40:1o:7:ARG:HH12	40:1o:17:ASP:HA	1.79	0.48
3:1C:33:LEU:O	3:1C:37:VAL:HG22	2.13	0.48
4:1D:83:LEU:HD23	4:1D:426:GLY:HA2	1.95	0.48
6:1F:118:LEU:HD21	6:1F:136:ILE:HG21	1.96	0.48
7:1G:55:CYS:SG	7:1G:68:ALA:N	2.86	0.48
7:1G:439:PHE:HD1	7:1G:442:ILE:HD11	1.79	0.48
7:1G:591:GLY:HA2	16:1P:6:ILE:HD13	1.95	0.48
12:1L:63:ILE:O	12:1L:65:ASN:ND2	2.36	0.48
15:1O:43:ALA:HB2	15:1O:123:VAL:HG11	1.95	0.48
16:1P:120:VAL:HA	16:1P:123:GLU:HB2	1.96	0.48
16:1P:243:GLN:OE1	16:1P:243:GLN:HA	2.14	0.48
22:1W:102:HIS:HA	22:1W:105:ARG:HH12	1.78	0.48
25:1Z:94:GLU:HA	25:1Z:97:ILE:HG22	1.94	0.48
32:1g:68:ILE:O	32:1g:72:LEU:HB3	2.13	0.48
45:1A:201:3PE:H2G2	27:1b:22:PHE:HD1	1.79	0.48
2:1B:66:ARG:HD3	9:1I:48:ILE:HG12	1.95	0.48
2:1B:68:ASP:HB3	2:1B:71:ARG:HB3	1.96	0.48
3:1C:136:ASP:HB3	3:1C:137:MET:HE2	1.96	0.48
4:1D:115:GLU:OE2	4:1D:192:ALA:HA	2.14	0.48
4:1D:169:TRP:CZ3	9:1I:36:MET:HE1	2.49	0.48
6:1F:254:LYS:HB3	6:1F:256:PHE:CZ	2.49	0.48
6:1F:391:SER:OG	43:1r:48:LEU:O	2.32	0.48
10:1J:150:GLY:HA2	30:1e:16:TRP:CH2	2.49	0.48
12:1L:375:ILE:HD11	35:1j:32:MET:HG2	1.95	0.48
13:1M:76:MET:HB3	13:1M:226:ALA:HB1	1.96	0.48
15:1O:174:VAL:HG22	15:1O:225:ALA:HB2	1.96	0.48
16:1P:318:LEU:HD23	16:1P:321:HIS:HB2	1.95	0.48
20:1T:27:PRO:HA	20:1T:30:LEU:HB3	1.96	0.48
21:1V:21:GLU:HA	21:1V:24:LYS:HD2	1.96	0.48
37:1l:27:TYR:CE2	37:1l:48:PRO:HD3	2.49	0.48
1:1A:60:ILE:HD12	1:1A:60:ILE:N	2.29	0.47
3:1C:55:ASP:OD1	3:1C:55:ASP:N	2.46	0.47
3:1C:74:SER:OG	3:1C:97:LEU:HB3	2.13	0.47
5:1E:103:CYS:SG	5:1E:144:CYS:HA	2.54	0.47
6:1F:30:ASP:OD1	6:1F:35:GLY:N	2.39	0.47
6:1F:216:PHE:HA	17:1Q:129:ARG:NH2	2.29	0.47
7:1G:54:MET:HE1	7:1G:94:MET:HE2	1.95	0.47
7:1G:240:VAL:HG22	7:1G:250:ILE:HD12	1.94	0.47
7:1G:248:MET:N	7:1G:248:MET:SD	2.87	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:339:ASP:OD1	19:1S:70:PHE:N	2.46	0.47
7:1G:615:THR:OG1	7:1G:618:GLN:NE2	2.43	0.47
10:1J:33:LEU:HD12	10:1J:34:ILE:N	2.29	0.47
12:1L:10:THR:O	12:1L:14:ILE:HD12	2.13	0.47
12:1L:489:THR:HA	12:1L:492:ILE:HG22	1.96	0.47
12:1L:561:ILE:HG23	12:1L:562:LEU:HD12	1.95	0.47
17:1Q:54:LYS:HE3	17:1Q:87:SER:HA	1.96	0.47
20:1U:23:ASP:OD1	20:1U:24:LYS:N	2.47	0.47
24:1Y:92:GLY:HA2	24:1Y:95:ALA:HB3	1.95	0.47
38:1m:21:GLU:HA	38:1m:24:ILE:HD11	1.95	0.47
1:1A:1:FME:HA	1:1A:1:FME:HE3	1.96	0.47
2:1B:91:THR:HA	2:1B:119:CYS:HB3	1.97	0.47
2:1B:114:VAL:HG22	2:1B:144:ILE:HB	1.94	0.47
3:1C:39:GLN:NE2	43:1r:67:ILE:HG23	2.29	0.47
4:1D:154:VAL:HG11	4:1D:225:LEU:HD11	1.96	0.47
4:1D:169:TRP:HB2	4:1D:170:MET:HE2	1.96	0.47
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.95	0.47
5:1E:27:ASN:O	5:1E:31:ILE:HG12	2.14	0.47
6:1F:51:LYS:HG2	6:1F:55:TRP:CD1	2.49	0.47
6:1F:308:PRO:HD3	6:1F:421:HIS:ND1	2.30	0.47
7:1G:125:SER:OG	7:1G:126:ASP:N	2.48	0.47
7:1G:255:HIS:CD2	7:1G:258:ILE:HB	2.49	0.47
7:1G:359:ARG:HA	7:1G:359:ARG:NH1	2.29	0.47
13:1M:181:TYR:CE1	41:1p:88:GLU:HG3	2.49	0.47
13:1M:205:VAL:HG22	13:1M:212:LEU:HD13	1.96	0.47
16:1P:172:PHE:HD2	16:1P:204:PRO:HB2	1.79	0.47
20:1T:45:LEU:O	20:1T:45:LEU:HD12	2.14	0.47
20:1U:33:ASN:OD1	20:1U:33:ASN:N	2.47	0.47
20:1U:37:MET:SD	20:1U:71:MET:HE1	2.54	0.47
32:1g:37:LEU:HD22	32:1g:46:GLY:HA2	1.95	0.47
41:1p:166:ARG:HD2	41:1p:170:LYS:HE3	1.96	0.47
44:1s:34:ASP:HB2	44:1s:39:ARG:HH22	1.80	0.47
3:1C:90:PHE:CE1	3:1C:113:GLU:HG3	2.49	0.47
4:1D:161:ILE:HG13	4:1D:238:ARG:CZ	2.45	0.47
4:1D:394:PRO:HD2	4:1D:427:GLU:OE2	2.13	0.47
6:1F:383:ASP:HA	6:1F:433:PHE:CE2	2.50	0.47
12:1L:583:LEU:HD12	12:1L:586:LEU:HD11	1.95	0.47
13:1M:11:LEU:HD22	13:1M:100:ILE:HD12	1.96	0.47
13:1M:89:THR:O	13:1M:93:LYS:HG2	2.14	0.47
14:1N:265:MET:HG3	14:1N:343:LEU:HD11	1.95	0.47
15:1O:57:HIS:HD2	15:1O:68:PRO:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:30:ASP:C	18:1R:31:ARG:HD3	2.39	0.47
23:1X:81:PHE:HD2	23:1X:85:TRP:HD1	1.63	0.47
34:1i:32:PRO:HB3	39:1n:114:TYR:CE1	2.49	0.47
4:1D:180:PHE:O	4:1D:184:VAL:HG22	2.14	0.47
5:1E:76:PRO:HB3	7:1G:170:ASP:HB3	1.96	0.47
7:1G:372:GLU:HA	7:1G:398:SER:HB3	1.95	0.47
7:1G:403:ASP:OD1	17:1Q:127:ARG:NH2	2.48	0.47
7:1G:627:SER:OG	7:1G:629:ASN:OD1	2.32	0.47
12:1L:53:MET:O	12:1L:57:THR:OG1	2.30	0.47
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.96	0.47
13:1M:263:MET:HE1	38:1m:104:PHE:CD2	2.49	0.47
13:1M:437:MET:O	13:1M:441:ILE:HG22	2.14	0.47
16:1P:13:ARG:NH1	16:1P:63:GLY:O	2.47	0.47
20:1U:88:GLU:OE2	34:1i:19:ARG:NH1	2.47	0.47
22:1W:42:GLU:O	22:1W:46:THR:HG23	2.13	0.47
37:1l:14:PRO:HA	37:1l:19:GLU:OE1	2.15	0.47
3:1C:24:ALA:HB1	43:1r:94:VAL:HG11	1.95	0.47
6:1F:144:ASN:HB3	44:1s:43:HIS:HB2	1.96	0.47
7:1G:99:ALA:HB1	7:1G:130:PHE:CE2	2.49	0.47
14:1N:96:THR:O	14:1N:100:MET:HE2	2.14	0.47
14:1N:122:ILE:HD11	14:1N:127:GLY:HA2	1.96	0.47
18:1R:32:GLN:NE2	18:1R:34:GLU:OE1	2.48	0.47
21:1V:24:LYS:O	21:1V:28:THR:HG23	2.14	0.47
6:1F:206:LYS:HB3	6:1F:207:PRO:HD3	1.95	0.47
7:1G:277:GLN:NE2	42:1q:137:TRP:HD1	2.12	0.47
7:1G:325:ALA:O	7:1G:329:VAL:HG23	2.14	0.47
7:1G:467:LEU:HA	7:1G:470:VAL:HG12	1.94	0.47
8:1H:114:TYR:OH	10:1J:61:LEU:O	2.20	0.47
12:1L:6:SER:O	12:1L:10:THR:HG23	2.15	0.47
12:1L:575:ILE:O	12:1L:579:ASN:ND2	2.46	0.47
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.79	0.47
20:1U:42:LEU:HD21	20:1U:46:ASP:HB3	1.95	0.47
23:1X:79:GLU:O	23:1X:82:THR:OG1	2.23	0.47
30:1e:16:TRP:CE3	30:1e:17:MET:HB3	2.50	0.47
2:1B:82:GLN:OE1	2:1B:82:GLN:N	2.47	0.47
6:1F:282:LYS:HG3	6:1F:283:HIS:CD2	2.50	0.47
6:1F:306:LEU:HD23	6:1F:418:LEU:HD21	1.95	0.47
7:1G:321:GLY:HA2	7:1G:496:ILE:HG23	1.97	0.47
8:1H:285:LEU:HD12	8:1H:285:LEU:O	2.15	0.47
10:1J:106:TYR:CD2	10:1J:113:VAL:HG12	2.49	0.47
11:1K:37:MET:HA	11:1K:40:LEU:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:271:LYS:O	12:1L:274:GLN:HG2	2.14	0.47
45:1L:703:3PE:H32	45:1L:703:3PE:H322	1.52	0.47
13:1M:30:HIS:HA	13:1M:33:LEU:HB2	1.95	0.47
15:1O:33:SER:HA	15:1O:182:ARG:HH22	1.80	0.47
15:1O:70:ASP:HB3	15:1O:73:LEU:HB2	1.96	0.47
15:1O:301:GLY:O	15:1O:309:ASN:ND2	2.48	0.47
16:1P:133:SER:HB3	16:1P:165:ILE:HD11	1.94	0.47
17:1Q:116:LYS:HD3	17:1Q:116:LYS:HA	1.60	0.47
19:1S:62:PRO:C	19:1S:78:LEU:HB3	2.40	0.47
21:1V:15:VAL:HG22	21:1V:77:GLU:HG2	1.97	0.47
21:1V:71:LEU:HD13	21:1V:79:VAL:HG11	1.96	0.47
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.44	0.47
22:1W:99:GLN:OE1	22:1W:99:GLN:HA	2.14	0.47
23:1X:101:LYS:O	23:1X:105:LYS:HG2	2.15	0.47
32:1g:92:GLU:OE1	41:1p:64:HIS:NE2	2.35	0.47
32:1g:108:MET:HE1	41:1p:141:ARG:HD2	1.96	0.47
38:1m:40:SER:OG	39:1n:148:PRO:O	2.31	0.47
38:1m:44:ARG:NH1	38:1m:44:ARG:O	2.47	0.47
39:1n:106:TRP:CE3	39:1n:110:GLU:HB3	2.49	0.47
39:1n:120:LYS:HA	39:1n:123:GLN:HG2	1.97	0.47
40:1o:30:PHE:HZ	40:1o:103:ARG:HD2	1.79	0.47
4:1D:152:MET:O	4:1D:156:THR:OG1	2.22	0.47
4:1D:347:HIS:NE2	7:1G:125:SER:O	2.39	0.47
7:1G:400:LEU:O	17:1Q:127:ARG:HB2	2.15	0.47
9:1I:50:TYR:CD1	9:1I:51:PRO:HA	2.50	0.47
10:1J:171:ILE:HD13	11:1K:77:LEU:HD23	1.97	0.47
16:1P:249:ALA:HB2	16:1P:318:LEU:HD21	1.95	0.47
20:1T:7:THR:O	20:1T:11:ILE:HG12	2.15	0.47
20:1T:56:ASP:OD1	20:1T:57:GLU:N	2.48	0.47
20:1U:35:HIS:HE1	20:1U:37:MET:HG2	1.80	0.47
32:1g:54:ASP:OD1	32:1g:55:LEU:N	2.48	0.47
37:1l:77:ILE:HB	38:1m:67:TRP:HB2	1.96	0.47
37:1l:129:GLY:H	40:1o:97:ARG:HB3	1.80	0.47
5:1E:111:ARG:HE	5:1E:151:ALA:HA	1.80	0.47
6:1F:31:TRP:HD1	6:1F:113:HIS:HA	1.80	0.47
6:1F:256:PHE:HD2	6:1F:270:GLU:HB3	1.79	0.47
7:1G:365:ASN:HD22	7:1G:488:LYS:HD2	1.79	0.47
7:1G:385:ARG:HG3	7:1G:415:LEU:HA	1.97	0.47
7:1G:673:MET:HG2	7:1G:688:VAL:HG11	1.97	0.47
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.49	0.47
8:1H:186:PHE:CD2	50:1H:401:PC1:H2E1	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:383:MET:HG3	12:1L:386:LEU:HB2	1.97	0.47
15:1O:110:ASP:OD1	15:1O:266:LYS:NZ	2.38	0.47
16:1P:194:ILE:O	16:1P:288:HIS:NE2	2.48	0.47
16:1P:341:ASN:OD1	16:1P:341:ASN:N	2.46	0.47
17:1Q:95:PHE:HA	17:1Q:98:LYS:HD3	1.97	0.47
20:1U:61:GLU:OE1	39:1n:81:PHE:HB2	2.14	0.47
1:1A:65:PHE:HA	1:1A:68:GLU:OE2	2.15	0.47
3:1C:204:GLU:HA	17:1Q:50:ASN:HD21	1.77	0.47
8:1H:29:GLY:HA2	8:1H:34:ARG:HE	1.80	0.47
9:1I:68:ARG:HH12	9:1I:76:ARG:HD2	1.79	0.47
10:1J:78:MET:HE3	10:1J:78:MET:C	2.40	0.47
13:1M:215:TRP:CD1	13:1M:215:TRP:H	2.32	0.47
15:1O:78:SER:HB3	15:1O:81:LYS:HB2	1.97	0.47
17:1Q:67:ASN:HD22	17:1Q:72:TRP:HD1	1.62	0.47
18:1R:19:ASP:N	18:1R:22:ASP:OD2	2.48	0.47
18:1R:28:PHE:CE2	18:1R:33:LYS:HG3	2.50	0.47
20:1T:22:TYR:CD2	20:1T:23:ASP:N	2.83	0.47
30:1e:85:LEU:HA	30:1e:88:GLU:OE2	2.15	0.47
34:1i:82:HIS:O	34:1i:86:LYS:HB2	2.15	0.47
37:1l:11:GLY:O	38:1m:78:ASN:ND2	2.48	0.47
39:1n:149:ARG:HD2	39:1n:149:ARG:HA	1.71	0.47
4:1D:270:ARG:NH1	4:1D:368:GLU:HG2	2.30	0.46
5:1E:100:ILE:HD12	5:1E:156:ILE:HG22	1.97	0.46
6:1F:103:GLY:HA3	6:1F:335:ILE:HD11	1.97	0.46
6:1F:276:LEU:O	6:1F:280:ILE:HD12	2.15	0.46
7:1G:323:VAL:HG11	7:1G:525:LEU:HD22	1.98	0.46
7:1G:626:VAL:HA	19:1S:19:ARG:NH2	2.30	0.46
8:1H:112:ALA:O	8:1H:116:ILE:HG12	2.15	0.46
10:1J:68:PHE:CD2	11:1K:75:LEU:HD21	2.50	0.46
11:1K:55:LEU:H	30:1e:24:GLN:HE22	1.63	0.46
11:1K:89:TYR:HB3	11:1K:91:GLN:OE1	2.15	0.46
12:1L:444:ASN:HD21	35:1j:7:ILE:HD13	1.80	0.46
14:1N:109:SER:HB3	14:1N:157:MET:HG3	1.96	0.46
16:1P:182:PHE:HA	16:1P:185:MET:HG2	1.97	0.46
16:1P:204:PRO:HG2	16:1P:310:LEU:HD12	1.97	0.46
21:1V:63:ASP:H	21:1V:66:LYS:HZ1	1.63	0.46
23:1X:46:ARG:NH1	25:1Z:76:GLN:OE1	2.48	0.46
33:1h:91:MET:HE1	41:1p:82:LEU:HA	1.96	0.46
5:1E:124:LEU:HD23	5:1E:173:ILE:HD12	1.97	0.46
6:1F:102:PRO:HG2	6:1F:302:SER:HB3	1.97	0.46
7:1G:646:ASN:O	7:1G:650:LYS:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:215:TYR:C	8:1H:220:PHE:HB2	2.40	0.46
9:1I:68:ARG:NH1	9:1I:76:ARG:HD2	2.30	0.46
11:1K:40:LEU:HD21	14:1N:72:MET:HB2	1.97	0.46
12:1L:279:CYS:HA	37:1I:116:PHE:CZ	2.50	0.46
13:1M:1:FME:HG3	13:1M:52:PHE:CD2	2.50	0.46
14:1N:210:THR:OG1	14:1N:211:MET:SD	2.72	0.46
15:1O:57:HIS:CD2	15:1O:68:PRO:HB3	2.51	0.46
16:1P:46:ILE:O	16:1P:46:ILE:HG22	2.15	0.46
16:1P:54:TYR:O	16:1P:57:MET:HB2	2.14	0.46
19:1S:12:LYS:HB2	19:1S:98:ALA:C	2.40	0.46
24:1Y:139:LYS:HG3	33:1h:112:ARG:HG3	1.95	0.46
30:1e:50:ARG:NH2	30:1e:54:GLU:OE2	2.49	0.46
32:1g:36:ASN:HB3	32:1g:39:GLU:OE2	2.14	0.46
3:1C:39:GLN:HE21	43:1r:67:ILE:HG23	1.80	0.46
4:1D:393:ALA:HB3	4:1D:396:PHE:HB2	1.98	0.46
6:1F:16:LYS:HA	6:1F:16:LYS:HD3	1.81	0.46
7:1G:276:ARG:CZ	7:1G:682:GLN:HE21	2.29	0.46
8:1H:52:ALA:O	8:1H:56:VAL:HG23	2.15	0.46
12:1L:268:GLU:N	12:1L:268:GLU:OE1	2.48	0.46
14:1N:155:LEU:HD22	14:1N:278:MET:HE2	1.97	0.46
16:1P:241:LEU:O	16:1P:245:ILE:HG22	2.16	0.46
30:1e:93:PRO:HB2	30:1e:98:LEU:HD21	1.97	0.46
33:1h:87:TYR:OH	41:1p:86:GLU:OE1	2.26	0.46
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.98	0.46
42:1q:13:GLN:HB3	42:1q:23:TYR:HE1	1.80	0.46
42:1q:29:ARG:NH2	42:1q:65:THR:O	2.48	0.46
43:1r:105:LEU:HD21	43:1r:111:TYR:CE1	2.51	0.46
1:1A:22:PHE:HZ	8:1H:62:ARG:HH11	1.63	0.46
3:1C:181:LYS:HG2	16:1P:174:ARG:NH2	2.30	0.46
4:1D:176:LYS:HG2	43:1r:26:ARG:NH1	2.30	0.46
6:1F:347:ILE:HG12	6:1F:418:LEU:HD12	1.98	0.46
7:1G:175:THR:N	7:1G:182:GLN:O	2.49	0.46
12:1L:478:PRO:HG3	40:1o:86:TRP:CH2	2.50	0.46
18:1R:68:HIS:CG	18:1R:86:TYR:HB3	2.51	0.46
19:1S:23:CYS:HA	19:1S:57:CYS:O	2.14	0.46
37:1I:82:ASP:HB2	37:1I:88:ARG:HH12	1.81	0.46
39:1n:41:CYS:HA	39:1n:44:ARG:HB3	1.96	0.46
41:1p:54:GLN:HE22	41:1p:55:HIS:HD2	1.63	0.46
41:1p:139:GLN:O	41:1p:157:LYS:NZ	2.47	0.46
43:1r:51:ASN:HB3	43:1r:56:ARG:HH22	1.81	0.46
4:1D:372:GLY:HA3	4:1D:394:PRO:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:195:LEU:HD11	7:1G:393:ALA:HB2	1.98	0.46
7:1G:362:TYR:HH	7:1G:504:ASP:CG	2.22	0.46
8:1H:200:LEU:O	8:1H:200:LEU:HD23	2.15	0.46
8:1H:201:THR:HG22	8:1H:211:PHE:HD1	1.80	0.46
10:1J:35:VAL:O	10:1J:39:VAL:HG12	2.16	0.46
12:1L:33:PRO:HB3	12:1L:118:PHE:CE1	2.50	0.46
12:1L:293:ILE:HD11	45:1L:704:3PE:H242	1.97	0.46
13:1M:306:PRO:HA	13:1M:458:LEU:HD13	1.96	0.46
14:1N:112:HIS:CE1	14:1N:164:ILE:HG21	2.50	0.46
16:1P:8:HIS:ND1	17:1Q:65:TRP:HB2	2.30	0.46
16:1P:236:TYR:HB2	16:1P:241:LEU:CD2	2.45	0.46
16:1P:245:ILE:O	16:1P:249:ALA:N	2.40	0.46
16:1P:256:TYR:HE2	16:1P:258:LEU:HD23	1.81	0.46
23:1X:73:ILE:HD12	26:1a:66:LEU:HD21	1.97	0.46
30:1e:60:ASP:HA	30:1e:63:VAL:HG12	1.98	0.46
31:1f:43:LEU:HD23	33:1h:87:TYR:CE2	2.50	0.46
42:1q:76:ASP:OD1	42:1q:76:ASP:O	2.34	0.46
4:1D:326:ASP:OD2	43:1r:46:HIS:ND1	2.48	0.46
4:1D:399:LEU:HD23	4:1D:428:VAL:HG11	1.98	0.46
8:1H:108:MET:HA	8:1H:108:MET:HE3	1.98	0.46
12:1L:478:PRO:HG2	40:1o:90:GLU:HG3	1.98	0.46
12:1L:594:THR:OG1	24:1Y:38:TYR:OH	2.29	0.46
14:1N:324:LYS:HA	14:1N:324:LYS:HD2	1.62	0.46
15:1O:51:PHE:HD2	15:1O:107:GLN:HE21	1.64	0.46
15:1O:168:VAL:HG13	15:1O:221:LEU:HD13	1.96	0.46
18:1R:32:GLN:NE2	42:1q:122:GLN:O	2.44	0.46
18:1R:75:LEU:HD21	18:1R:91:PHE:O	2.16	0.46
20:1T:84:LYS:NZ	20:1T:86:VAL:O	2.47	0.46
22:1W:17:VAL:HB	22:1W:77:ARG:CZ	2.45	0.46
23:1X:48:GLU:OE1	27:1b:57:ARG:NH1	2.48	0.46
29:1d:94:VAL:HG23	29:1d:101:PHE:CD2	2.51	0.46
39:1n:57:VAL:O	39:1n:61:GLN:HG2	2.16	0.46
40:1o:61:TYR:HB3	40:1o:86:TRP:HA	1.96	0.46
1:1A:85:LYS:HE2	1:1A:85:LYS:HB3	1.64	0.46
5:1E:14:GLU:O	5:1E:19:THR:OG1	2.27	0.46
5:1E:48:LEU:O	5:1E:90:TYR:OH	2.27	0.46
6:1F:50:LEU:O	6:1F:127:ARG:NH2	2.49	0.46
6:1F:215:VAL:HG22	6:1F:220:THR:HG1	1.80	0.46
6:1F:435:LEU:HD23	6:1F:435:LEU:HA	1.79	0.46
45:1L:702:3PE:C24	37:1l:88:ARG:HD3	2.43	0.46
15:1O:80:GLU:HB3	15:1O:190:HIS:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:31:GLY:O	16:1P:35:VAL:HG22	2.15	0.46
17:1Q:52:THR:O	17:1Q:53:LYS:HD3	2.15	0.46
20:1U:19:LEU:HD12	20:1U:19:LEU:H	1.79	0.46
20:1U:35:HIS:CE1	20:1U:37:MET:HG2	2.51	0.46
29:1d:91:PHE:HA	29:1d:94:VAL:HG12	1.98	0.46
36:1k:48:GLU:HB3	36:1k:51:ARG:HD2	1.98	0.46
37:1l:122:TYR:HB3	40:1o:8:TYR:CE2	2.51	0.46
4:1D:387:TYR:CE2	21:1V:113:TRP:HH2	2.33	0.46
5:1E:39:PRO:HB3	44:1s:66:PRO:HD2	1.98	0.46
6:1F:349:ARG:HD2	6:1F:349:ARG:HA	1.68	0.46
7:1G:206:GLY:N	46:1G:801:SF4:S1	2.86	0.46
7:1G:514:ILE:HD12	7:1G:519:PRO:HG3	1.98	0.46
9:1I:53:GLU:HG2	42:1q:61:TRP:HB3	1.98	0.46
10:1J:25:SER:HB2	10:1J:81:GLU:HB3	1.97	0.46
10:1J:129:ASP:OD2	10:1J:129:ASP:C	2.59	0.46
11:1K:61:ILE:O	11:1K:65:VAL:HG23	2.16	0.46
14:1N:108:LEU:HD22	14:1N:191:THR:HG21	1.98	0.46
15:1O:75:GLY:C	15:1O:77:CYS:H	2.24	0.46
20:1U:75:GLU:N	20:1U:75:GLU:OE1	2.48	0.46
22:1W:57:LYS:HE3	22:1W:57:LYS:HB3	1.72	0.46
22:1W:111:GLU:HG2	22:1W:114:ARG:NH2	2.31	0.46
25:1Z:68:ARG:HB2	26:1a:43:TYR:CE2	2.50	0.46
30:1e:90:LYS:HD3	30:1e:90:LYS:HA	1.67	0.46
34:1i:48:LYS:HG2	34:1i:49:PHE:CD2	2.51	0.46
2:1B:101:ARG:HD2	2:1B:101:ARG:HA	1.64	0.46
7:1G:53:ARG:HH21	7:1G:56:LEU:HD21	1.81	0.46
7:1G:74:MET:HB3	7:1G:77:TRP:CE3	2.51	0.46
7:1G:252:PRO:HG2	17:1Q:44:ASN:ND2	2.29	0.46
7:1G:628:PRO:HG2	19:1S:57:CYS:HB3	1.97	0.46
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.81	0.46
11:1K:91:GLN:O	11:1K:94:ASN:ND2	2.49	0.46
12:1L:386:LEU:HD13	35:1j:36:ILE:HD11	1.98	0.46
12:1L:500:LEU:HD11	45:1L:704:3PE:H362	1.97	0.46
13:1M:10:MET:HG3	31:1f:15:LEU:HD21	1.98	0.46
14:1N:44:LEU:HD23	14:1N:56:ALA:HA	1.97	0.46
16:1P:171:ILE:HG12	16:1P:210:VAL:HG21	1.98	0.46
17:1Q:39:VAL:HG11	17:1Q:108:ARG:HE	1.81	0.46
19:1S:20:ILE:HD13	19:1S:22:LEU:HD22	1.96	0.46
19:1S:24:GLN:CB	19:1S:25:ARG:HH12	2.27	0.46
20:1T:11:ILE:HD12	20:1T:80:ILE:HG22	1.98	0.46
20:1T:36:PHE:O	20:1T:41:GLY:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:76:HIS:O	23:1X:78:ALA:N	2.48	0.46
27:1b:31:LEU:O	27:1b:35:SER:N	2.49	0.46
27:1b:77:LEU:HA	27:1b:79:TRP:NE1	2.30	0.46
41:1p:145:LEU:HB3	41:1p:149:TYR:HB3	1.97	0.46
1:1A:73:LEU:HD13	8:1H:103:LEU:HD11	1.98	0.46
4:1D:228:MET:HE2	4:1D:228:MET:HB2	1.77	0.46
5:1E:149:VAL:HG21	6:1F:267:THR:HG22	1.98	0.46
5:1E:169:ILE:HD12	5:1E:172:ILE:HB	1.97	0.46
7:1G:104:ASP:O	7:1G:108:CYS:N	2.48	0.46
7:1G:284:ILE:HD11	7:1G:299:ALA:HA	1.98	0.46
7:1G:306:MET:HG2	7:1G:542:PHE:CG	2.51	0.46
7:1G:367:THR:HG22	7:1G:370:GLY:H	1.80	0.46
7:1G:427:LYS:O	7:1G:430:GLN:HG3	2.16	0.46
7:1G:622:ARG:HA	7:1G:625:GLU:HG2	1.98	0.46
10:1J:132:ASP:C	10:1J:132:ASP:OD1	2.59	0.46
14:1N:261:MET:HB2	14:1N:337:LEU:HD12	1.97	0.46
14:1N:314:LYS:NZ	15:1O:270:LEU:O	2.50	0.46
15:1O:154:GLU:HA	15:1O:157:LYS:NZ	2.31	0.46
23:1X:81:PHE:CD2	23:1X:85:TRP:HD1	2.34	0.46
24:1Y:93:GLY:O	24:1Y:97:GLY:N	2.39	0.46
25:1Z:74:LEU:O	25:1Z:78:GLU:HG2	2.16	0.46
2:1B:81:ARG:HH12	8:1H:63:PRO:HD3	1.81	0.45
3:1C:101:PHE:CE1	43:1r:99:PRO:HB3	2.50	0.45
4:1D:14:PHE:N	4:1D:14:PHE:CD1	2.83	0.45
5:1E:51:LEU:HD21	5:1E:84:ALA:HB2	1.98	0.45
6:1F:378:ARG:NH1	7:1G:131:LEU:HG	2.31	0.45
7:1G:387:GLU:OE2	7:1G:665:GLN:HG2	2.16	0.45
8:1H:170:GLU:HG2	8:1H:171:HIS:ND1	2.32	0.45
12:1L:530:PRO:O	12:1L:534:HIS:HB2	2.16	0.45
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.41	0.45
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.33	0.45
16:1P:262:ALA:HA	16:1P:265:TRP:CD1	2.40	0.45
17:1Q:130:VAL:HG12	17:1Q:132:THR:H	1.79	0.45
26:1a:27:HIS:NE2	26:1a:36:LYS:HE3	2.31	0.45
33:1h:7:ARG:HH22	34:1i:26:GLU:HA	1.81	0.45
36:1k:70:PHE:HD2	36:1k:74:PHE:HE1	1.63	0.45
41:1p:22:GLN:H	41:1p:22:GLN:HG3	1.62	0.45
1:1A:109:LYS:CG	1:1A:110:GLY:H	2.29	0.45
3:1C:161:PRO:HA	3:1C:166:PHE:CG	2.51	0.45
4:1D:95:THR:HA	4:1D:385:ARG:HG2	1.97	0.45
5:1E:82:GLU:HA	5:1E:85:THR:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:189:LYS:HD3	7:1G:190:MET:H	1.81	0.45
7:1G:252:PRO:O	17:1Q:44:ASN:ND2	2.49	0.45
10:1J:103:MET:C	10:1J:103:MET:HE2	2.40	0.45
11:1K:33:LEU:O	11:1K:36:MET:HG2	2.16	0.45
13:1M:2:LEU:HD13	31:1f:26:LEU:HB3	1.97	0.45
15:1O:14:THR:HB	15:1O:256:PHE:HD2	1.81	0.45
16:1P:146:LEU:HD11	16:1P:289:MET:HG2	1.98	0.45
16:1P:196:LEU:HG	16:1P:257:PRO:HB3	1.98	0.45
37:1l:118:VAL:HA	37:1l:121:ILE:HG12	1.98	0.45
39:1n:12:GLN:H	39:1n:12:GLN:CD	2.23	0.45
39:1n:121:ARG:O	39:1n:125:LYS:HG2	2.17	0.45
42:1q:94:THR:HG23	43:1r:34:THR:HG22	1.98	0.45
2:1B:145:TYR:HB2	9:1l:141:THR:HG23	1.98	0.45
3:1C:113:GLU:H	3:1C:113:GLU:CD	2.20	0.45
5:1E:193:CYS:H	6:1F:26:TYR:HE1	1.63	0.45
7:1G:454:GLY:HA2	7:1G:493:LEU:HB2	1.99	0.45
13:1M:120:ILE:HG23	14:1N:255:PRO:HB3	1.96	0.45
13:1M:305:THR:HB	13:1M:308:SER:HB2	1.97	0.45
16:1P:26:ALA:HA	16:1P:31:GLY:HA3	1.98	0.45
34:1i:105:PRO:HG3	40:1o:44:GLU:HG2	1.97	0.45
37:1l:134:PRO:CB	40:1o:38:MET:HE2	2.35	0.45
39:1n:103:LEU:HA	39:1n:103:LEU:HD23	1.72	0.45
41:1p:161:ARG:HG2	41:1p:161:ARG:HH11	1.81	0.45
3:1C:95:ASN:ND2	3:1C:106:ARG:HG3	2.31	0.45
7:1G:134:LYS:H	18:1R:72:TYR:HE2	1.64	0.45
7:1G:145:LEU:HD23	7:1G:145:LEU:H	1.80	0.45
7:1G:290:LEU:HD13	7:1G:291:LEU:O	2.17	0.45
7:1G:377:ILE:HG13	7:1G:450:MET:HB3	1.97	0.45
10:1J:71:THR:O	10:1J:74:MET:HG3	2.16	0.45
13:1M:447:LEU:HD21	13:1M:454:ILE:HG21	1.98	0.45
16:1P:35:VAL:HG21	16:1P:59:LEU:HD12	1.98	0.45
21:1V:26:LEU:O	21:1V:30:ILE:HG23	2.16	0.45
28:1c:28:TRP:O	28:1c:32:ILE:HG23	2.16	0.45
2:1B:70:ASP:HA	2:1B:74:VAL:O	2.17	0.45
5:1E:204:GLU:CD	6:1F:17:ASP:HB2	2.42	0.45
8:1H:96:ILE:HG23	25:1Z:144:THR:OG1	2.15	0.45
9:1I:163:ALA:HB1	42:1q:103:PRO:HB3	1.97	0.45
10:1J:95:SER:O	10:1J:98:MET:N	2.47	0.45
10:1J:109:LYS:O	10:1J:111:GLU:HG2	2.17	0.45
10:1J:163:ILE:HG13	14:1N:12:THR:HG21	1.98	0.45
12:1L:264:TYR:N	12:1L:265:PRO:HD2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:400:ASN:HD21	51:1L:701:MYR:H62	1.82	0.45
13:1M:388:TRP:C	38:1m:111:LYS:HZ1	2.24	0.45
13:1M:396:MET:HE3	13:1M:396:MET:HB2	1.86	0.45
14:1N:11:MET:C	14:1N:11:MET:HE3	2.42	0.45
14:1N:262:PRO:O	14:1N:266:ILE:HG12	2.15	0.45
15:1O:211:LEU:HD12	15:1O:220:VAL:HG13	1.98	0.45
15:1O:237:ASP:OD2	15:1O:237:ASP:N	2.36	0.45
16:1P:57:MET:HA	16:1P:57:MET:HE3	1.97	0.45
16:1P:77:ASP:OD2	16:1P:80:SER:N	2.49	0.45
16:1P:91:VAL:HG12	16:1P:126:VAL:HG21	1.97	0.45
20:1U:63:PRO:HD2	20:1U:79:TYR:OH	2.17	0.45
28:1c:28:TRP:NE1	29:1d:66:THR:HG22	2.32	0.45
34:1i:1:SAC:O	34:1i:2:GLY:N	2.50	0.45
35:1j:60:THR:N	35:1j:63:GLU:OE2	2.50	0.45
35:1j:63:GLU:HG2	35:1j:64:LEU:HD22	1.99	0.45
39:1n:107:HIS:O	39:1n:111:LYS:HG3	2.16	0.45
1:1A:78:ALA:HA	10:1J:144:ALA:HB1	1.98	0.45
2:1B:81:ARG:HD3	8:1H:214:GLU:CG	2.46	0.45
5:1E:98:TYR:HA	5:1E:157:ASN:CG	2.42	0.45
5:1E:194:GLU:HB3	6:1F:26:TYR:CE1	2.52	0.45
6:1F:107:ASP:HA	6:1F:110:ILE:HG22	1.99	0.45
7:1G:38:PRO:HB2	7:1G:54:MET:HG3	1.99	0.45
7:1G:249:ARG:NH1	7:1G:251:LEU:HD21	2.32	0.45
7:1G:673:MET:HE1	7:1G:679:ARG:HA	1.99	0.45
8:1H:189:THR:O	8:1H:193:THR:HG23	2.16	0.45
12:1L:140:LEU:HB3	12:1L:182:PHE:HZ	1.81	0.45
12:1L:331:MET:HE1	12:1L:468:ILE:HD12	1.98	0.45
12:1L:387:THR:OG1	12:1L:461:SER:O	2.24	0.45
12:1L:562:LEU:HB2	12:1L:563:PRO:HD3	1.97	0.45
15:1O:92:ASN:O	15:1O:96:LEU:HB2	2.17	0.45
15:1O:226:ARG:H	15:1O:226:ARG:NE	2.14	0.45
20:1U:9:GLU:OE1	20:1U:9:GLU:N	2.38	0.45
21:1V:102:LEU:H	21:1V:102:LEU:HD22	1.81	0.45
33:1h:8:LEU:HB2	34:1i:25:GLN:O	2.17	0.45
43:1r:34:THR:O	43:1r:35:GLN:NE2	2.49	0.45
2:1B:147:PRO:HG3	9:1I:147:LEU:HD21	1.97	0.45
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.50	0.45
4:1D:270:ARG:HH11	4:1D:270:ARG:HG3	1.81	0.45
4:1D:357:GLN:OE1	7:1G:122:MET:HE1	2.17	0.45
7:1G:465:ALA:O	7:1G:469:ALA:N	2.44	0.45
7:1G:692:THR:OG1	7:1G:693:GLU:OE2	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:9:GLU:H	9:1I:9:GLU:CD	2.22	0.45
10:1J:118:LYS:HD2	10:1J:119:PHE:N	2.32	0.45
12:1L:371:THR:O	12:1L:375:ILE:HG12	2.17	0.45
13:1M:147:LEU:HD23	14:1N:294:MET:HE3	1.99	0.45
13:1M:181:TYR:HE1	41:1p:88:GLU:HG3	1.82	0.45
14:1N:154:MET:HA	14:1N:154:MET:HE3	1.98	0.45
16:1P:113:ILE:HG13	16:1P:114:PRO:HD3	1.98	0.45
17:1Q:40:PRO:HG2	17:1Q:51:ASN:O	2.17	0.45
18:1R:18:TYR:HE1	18:1R:24:ARG:HE	1.65	0.45
23:1X:122:GLY:HA3	27:1b:77:LEU:HD22	1.99	0.45
30:1e:75:LEU:O	30:1e:78:ILE:HG22	2.17	0.45
32:1g:99:TYR:O	32:1g:103:ASN:ND2	2.47	0.45
34:1i:110:LEU:HD23	34:1i:111:GLU:OE1	2.17	0.45
39:1n:113:MET:HE3	39:1n:113:MET:HB2	1.83	0.45
41:1p:100:GLU:HA	41:1p:103:ASN:HD22	1.82	0.45
2:1B:34:ASP:O	2:1B:38:ASN:ND2	2.50	0.45
3:1C:40:VAL:HG22	43:1r:69:MET:HB3	1.98	0.45
3:1C:89:ARG:HG3	3:1C:90:PHE:CD1	2.51	0.45
3:1C:203:TRP:CZ3	7:1G:38:PRO:HA	2.51	0.45
4:1D:104:ASP:OD1	4:1D:111:MET:HB3	2.17	0.45
4:1D:258:VAL:HG23	4:1D:261:ARG:HH21	1.82	0.45
6:1F:393:TRP:CE3	6:1F:419:ILE:HG21	2.52	0.45
7:1G:100:ASN:HB3	7:1G:135:ARG:HG2	1.99	0.45
7:1G:238:ILE:HG22	7:1G:252:PRO:HA	1.98	0.45
7:1G:601:ARG:NH2	7:1G:614:ASP:OD2	2.50	0.45
7:1G:661:LEU:H	7:1G:661:LEU:HD12	1.82	0.45
8:1H:206:GLU:HG3	8:1H:207:LEU:HD12	1.99	0.45
9:1I:175:TYR:CE1	43:1r:38:PRO:HG3	2.52	0.45
10:1J:139:GLU:O	10:1J:143:ILE:HG12	2.17	0.45
12:1L:117:PHE:HE1	12:1L:243:VAL:HG22	1.82	0.45
12:1L:131:LEU:HB2	12:1L:143:GLY:HA3	1.99	0.45
13:1M:19:LYS:HB2	13:1M:19:LYS:HE3	1.75	0.45
13:1M:154:LEU:HA	13:1M:154:LEU:HD12	1.80	0.45
13:1M:403:THR:HA	13:1M:406:TYR:HE2	1.82	0.45
52:1M:501:PGT:H121	52:1M:501:PGT:H32	1.69	0.45
20:1T:9:GLU:HA	20:1T:12:LYS:HZ2	1.82	0.45
22:1W:92:GLU:OE2	22:1W:98:LYS:NZ	2.50	0.45
23:1X:36:ASP:OD2	23:1X:40:LYS:HG2	2.16	0.45
33:1h:23:LYS:HG2	33:1h:26:ARG:HH12	1.81	0.45
35:1j:60:THR:OG1	35:1j:63:GLU:OE1	2.27	0.45
4:1D:67:GLU:OE1	4:1D:74:ARG:NH2	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:76:CYS:SG	4:1D:403:ASP:HA	2.57	0.45
4:1D:146:ARG:HE	4:1D:370:PRO:HB3	1.82	0.45
4:1D:171:PHE:HA	4:1D:174:ARG:HD3	1.98	0.45
6:1F:252:GLY:O	6:1F:272:MET:HB3	2.16	0.45
7:1G:80:LEU:HB3	7:1G:83:SER:HB2	1.98	0.45
7:1G:362:TYR:CG	7:1G:362:TYR:O	2.69	0.45
7:1G:575:ASN:HD21	7:1G:579:ARG:HB3	1.81	0.45
9:1I:114:THR:O	9:1I:114:THR:OG1	2.34	0.45
10:1J:32:GLY:O	10:1J:36:SER:OG	2.33	0.45
12:1L:37:LYS:HD3	12:1L:98:TRP:HE1	1.81	0.45
12:1L:503:GLU:O	12:1L:507:THR:OG1	2.32	0.45
13:1M:51:ASN:ND2	33:1h:90:THR:OG1	2.49	0.45
15:1O:179:ILE:O	15:1O:183:ILE:HG13	2.17	0.45
15:1O:266:LYS:O	15:1O:269:VAL:HG22	2.17	0.45
16:1P:2:HIS:HB3	16:1P:5:LEU:HD23	1.98	0.45
20:1U:17:TYR:OH	36:1k:16:PRO:O	2.26	0.45
21:1V:19:PRO:HB2	21:1V:76:ILE:HG21	1.99	0.45
21:1V:109:ASN:HA	21:1V:112:LYS:NZ	2.31	0.45
24:1Y:8:TYR:O	24:1Y:20:LYS:NZ	2.47	0.45
29:1d:114:GLU:OE2	41:1p:152:ARG:NH1	2.49	0.45
34:1i:3:TYR:HD1	34:1i:7:GLU:HG2	1.82	0.45
34:1i:68:ILE:O	34:1i:72:THR:HG22	2.16	0.45
37:1l:14:PRO:HD3	37:1l:46:ASP:HA	1.98	0.45
40:1o:98:MET:O	40:1o:102:GLU:HG2	2.17	0.45
4:1D:233:ARG:HB3	9:1I:30:LEU:HD21	1.98	0.45
5:1E:102:VAL:HG21	5:1E:117:LEU:HB3	1.99	0.45
6:1F:242:PHE:CE2	6:1F:252:GLY:HA3	2.52	0.45
7:1G:285:ARG:HD2	7:1G:291:LEU:HD13	1.98	0.45
7:1G:298:ASP:OD2	7:1G:302:ARG:NH2	2.49	0.45
7:1G:314:ASP:HA	7:1G:520:LYS:HD3	1.99	0.45
8:1H:107:ALA:HB1	10:1J:57:PHE:HB3	1.99	0.45
8:1H:126:LYS:O	8:1H:130:ILE:HG13	2.17	0.45
8:1H:139:THR:OG1	8:1H:192:GLU:OE1	2.35	0.45
9:1I:35:GLY:HA3	50:1I:203:PC1:H331	1.99	0.45
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.52	0.45
12:1L:154:LEU:HD23	12:1L:154:LEU:HA	1.77	0.45
13:1M:45:LEU:HG	13:1M:50:LEU:HD11	1.99	0.45
13:1M:160:LEU:O	13:1M:164:LEU:HD12	2.16	0.45
15:1O:3:TYR:HB2	15:1O:260:ARG:HE	1.81	0.45
15:1O:272:TYR:O	15:1O:275:ILE:HG12	2.17	0.45
20:1T:11:ILE:HD12	20:1T:80:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:5:PRO:HD3	35:1j:1:ALA:N	2.32	0.45
22:1W:34:GLU:OE1	22:1W:35:LEU:N	2.50	0.45
34:1i:24:ASP:CG	39:1n:124:TRP:HE1	2.25	0.45
40:1o:25:PRO:HB2	40:1o:28:TYR:HB3	1.99	0.45
3:1C:164:LYS:HB3	17:1Q:84:LEU:HD11	2.00	0.44
4:1D:281:VAL:HG13	4:1D:283:PHE:HE1	1.81	0.44
5:1E:33:ALA:O	5:1E:36:LYS:HG2	2.17	0.44
5:1E:78:MET:O	5:1E:81:TYR:HB2	2.17	0.44
5:1E:145:LEU:HD21	5:1E:153:MET:HG2	1.99	0.44
6:1F:134:ALA:O	6:1F:176:PHE:N	2.31	0.44
6:1F:162:ILE:HD13	6:1F:175:VAL:HG12	1.98	0.44
7:1G:290:LEU:HG	42:1q:142:THR:C	2.42	0.44
8:1H:26:LYS:NZ	8:1H:35:LYS:O	2.50	0.44
12:1L:21:MET:HA	12:1L:21:MET:HE3	1.99	0.44
12:1L:162:THR:OG1	37:1l:86:ARG:NH1	2.50	0.44
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.98	0.44
13:1M:3:LYS:HB2	13:1M:3:LYS:HE3	1.76	0.44
13:1M:336:ARG:HD2	13:1M:426:ILE:HG23	1.98	0.44
15:1O:27:VAL:HA	15:1O:170:VAL:HB	1.99	0.44
15:1O:63:THR:HG23	15:1O:302:ARG:HH22	1.80	0.44
15:1O:183:ILE:HD12	15:1O:184:GLN:N	2.32	0.44
16:1P:253:PHE:CZ	16:1P:255:PRO:HB3	2.52	0.44
17:1Q:14:ASP:OD1	17:1Q:14:ASP:N	2.43	0.44
17:1Q:55:TRP:CZ2	17:1Q:108:ARG:HD2	2.51	0.44
21:1V:29:LYS:O	21:1V:33:VAL:HG22	2.17	0.44
23:1X:136:LEU:HD12	23:1X:137:PRO:HD2	1.98	0.44
26:1a:65:GLY:N	26:1a:67:GLU:OE2	2.50	0.44
37:1l:126:GLN:O	37:1l:128:VAL:N	2.50	0.44
39:1n:125:LYS:O	39:1n:129:ARG:HG2	2.16	0.44
3:1C:56:GLY:C	3:1C:59:PRO:HD2	2.43	0.44
3:1C:149:ARG:HD2	22:1W:97:TRP:HZ3	1.81	0.44
5:1E:200:THR:OG1	6:1F:283:HIS:ND1	2.48	0.44
6:1F:205:LEU:HG	6:1F:404:ILE:HD12	1.98	0.44
6:1F:309:LYS:HE3	6:1F:309:LYS:HB3	1.64	0.44
6:1F:394:GLU:HB2	7:1G:129:ARG:HH22	1.82	0.44
7:1G:20:VAL:HG21	7:1G:73:VAL:HG11	1.99	0.44
7:1G:285:ARG:HB3	42:1q:144:TYR:H	1.81	0.44
7:1G:666:LEU:HD12	7:1G:666:LEU:HA	1.84	0.44
11:1K:47:ILE:HG12	14:1N:79:LEU:HD13	1.99	0.44
12:1L:149:ILE:HD12	12:1L:172:ILE:HD11	1.99	0.44
12:1L:236:ALA:HB1	12:1L:248:HIS:CE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:316:THR:HB	12:1L:395:ILE:HD12	2.00	0.44
12:1L:432:LEU:HD21	36:1k:65:ALA:HB2	1.98	0.44
14:1N:40:MET:SD	14:1N:134:GLN:NE2	2.91	0.44
14:1N:80:TYR:HA	30:1e:67:LEU:HD21	1.98	0.44
15:1O:104:ARG:NH1	54:1O:401:GTP:N7	2.64	0.44
16:1P:38:LEU:O	16:1P:43:SER:OG	2.30	0.44
16:1P:256:TYR:CE2	16:1P:258:LEU:HD23	2.51	0.44
17:1Q:112:LYS:O	17:1Q:114:LYS:NZ	2.45	0.44
25:1Z:6:VAL:HG21	43:1r:41:PRO:HB3	1.99	0.44
33:1h:70:PRO:HA	33:1h:73:ARG:HD3	2.00	0.44
34:1i:86:LYS:HB3	34:1i:87:TYR:CD1	2.53	0.44
38:1m:5:TYR:HE2	38:1m:14:PRO:HD3	1.81	0.44
2:1B:59:MET:HA	2:1B:156:LEU:HD21	1.99	0.44
4:1D:202:ASP:CG	43:1r:40:LEU:HD11	2.43	0.44
7:1G:58:GLU:HB3	7:1G:65:VAL:HG22	1.99	0.44
7:1G:259:ASN:HA	7:1G:390:LEU:HD22	1.98	0.44
7:1G:383:ASN:C	7:1G:387:GLU:HG2	2.42	0.44
9:1I:168:ASN:HD21	42:1q:93:MET:HE1	1.82	0.44
12:1L:150:MET:HE3	12:1L:153:LEU:HD12	1.98	0.44
12:1L:217:LEU:HD12	12:1L:277:THR:HG22	1.98	0.44
12:1L:298:ILE:HG22	12:1L:354:GLN:O	2.17	0.44
12:1L:306:THR:HG22	12:1L:336:LYS:HD2	1.99	0.44
13:1M:364:LEU:HG	13:1M:369:LEU:HD22	1.99	0.44
13:1M:421:HIS:HB3	38:1m:50:TYR:OH	2.17	0.44
15:1O:257:HIS:O	15:1O:261:MET:HG2	2.17	0.44
16:1P:237:LEU:HB3	16:1P:240:ASP:HB2	1.99	0.44
21:1V:27:TYR:HD2	21:1V:55:LEU:HB2	1.83	0.44
22:1W:24:ASP:CG	22:1W:25:MET:N	2.74	0.44
25:1Z:144:THR:O	26:1a:36:LYS:NZ	2.50	0.44
33:1h:49:GLU:OE2	33:1h:69:HIS:NE2	2.48	0.44
37:1l:43:GLY:HA3	38:1m:75:ILE:HG13	1.99	0.44
37:1l:139:TYR:CE1	37:1l:144:GLY:HA3	2.52	0.44
41:1p:69:ARG:NH2	41:1p:94:ASP:OD1	2.50	0.44
3:1C:152:LEU:HD22	4:1D:84:HIS:ND1	2.32	0.44
6:1F:26:TYR:HD2	6:1F:28:ARG:HG2	1.82	0.44
7:1G:159:CYS:HA	7:1G:199:ILE:HD11	2.00	0.44
7:1G:396:ARG:HA	7:1G:399:TRP:HB3	2.00	0.44
7:1G:539:LYS:HB3	7:1G:540:ASP:OD1	2.18	0.44
8:1H:260:VAL:HG21	26:1a:17:PHE:HA	2.00	0.44
8:1H:281:ARG:HG3	8:1H:281:ARG:HH11	1.82	0.44
8:1H:287:HIS:NE2	50:1H:401:PC1:H141	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:447:LEU:HD11	13:1M:454:ILE:HG23	2.00	0.44
16:1P:28:GLY:HA3	56:1P:501:NDP:O1N	2.18	0.44
21:1V:81:LEU:O	21:1V:84:GLU:HG3	2.17	0.44
22:1W:23:ARG:HH21	22:1W:27:GLU:HG2	1.81	0.44
23:1X:23:VAL:HG13	23:1X:81:PHE:CZ	2.53	0.44
24:1Y:23:ALA:O	24:1Y:26:SER:OG	2.32	0.44
33:1h:30:LEU:HD12	33:1h:34:ILE:HG23	1.99	0.44
34:1i:118:LEU:HD23	34:1i:118:LEU:H	1.82	0.44
1:1A:87:MET:HA	10:1J:147:TYR:HB3	1.99	0.44
3:1C:82:ASP:HB2	3:1C:138:PHE:HE2	1.83	0.44
4:1D:246:THR:OG1	21:1V:12:GLY:HA3	2.18	0.44
4:1D:305:ARG:NH2	25:1Z:23:ARG:HG3	2.32	0.44
4:1D:345:LEU:HD22	7:1G:103:LEU:HD23	1.99	0.44
6:1F:89:ARG:HG2	17:1Q:124:TRP:HB2	1.99	0.44
6:1F:136:ILE:CD1	6:1F:177:VAL:HA	2.48	0.44
7:1G:296:TRP:HZ3	7:1G:561:LEU:HD22	1.83	0.44
7:1G:640:ASN:CG	7:1G:641:TYR:N	2.75	0.44
7:1G:688:VAL:O	7:1G:692:THR:OG1	2.36	0.44
8:1H:303:TRP:NE1	25:1Z:47:TYR:OH	2.48	0.44
9:1I:56:PRO:O	9:1I:57:LEU:HD13	2.17	0.44
12:1L:145:GLU:OE2	12:1L:176:ARG:NE	2.50	0.44
12:1L:481:THR:C	12:1L:482:MET:HE3	2.42	0.44
12:1L:485:TYR:CE2	51:1L:701:MYR:H52	2.52	0.44
12:1L:511:LEU:HD11	39:1n:38:TYR:CE1	2.53	0.44
14:1N:92:PRO:O	14:1N:96:THR:HG23	2.18	0.44
14:1N:209:ILE:HG23	14:1N:213:LEU:HD23	1.99	0.44
16:1P:9:GLY:HA3	16:1P:15:SER:HB3	2.00	0.44
16:1P:84:VAL:HG23	16:1P:85:VAL:HG13	2.00	0.44
16:1P:112:LYS:O	16:1P:115:HIS:ND1	2.51	0.44
16:1P:132:ILE:HG22	16:1P:166:ILE:HB	2.00	0.44
16:1P:196:LEU:HB3	16:1P:239:PHE:CE2	2.51	0.44
22:1W:21:PHE:O	22:1W:23:ARG:NH1	2.49	0.44
39:1n:82:PRO:HA	39:1n:87:GLY:HA3	2.00	0.44
2:1B:49:THR:HA	2:1B:87:ILE:HB	2.00	0.44
2:1B:116:MET:HG3	2:1B:151:PRO:HG2	1.99	0.44
2:1B:127:HIS:ND1	9:1I:115:LYS:HD3	2.32	0.44
3:1C:41:GLN:NE2	43:1r:65:PRO:O	2.45	0.44
3:1C:129:TRP:HZ2	4:1D:78:PRO:HD2	1.83	0.44
3:1C:198:ASP:OD1	3:1C:198:ASP:N	2.50	0.44
4:1D:116:GLN:NE2	4:1D:138:ARG:HG2	2.31	0.44
4:1D:317:LYS:HA	4:1D:317:LYS:HD2	1.92	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:249:ARG:HD2	7:1G:251:LEU:HD11	2.00	0.44
7:1G:332:LYS:HB2	7:1G:507:TYR:HE1	1.83	0.44
8:1H:86:TRP:HA	8:1H:89:LEU:HD23	2.00	0.44
11:1K:48:ILE:HG13	11:1K:48:ILE:H	1.60	0.44
16:1P:185:MET:HA	16:1P:188:PHE:CD2	2.52	0.44
17:1Q:127:ARG:HH11	44:1s:70:ARG:CZ	2.31	0.44
20:1T:17:TYR:HB2	20:1T:20:LYS:HE3	2.00	0.44
20:1T:43:ASP:OD1	20:1T:46:ASP:N	2.33	0.44
23:1X:77:CYS:SG	23:1X:113:LYS:NZ	2.91	0.44
40:1o:32:GLU:OE2	40:1o:32:GLU:N	2.51	0.44
3:1C:155:TYR:HB2	22:1W:102:HIS:CE1	2.52	0.44
6:1F:22:PHE:HD1	6:1F:117:LYS:HD2	1.83	0.44
7:1G:326:GLU:OE1	7:1G:572:THR:N	2.50	0.44
7:1G:386:PHE:HB2	7:1G:665:GLN:HB3	2.00	0.44
8:1H:181:LEU:HA	8:1H:184:MET:HB2	1.98	0.44
10:1J:61:LEU:HA	10:1J:61:LEU:HD12	1.70	0.44
10:1J:152:TRP:CD2	30:1e:13:LEU:HD11	2.53	0.44
12:1L:293:ILE:HG22	12:1L:422:TYR:HB3	2.00	0.44
13:1M:47:GLU:OE1	13:1M:47:GLU:N	2.51	0.44
13:1M:70:THR:HA	13:1M:103:GLN:NE2	2.32	0.44
45:1N:401:3PE:O14	15:1O:303:LYS:NZ	2.44	0.44
16:1P:172:PHE:HB2	16:1P:179:LEU:HD22	2.00	0.44
16:1P:201:VAL:O	16:1P:290:SER:OG	2.35	0.44
16:1P:202:LYS:HA	16:1P:291:ASP:HB3	2.00	0.44
33:1h:41:THR:O	33:1h:45:VAL:HG22	2.18	0.44
34:1i:107:ASP:H	40:1o:67:LYS:NZ	2.16	0.44
35:1j:26:GLU:H	35:1j:26:GLU:HG2	1.69	0.44
41:1p:119:SER:OG	41:1p:123:ASN:ND2	2.50	0.44
2:1B:52:LEU:HD12	2:1B:89:ALA:O	2.17	0.44
2:1B:55:CYS:SG	2:1B:117:GLY:HA3	2.57	0.44
3:1C:67:HIS:HB3	3:1C:70:ALA:HB3	2.00	0.44
3:1C:149:ARG:HA	22:1W:88:MET:CE	2.47	0.44
6:1F:121:GLY:HA3	6:1F:228:VAL:O	2.18	0.44
6:1F:279:LEU:HD22	6:1F:317:MET:HE1	1.99	0.44
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.98	0.44
7:1G:378:LEU:HB3	7:1G:451:VAL:HG13	2.00	0.44
7:1G:386:PHE:CZ	7:1G:668:ILE:HD12	2.53	0.44
7:1G:389:PRO:CD	7:1G:390:LEU:N	2.80	0.44
8:1H:15:LEU:HB3	26:1a:15:CYS:SG	2.58	0.44
9:1I:33:GLY:O	9:1I:37:THR:HG23	2.18	0.44
12:1L:335:PHE:CE1	12:1L:380:LEU:HD23	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1M:501:PGT:H181	52:1M:501:PGT:H152	1.63	0.44
16:1P:170:ASP:O	16:1P:204:PRO:HA	2.18	0.44
19:1S:17:GLU:CD	19:1S:53:LEU:HG	2.42	0.44
19:1S:35:PHE:CD1	19:1S:35:PHE:C	2.96	0.44
20:1T:58:PHE:HB3	20:1T:60:PHE:CE2	2.53	0.44
20:1T:60:PHE:CD1	20:1T:60:PHE:C	2.96	0.44
21:1V:39:LYS:HD3	21:1V:44:ARG:HD3	2.00	0.44
21:1V:79:VAL:HA	21:1V:82:GLN:HE22	1.82	0.44
40:1o:51:MET:O	40:1o:55:ARG:HG3	2.17	0.44
41:1p:29:VAL:O	41:1p:33:THR:OG1	2.32	0.44
42:1q:5:GLN:O	42:1q:9:ARG:HG3	2.17	0.44
1:1A:18:VAL:HG21	8:1H:76:ILE:HD11	2.00	0.44
2:1B:41:ARG:HH11	2:1B:110:PRO:HG3	1.83	0.44
4:1D:4:TRP:CE2	13:1M:140:THR:HG23	2.52	0.44
4:1D:98:GLN:O	4:1D:101:PRO:HD2	2.18	0.44
5:1E:97:LYS:HD2	5:1E:97:LYS:HA	1.70	0.44
6:1F:371:TRP:HZ2	7:1G:130:PHE:HA	1.82	0.44
10:1J:57:PHE:CE2	10:1J:61:LEU:HD23	2.53	0.44
10:1J:151:THR:OG1	50:1J:201:PC1:H32	2.17	0.44
12:1L:3:PRO:HB3	41:1p:36:PHE:CE2	2.53	0.44
12:1L:496:MET:O	12:1L:500:LEU:HG	2.17	0.44
13:1M:278:ARG:NH1	37:1l:83:MET:HE3	2.33	0.44
14:1N:194:LEU:HD23	14:1N:201:THR:HG21	2.00	0.44
16:1P:234:ASN:C	16:1P:234:ASN:OD1	2.61	0.44
56:1P:501:NDP:H51A	56:1P:501:NDP:C8A	2.44	0.44
19:1S:20:ILE:HD11	19:1S:54:ILE:HG23	2.00	0.44
20:1T:22:TYR:HD2	20:1T:23:ASP:N	2.16	0.44
22:1W:53:ASP:N	22:1W:53:ASP:OD1	2.51	0.44
24:1Y:31:THR:O	24:1Y:35:VAL:HG12	2.17	0.44
29:1d:96:SER:OG	29:1d:97:HIS:ND1	2.49	0.44
35:1j:44:SER:O	35:1j:48:LEU:HD23	2.18	0.44
40:1o:72:SER:HA	41:1p:23:THR:OG1	2.18	0.44
42:1q:6:VAL:HG22	42:1q:9:ARG:HH21	1.83	0.44
6:1F:261:HIS:N	6:1F:336:VAL:O	2.46	0.43
6:1F:262:VAL:HG13	6:1F:265:PRO:HG3	2.00	0.43
7:1G:199:ILE:HD12	7:1G:199:ILE:HA	1.85	0.43
7:1G:496:ILE:HB	7:1G:499:GLN:HB2	2.00	0.43
7:1G:569:LYS:HZ3	7:1G:571:ALA:HB3	1.82	0.43
8:1H:281:ARG:HD3	8:1H:281:ARG:HA	1.87	0.43
11:1K:27:MET:O	11:1K:31:LEU:HD12	2.18	0.43
13:1M:84:LEU:O	13:1M:86:LYS:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:97:GLN:HG2	15:1O:135:LEU:HB2	1.99	0.43
16:1P:195:SER:O	16:1P:195:SER:OG	2.36	0.43
16:1P:238:LEU:O	16:1P:242:VAL:HG23	2.17	0.43
22:1W:90:LEU:O	22:1W:94:ILE:HD12	2.18	0.43
23:1X:25:LYS:HA	23:1X:28:ALA:HB2	2.00	0.43
24:1Y:28:GLY:O	24:1Y:62:SER:OG	2.29	0.43
40:1o:88:TYR:CZ	40:1o:92:LEU:HD11	2.53	0.43
41:1p:27:ASN:HD21	41:1p:29:VAL:HB	1.82	0.43
41:1p:73:ILE:HA	41:1p:76:CYS:HB2	1.98	0.43
3:1C:147:ASP:OD2	3:1C:149:ARG:NH1	2.42	0.43
3:1C:206:PHE:CE1	4:1D:360:PRO:HD3	2.53	0.43
5:1E:149:VAL:O	6:1F:265:PRO:HB2	2.17	0.43
6:1F:351:ILE:HA	6:1F:354:TYR:HB2	2.00	0.43
9:1I:73:GLY:HA2	42:1q:108:TYR:HE1	1.83	0.43
9:1I:141:THR:OG1	9:1I:146:GLU:OE2	2.36	0.43
10:1J:87:LYS:HA	10:1J:87:LYS:HD3	1.79	0.43
12:1L:141:PHE:HB2	12:1L:186:MET:HE1	1.99	0.43
12:1L:331:MET:N	12:1L:331:MET:SD	2.91	0.43
12:1L:386:LEU:HD12	12:1L:386:LEU:HA	1.82	0.43
12:1L:495:ILE:O	12:1L:499:MET:HG3	2.18	0.43
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	2.00	0.43
13:1M:14:MET:HG3	31:1f:12:VAL:HB	2.00	0.43
15:1O:28:ASP:C	15:1O:35:LYS:HD2	2.43	0.43
16:1P:93:ASN:OD1	16:1P:94:LEU:N	2.51	0.43
17:1Q:22:LEU:HB3	22:1W:82:LEU:HD21	1.99	0.43
18:1R:28:PHE:N	18:1R:28:PHE:CD1	2.86	0.43
20:1U:9:GLU:HA	20:1U:12:LYS:HE3	1.99	0.43
20:1U:47:GLN:HA	20:1U:50:ILE:HG12	2.00	0.43
30:1e:46:ILE:HG23	30:1e:50:ARG:NH1	2.33	0.43
1:1A:55:PHE:HB2	10:1J:70:TYR:OH	2.18	0.43
2:1B:93:THR:HG23	2:1B:96:MET:H	1.82	0.43
3:1C:127:ALA:HA	3:1C:130:TYR:CD1	2.52	0.43
3:1C:150:ARG:NH2	3:1C:157:PHE:O	2.52	0.43
5:1E:34:ILE:HD13	5:1E:34:ILE:HA	1.88	0.43
5:1E:165:THR:N	5:1E:168:ASP:OD2	2.47	0.43
6:1F:31:TRP:CZ2	6:1F:148:ASN:HB3	2.53	0.43
6:1F:256:PHE:CD2	6:1F:270:GLU:HB3	2.54	0.43
7:1G:315:VAL:HG13	7:1G:340:SER:HB2	1.99	0.43
7:1G:386:PHE:HB3	7:1G:671:PHE:CD1	2.53	0.43
7:1G:652:VAL:HG22	7:1G:653:ASN:N	2.27	0.43
8:1H:136:VAL:O	8:1H:140:ILE:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:190:LEU:H	8:1H:190:LEU:HD12	1.84	0.43
8:1H:235:ASN:O	8:1H:239:ALA:N	2.32	0.43
9:1I:146:GLU:HA	42:1q:124:TYR:HD2	1.83	0.43
10:1J:129:ASP:OD1	11:1K:52:HIS:NE2	2.51	0.43
12:1L:121:LEU:HD23	12:1L:121:LEU:HA	1.84	0.43
12:1L:556:ILE:HD13	12:1L:556:ILE:HA	1.88	0.43
13:1M:30:HIS:CD2	31:1f:16:VAL:HB	2.54	0.43
13:1M:214:LEU:HD23	13:1M:214:LEU:HA	1.68	0.43
14:1N:2:ASN:HB3	14:1N:5:ILE:CD1	2.48	0.43
14:1N:7:THR:HA	53:1N:402:CDL:H112	2.00	0.43
14:1N:190:MET:H	14:1N:190:MET:HG2	1.56	0.43
14:1N:338:PRO:O	23:1X:169:TRP:NE1	2.51	0.43
16:1P:97:ARG:HA	16:1P:97:ARG:HD3	1.79	0.43
35:1j:64:LEU:HD13	35:1j:64:LEU:HA	1.80	0.43
36:1k:39:GLY:O	36:1k:40:LEU:HD23	2.18	0.43
38:1m:38:ILE:HG22	38:1m:41:ARG:NH2	2.33	0.43
40:1o:41:THR:OG1	40:1o:42:GLN:N	2.51	0.43
3:1C:126:ALA:HB2	4:1D:252:ASN:O	2.18	0.43
4:1D:46:ASN:HA	4:1D:68:LEU:O	2.18	0.43
5:1E:9:HIS:NE2	5:1E:63:ILE:HG13	2.34	0.43
10:1J:78:MET:C	10:1J:80:PRO:HD3	2.43	0.43
11:1K:43:MET:O	11:1K:47:ILE:HD12	2.18	0.43
12:1L:287:PHE:CZ	12:1L:527:GLY:HA3	2.53	0.43
12:1L:578:SER:HB2	14:1N:172:GLN:NE2	2.29	0.43
13:1M:75:LEU:HD23	13:1M:78:MET:HE3	1.99	0.43
13:1M:420:THR:HB	13:1M:423:ILE:HD12	1.99	0.43
14:1N:331:VAL:HG21	29:1d:41:SER:HA	1.99	0.43
15:1O:136:GLU:O	15:1O:140:ARG:HG2	2.19	0.43
19:1S:35:PHE:C	19:1S:35:PHE:HD1	2.27	0.43
20:1T:11:ILE:HG22	20:1T:77:VAL:HG13	1.99	0.43
25:1Z:113:THR:HG22	25:1Z:115:ARG:H	1.84	0.43
34:1i:87:TYR:CZ	41:1p:48:ARG:HG2	2.53	0.43
37:1l:10:PRO:HD2	38:1m:69:TYR:HD2	1.82	0.43
37:1l:138:LEU:HD12	37:1l:142:ARG:NH1	2.32	0.43
39:1n:137:LYS:HB3	39:1n:137:LYS:HE3	1.55	0.43
40:1o:50:LEU:O	40:1o:55:ARG:NE	2.34	0.43
41:1p:54:GLN:NE2	41:1p:55:HIS:HD2	2.17	0.43
43:1r:54:CYS:HA	43:1r:57:ASP:HB2	2.01	0.43
43:1r:92:LYS:HE2	43:1r:92:LYS:H	1.83	0.43
2:1B:32:LYS:HA	2:1B:32:LYS:HD2	1.91	0.43
2:1B:48:MET:O	2:1B:87:ILE:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:209:ASP:OD1	25:1Z:16:TYR:OH	2.36	0.43
4:1D:270:ARG:HB3	4:1D:283:PHE:CZ	2.53	0.43
6:1F:129:MET:HG3	6:1F:131:ALA:H	1.84	0.43
7:1G:100:ASN:OD1	7:1G:135:ARG:NH1	2.52	0.43
10:1J:6:ALA:HA	10:1J:9:LEU:HB2	1.99	0.43
11:1K:90:VAL:HA	11:1K:93:LEU:HB2	2.01	0.43
13:1M:455:LEU:HA	13:1M:455:LEU:HD23	1.72	0.43
14:1N:219:LEU:O	14:1N:223:SER:N	2.51	0.43
15:1O:97:GLN:NE2	54:1O:401:GTP:HN1	2.16	0.43
15:1O:186:LYS:HB2	15:1O:191:GLU:OE2	2.18	0.43
19:1S:36:ILE:HA	19:1S:40:TYR:HB2	2.00	0.43
21:1V:31:LEU:HD23	21:1V:31:LEU:HA	1.88	0.43
34:1i:123:PRO:HB2	34:1i:125:GLN:OE1	2.18	0.43
37:1l:93:PRO:HB3	38:1m:14:PRO:HG3	2.00	0.43
37:1l:112:MET:O	37:1l:116:PHE:HB2	2.19	0.43
43:1r:12:ASN:O	43:1r:16:GLY:N	2.49	0.43
43:1r:105:LEU:HD12	43:1r:105:LEU:HA	1.84	0.43
7:1G:106:PRO:O	9:1I:104:ARG:NH2	2.51	0.43
7:1G:395:ILE:O	7:1G:399:TRP:N	2.39	0.43
8:1H:132:ALA:O	8:1H:136:VAL:HG13	2.17	0.43
11:1K:67:ALA:HA	11:1K:70:GLU:OE1	2.18	0.43
12:1L:119:LYS:HB3	12:1L:119:LYS:HE2	1.77	0.43
30:1e:29:PRO:HB3	33:1h:138:LYS:HG3	2.00	0.43
32:1g:66:PHE:HB2	33:1h:28:TYR:HE2	1.81	0.43
36:1k:50:TRP:CE2	36:1k:51:ARG:HG2	2.53	0.43
37:1l:60:PRO:HG3	37:1l:70:ARG:NH2	2.33	0.43
40:1o:30:PHE:CZ	40:1o:103:ARG:HD2	2.54	0.43
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	2.00	0.43
4:1D:103:PHE:HA	4:1D:106:LEU:HB2	1.99	0.43
7:1G:232:ASP:OD2	7:1G:388:ALA:HA	2.19	0.43
8:1H:59:GLU:HA	8:1H:60:PRO:HD3	1.80	0.43
9:1I:8:ARG:NH1	9:1I:8:ARG:HA	2.34	0.43
12:1L:3:PRO:O	12:1L:7:LEU:HD23	2.18	0.43
12:1L:88:MET:HE2	12:1L:88:MET:HA	2.00	0.43
12:1L:250:SER:CB	12:1L:333:ALA:HA	2.47	0.43
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	2.01	0.43
14:1N:321:LYS:HD3	14:1N:323:MET:HB3	2.00	0.43
16:1P:175:GLU:OE2	16:1P:175:GLU:N	2.52	0.43
16:1P:234:ASN:HB2	16:1P:341:ASN:HB3	2.01	0.43
16:1P:280:THR:H	16:1P:283:LYS:HE2	1.83	0.43
17:1Q:112:LYS:HB3	17:1Q:114:LYS:NZ	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:83:ALA:O	19:1S:87:THR:OG1	2.37	0.43
21:1V:81:LEU:O	21:1V:85:ASN:ND2	2.52	0.43
23:1X:12:LEU:HD23	23:1X:12:LEU:H	1.84	0.43
40:1o:14:LYS:HE2	40:1o:112:LYS:NZ	2.34	0.43
43:1r:56:ARG:O	43:1r:58:GLY:N	2.51	0.43
1:1A:1:FME:O1	1:1A:2:ASN:N	2.52	0.43
1:1A:81:THR:O	27:1b:45:ASN:ND2	2.52	0.43
3:1C:39:GLN:HB3	3:1C:51:PHE:CD2	2.53	0.43
3:1C:66:ASP:HB2	21:1V:89:LEU:HD12	2.01	0.43
3:1C:78:LEU:HA	3:1C:93:VAL:O	2.19	0.43
5:1E:37:ASN:OD1	44:1s:62:ARG:NH2	2.52	0.43
6:1F:422:PHE:HB3	6:1F:425:GLU:HB2	2.01	0.43
7:1G:9:ILE:HG12	7:1G:22:PRO:HG3	2.00	0.43
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.58	0.43
7:1G:110:GLN:HG3	7:1G:205:VAL:C	2.44	0.43
7:1G:230:VAL:HG11	7:1G:566:TYR:CD1	2.54	0.43
11:1K:42:ILE:O	11:1K:46:LEU:HD23	2.19	0.43
12:1L:203:MET:HE2	41:1p:113:GLN:HG2	2.01	0.43
12:1L:572:LYS:O	12:1L:575:ILE:HB	2.18	0.43
13:1M:225:ILE:HD13	13:1M:331:ASN:HB2	1.99	0.43
15:1O:58:TYR:OH	15:1O:110:ASP:OD2	2.33	0.43
15:1O:144:ILE:HD12	15:1O:148:CYS:HB2	2.00	0.43
20:1U:7:THR:O	20:1U:11:ILE:HD12	2.19	0.43
20:1U:17:TYR:O	20:1U:21:LEU:HB2	2.19	0.43
22:1W:90:LEU:HD23	22:1W:91:GLU:OE1	2.19	0.43
25:1Z:143:TYR:HE2	26:1a:48:MET:SD	2.42	0.43
31:1f:37:PHE:O	33:1h:88:GLU:HB3	2.19	0.43
34:1i:112:THR:OG1	34:1i:114:GLU:HG3	2.18	0.43
40:1o:90:GLU:O	40:1o:94:TYR:HB2	2.19	0.43
3:1C:15:ASN:OD1	3:1C:15:ASN:C	2.61	0.43
7:1G:37:ILE:HD12	7:1G:37:ILE:N	2.34	0.43
7:1G:149:ILE:O	7:1G:149:ILE:HG22	2.18	0.43
7:1G:194:GLU:CD	7:1G:385:ARG:HH21	2.24	0.43
7:1G:467:LEU:HA	7:1G:467:LEU:HD12	1.89	0.43
12:1L:47:SER:C	12:1L:50:PRO:HD2	2.43	0.43
13:1M:243:MET:HB2	13:1M:301:ILE:HD12	2.01	0.43
14:1N:3:PRO:HA	14:1N:6:TYR:HB3	2.01	0.43
16:1P:219:LYS:HE3	16:1P:219:LYS:HB3	1.77	0.43
29:1d:16:ASN:HA	29:1d:19:ARG:HH21	1.84	0.43
35:1j:29:SER:O	35:1j:32:MET:HG3	2.19	0.43
38:1m:5:TYR:CE2	38:1m:14:PRO:HD3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:59:ARG:HD3	41:1p:59:ARG:HA	1.69	0.43
1:1A:68:GLU:HA	1:1A:71:LEU:HD23	2.00	0.43
2:1B:50:PHE:N	2:1B:87:ILE:O	2.33	0.43
2:1B:92:LEU:HD21	2:1B:100:LEU:HD23	2.01	0.43
2:1B:118:SER:N	46:1B:201:SF4:S1	2.91	0.43
3:1C:27:GLN:HA	3:1C:30:ALA:HB3	2.01	0.43
4:1D:101:PRO:HB3	4:1D:105:ARG:NH2	2.34	0.43
5:1E:131:THR:OG1	5:1E:138:THR:HG22	2.19	0.43
5:1E:195:PRO:HB3	6:1F:264:HIS:HB3	2.00	0.43
7:1G:105:CYS:HB2	7:1G:106:PRO:HD3	2.00	0.43
7:1G:147:LYS:HA	7:1G:147:LYS:HD3	1.78	0.43
7:1G:194:GLU:OE1	7:1G:385:ARG:NH2	2.39	0.43
7:1G:584:LYS:HA	7:1G:584:LYS:HD2	1.57	0.43
10:1J:68:PHE:CE1	11:1K:31:LEU:HG	2.54	0.43
12:1L:49:VAL:HA	12:1L:52:LEU:HD23	2.01	0.43
12:1L:141:PHE:HE2	13:1M:375:LEU:HD21	1.84	0.43
12:1L:294:THR:O	12:1L:524:ASN:ND2	2.51	0.43
12:1L:395:ILE:O	12:1L:399:VAL:HG13	2.19	0.43
12:1L:496:MET:HE3	12:1L:500:LEU:HD23	2.01	0.43
13:1M:86:LYS:H	13:1M:86:LYS:HG3	1.59	0.43
13:1M:354:LEU:HB2	33:1h:18:ASP:OD2	2.19	0.43
14:1N:170:LEU:O	14:1N:295:ARG:NH1	2.50	0.43
15:1O:95:ARG:HG3	15:1O:282:ILE:HG22	2.01	0.43
15:1O:223:TYR:OH	15:1O:237:ASP:OD1	2.28	0.43
16:1P:73:TRP:HZ2	56:1P:501:NDP:H2A	1.84	0.43
16:1P:149:LYS:O	16:1P:153:GLU:N	2.48	0.43
16:1P:226:LYS:HG3	16:1P:227:THR:H	1.84	0.43
21:1V:43:TYR:O	21:1V:47:THR:HG23	2.18	0.43
22:1W:90:LEU:C	22:1W:94:ILE:HD12	2.44	0.43
37:1l:30:ARG:HH22	38:1m:35:ARG:N	2.17	0.43
40:1o:7:ARG:HG2	40:1o:8:TYR:CD1	2.54	0.43
40:1o:57:TYR:HB2	40:1o:93:ASP:OD2	2.19	0.43
41:1p:159:LYS:O	41:1p:163:LEU:HD23	2.18	0.43
42:1q:86:TRP:CD1	42:1q:98:PRO:HG2	2.54	0.43
43:1r:32:LYS:HA	43:1r:32:LYS:HD3	1.88	0.43
3:1C:66:ASP:N	3:1C:66:ASP:OD1	2.52	0.42
3:1C:94:TYR:HB2	3:1C:107:VAL:CG2	2.47	0.42
3:1C:116:PRO:HB3	3:1C:141:PHE:CD2	2.54	0.42
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.53	0.42
4:1D:165:THR:OG1	8:1H:276:SER:HA	2.19	0.42
4:1D:373:GLU:C	4:1D:394:PRO:HG3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:25:THR:HG22	7:1G:28:GLN:HB2	2.01	0.42
7:1G:47:SER:OG	7:1G:48:VAL:N	2.52	0.42
7:1G:302:ARG:HG3	7:1G:542:PHE:HE2	1.84	0.42
7:1G:426:PRO:HB3	7:1G:466:ILE:HD11	2.00	0.42
7:1G:432:ILE:HG13	7:1G:440:SER:OG	2.19	0.42
10:1J:20:PHE:CE1	10:1J:33:LEU:HD23	2.54	0.42
12:1L:60:GLU:CD	12:1L:83:ASP:HA	2.44	0.42
45:1L:702:3PE:H231	37:1l:88:ARG:HA	2.00	0.42
13:1M:45:LEU:HD12	33:1h:86:ASN:HD22	1.84	0.42
13:1M:75:LEU:HD13	13:1M:440:HIS:NE2	2.33	0.42
15:1O:51:PHE:HB3	15:1O:107:GLN:HE21	1.84	0.42
16:1P:299:GLY:N	16:1P:302:ASP:OD1	2.50	0.42
21:1V:22:ARG:HA	21:1V:22:ARG:HD2	1.86	0.42
24:1Y:114:CYS:O	24:1Y:116:TYR:N	2.52	0.42
34:1i:121:GLU:OE1	34:1i:121:GLU:N	2.52	0.42
38:1m:91:LEU:O	38:1m:96:PRO:HD3	2.19	0.42
41:1p:77:GLU:HG3	41:1p:80:ASP:HB2	2.00	0.42
42:1q:14:VAL:HA	42:1q:23:TYR:HD1	1.84	0.42
2:1B:116:MET:SD	2:1B:156:LEU:HD22	2.59	0.42
2:1B:125:TYR:HB2	9:1I:117:ILE:HG23	2.02	0.42
3:1C:96:LEU:HB2	3:1C:105:ILE:HD12	2.00	0.42
6:1F:22:PHE:CE2	6:1F:255:LEU:HD11	2.54	0.42
7:1G:61:LYS:HD2	7:1G:61:LYS:O	2.18	0.42
7:1G:159:CYS:CB	7:1G:199:ILE:HD11	2.49	0.42
7:1G:278:ARG:HD3	7:1G:549:HIS:CE1	2.54	0.42
7:1G:283:MET:HE3	7:1G:291:LEU:C	2.44	0.42
7:1G:408:LEU:O	7:1G:421:HIS:HA	2.19	0.42
7:1G:524:LEU:O	7:1G:545:TYR:HA	2.18	0.42
7:1G:675:ASP:OD2	7:1G:676:SER:N	2.52	0.42
8:1H:151:LEU:O	8:1H:155:LEU:HB2	2.19	0.42
8:1H:299:ALA:HB1	27:1b:24:ILE:HB	2.01	0.42
9:1I:8:ARG:NH2	43:1r:112:LEU:O	2.53	0.42
11:1K:48:ILE:HG23	11:1K:53:PHE:HB3	2.01	0.42
12:1L:5:ALA:HB2	12:1L:61:MET:SD	2.59	0.42
12:1L:71:LEU:HD22	13:1M:307:TRP:CH2	2.54	0.42
13:1M:14:MET:HB2	31:1f:15:LEU:HD13	2.02	0.42
14:1N:25:HIS:O	14:1N:29:ILE:HG12	2.19	0.42
16:1P:93:ASN:HB3	16:1P:131:HIS:HA	2.01	0.42
20:1U:22:TYR:HE1	36:1k:43:PRO:HB2	1.84	0.42
22:1W:69:LYS:HB2	22:1W:69:LYS:HE2	1.73	0.42
25:1Z:68:ARG:HB2	26:1a:43:TYR:HE2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:2:GLU:HA	42:1q:5:GLN:NE2	2.33	0.42
4:1D:204:PRO:HA	9:1I:175:TYR:CE2	2.54	0.42
6:1F:111:ILE:HD13	6:1F:138:ILE:HD13	2.02	0.42
7:1G:211:LYS:O	7:1G:214:ALA:HB2	2.18	0.42
7:1G:215:PHE:CD2	9:1I:104:ARG:HD3	2.54	0.42
7:1G:230:VAL:HG23	7:1G:573:TYR:CE2	2.54	0.42
8:1H:1:FME:HA	8:1H:4:ILE:HD11	1.91	0.42
8:1H:196:ALA:N	8:1H:199:ASP:HB3	2.33	0.42
8:1H:222:MET:O	8:1H:226:ALA:N	2.43	0.42
10:1J:83:TRP:HB3	10:1J:90:PHE:HE1	1.84	0.42
13:1M:181:TYR:HB3	41:1p:84:MET:HE3	2.01	0.42
13:1M:203:PHE:CE1	13:1M:242:GLY:HA3	2.54	0.42
13:1M:329:LEU:HD23	13:1M:359:TRP:CD2	2.54	0.42
14:1N:125:GLN:HG3	14:1N:220:ILE:HD13	2.00	0.42
19:1S:68:TYR:HD1	19:1S:72:GLN:HE22	1.67	0.42
20:1U:28:GLU:OE2	20:1U:29:LYS:NZ	2.26	0.42
21:1V:88:SER:O	21:1V:92:LYS:HG2	2.20	0.42
21:1V:92:LYS:HB3	21:1V:96:TRP:CZ2	2.54	0.42
23:1X:125:SER:HA	27:1b:53:PRO:HG3	2.01	0.42
25:1Z:98:MET:HG3	25:1Z:101:VAL:HG21	2.00	0.42
38:1m:109:ASP:O	38:1m:112:GLU:HG3	2.20	0.42
4:1D:208:LEU:HA	4:1D:211:ILE:HD12	2.01	0.42
5:1E:55:GLN:NE2	5:1E:59:GLY:O	2.52	0.42
6:1F:150:GLN:HE21	6:1F:177:VAL:HG11	1.85	0.42
8:1H:240:ILE:HD13	8:1H:240:ILE:HA	1.92	0.42
12:1L:48:LEU:O	12:1L:51:LEU:HB2	2.19	0.42
12:1L:79:SER:HB2	12:1L:135:ASN:HB3	2.00	0.42
12:1L:202:PHE:CE1	12:1L:265:PRO:HG2	2.55	0.42
12:1L:587:TYR:OH	14:1N:117:GLU:OE2	2.35	0.42
13:1M:458:LEU:HD23	13:1M:458:LEU:HA	1.90	0.42
20:1T:60:PHE:HE1	20:1T:62:ILE:HG22	1.84	0.42
22:1W:46:THR:O	22:1W:50:PHE:HB2	2.20	0.42
26:1a:2:TRP:CD1	26:1a:2:TRP:H	2.36	0.42
34:1i:72:THR:HG23	34:1i:73:HIS:ND1	2.34	0.42
37:1l:130:PRO:HD3	40:1o:21:MET:HE1	2.02	0.42
2:1B:150:PRO:HG3	4:1D:189:MET:HE2	2.02	0.42
4:1D:217:ASN:O	4:1D:221:ARG:HG2	2.19	0.42
6:1F:37:GLN:HA	6:1F:41:ASP:O	2.20	0.42
7:1G:231:MET:HG2	7:1G:266:LYS:HD2	2.01	0.42
7:1G:260:GLU:OE2	7:1G:394:ARG:NH1	2.53	0.42
7:1G:275:LYS:HA	42:1q:134:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:95:GLU:HG3	9:1I:108:ARG:HB3	2.01	0.42
9:1I:96:ALA:HB2	9:1I:106:THR:HA	2.01	0.42
12:1L:76:LEU:HD11	12:1L:196:TRP:HZ3	1.84	0.42
12:1L:190:LEU:HD21	13:1M:307:TRP:CH2	2.55	0.42
12:1L:288:THR:HG21	12:1L:307:SER:OG	2.18	0.42
12:1L:338:MET:HE1	12:1L:461:SER:OG	2.19	0.42
12:1L:350:LEU:O	12:1L:350:LEU:HD23	2.20	0.42
16:1P:76:LYS:HD3	16:1P:76:LYS:HA	1.72	0.42
16:1P:249:ALA:HB1	16:1P:251:ARG:HG2	2.00	0.42
19:1S:87:THR:O	19:1S:91:GLU:HG2	2.20	0.42
22:1W:91:GLU:HA	22:1W:94:ILE:HD12	2.02	0.42
26:1a:28:LYS:HE3	26:1a:28:LYS:HB3	1.61	0.42
32:1g:96:LEU:HD11	32:1g:100:ARG:NH2	2.35	0.42
37:1l:46:ASP:OD1	37:1l:46:ASP:N	2.44	0.42
37:1l:82:ASP:HB2	37:1l:88:ARG:NH1	2.34	0.42
37:1l:139:TYR:CD2	37:1l:150:PRO:HG3	2.55	0.42
38:1m:112:GLU:OE2	38:1m:113:LYS:NZ	2.43	0.42
39:1n:128:ARG:HD2	39:1n:167:TRP:CD2	2.54	0.42
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	2.01	0.42
42:1q:1:MET:O	42:1q:4:VAL:HG12	2.20	0.42
43:1r:1:ALA:HB1	43:1r:23:LEU:HD22	2.02	0.42
2:1B:51:GLY:HA2	2:1B:89:ALA:O	2.19	0.42
4:1D:83:LEU:HD12	4:1D:83:LEU:HA	1.90	0.42
5:1E:124:LEU:H	5:1E:124:LEU:HG	1.72	0.42
7:1G:187:ILE:HD11	7:1G:189:LYS:HB2	2.01	0.42
7:1G:384:PRO:HD2	7:1G:415:LEU:HD11	2.00	0.42
7:1G:421:HIS:ND1	7:1G:421:HIS:O	2.53	0.42
7:1G:675:ASP:CG	7:1G:676:SER:N	2.78	0.42
10:1J:106:TYR:HA	10:1J:109:LYS:HG2	2.00	0.42
14:1N:319:HIS:CD2	14:1N:321:LYS:H	2.34	0.42
16:1P:107:GLU:O	16:1P:111:VAL:HG22	2.19	0.42
16:1P:143:SER:HB3	16:1P:146:LEU:HG	2.01	0.42
16:1P:335:LYS:HD2	16:1P:335:LYS:O	2.18	0.42
19:1S:23:CYS:HB3	19:1S:26:SER:HB3	2.01	0.42
19:1S:41:VAL:HG22	19:1S:45:LYS:HZ1	1.84	0.42
21:1V:6:LYS:HE2	21:1V:6:LYS:HB2	1.63	0.42
22:1W:62:LYS:HE3	22:1W:62:LYS:HB3	1.90	0.42
23:1X:34:GLN:HG3	23:1X:116:TRP:CD2	2.55	0.42
29:1d:116:PHE:CE2	41:1p:157:LYS:HG3	2.54	0.42
30:1e:37:LYS:HB3	30:1e:37:LYS:HE3	1.71	0.42
34:1i:31:GLU:OE1	39:1n:115:PRO:HD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:1k:24:GLU:H	36:1k:24:GLU:CD	2.26	0.42
39:1n:54:LYS:HA	39:1n:54:LYS:HD2	1.80	0.42
4:1D:145:THR:OG1	4:1D:181:TYR:OH	2.25	0.42
4:1D:162:GLY:HA3	8:1H:279:ARG:N	2.35	0.42
4:1D:285:VAL:HA	4:1D:286:PRO:HD3	1.88	0.42
6:1F:226:GLU:O	6:1F:230:VAL:HG13	2.20	0.42
7:1G:142:ILE:C	7:1G:190:MET:HE1	2.44	0.42
7:1G:161:ARG:HH11	7:1G:161:ARG:HG3	1.84	0.42
10:1J:130:THR:HG21	25:1Z:124:LEU:HD12	2.01	0.42
12:1L:8:THR:HG21	12:1L:82:MET:HG3	2.02	0.42
12:1L:279:CYS:HA	37:1l:116:PHE:CE2	2.55	0.42
12:1L:355:ASP:OD1	12:1L:357:ARG:NE	2.44	0.42
13:1M:293:HIS:NE2	13:1M:366:ASN:OD1	2.52	0.42
13:1M:373:ILE:HG21	13:1M:454:ILE:HD11	2.02	0.42
52:1M:501:PGT:H352	52:1M:501:PGT:H321	1.77	0.42
14:1N:88:LYS:HE3	14:1N:88:LYS:HB3	1.75	0.42
15:1O:73:LEU:HD21	15:1O:295:LYS:HD3	2.02	0.42
19:1S:82:SER:HB3	19:1S:85:GLN:HB3	2.01	0.42
20:1T:78:ASP:OD1	20:1T:79:TYR:N	2.52	0.42
20:1U:32:VAL:O	20:1U:74:GLN:N	2.53	0.42
22:1W:65:GLU:OE1	22:1W:66:MET:N	2.53	0.42
32:1g:66:PHE:O	32:1g:70:LEU:HB3	2.20	0.42
34:1i:93:PRO:HG3	41:1p:9:TYR:CE2	2.55	0.42
34:1i:125:GLN:HB2	40:1o:61:TYR:OH	2.20	0.42
35:1j:60:THR:O	35:1j:64:LEU:HD23	2.20	0.42
37:1l:97:SER:HA	38:1m:5:TYR:CD1	2.54	0.42
38:1m:84:LYS:HA	38:1m:84:LYS:HD3	1.68	0.42
39:1n:47:PHE:HA	39:1n:50:HIS:CE1	2.54	0.42
42:1q:52:ASN:OD1	42:1q:52:ASN:C	2.62	0.42
42:1q:106:ARG:HB2	42:1q:109:ILE:HG13	2.01	0.42
3:1C:84:PRO:HB2	17:1Q:86:PHE:HE1	1.84	0.42
4:1D:161:ILE:HG21	4:1D:235:TRP:CE3	2.55	0.42
4:1D:290:ARG:H	4:1D:290:ARG:HG3	1.70	0.42
5:1E:102:VAL:HA	5:1E:154:VAL:HG23	2.00	0.42
6:1F:247:ARG:NH1	6:1F:316:LEU:HD23	2.35	0.42
8:1H:314:ILE:HD11	27:1b:44:ILE:HD11	2.02	0.42
10:1J:17:PHE:CD1	10:1J:20:PHE:HE2	2.37	0.42
11:1K:27:MET:N	11:1K:88:ASP:OD2	2.52	0.42
12:1L:90:ILE:HB	12:1L:91:PRO:HD3	2.02	0.42
12:1L:226:GLN:OE1	12:1L:284:THR:HG21	2.20	0.42
13:1M:42:LEU:HD12	13:1M:453:MET:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:87:LYS:HZ1	15:1O:141:GLN:C	2.28	0.42
16:1P:340:VAL:O	16:1P:340:VAL:HG22	2.19	0.42
20:1T:58:PHE:O	20:1T:60:PHE:N	2.47	0.42
22:1W:102:HIS:HA	22:1W:105:ARG:NH1	2.35	0.42
29:1d:58:LEU:HD23	29:1d:58:LEU:HA	1.81	0.42
31:1f:44:PHE:CD2	33:1h:84:GLU:HB3	2.55	0.42
35:1j:18:THR:O	35:1j:22:LEU:HD12	2.19	0.42
39:1n:34:ASP:N	39:1n:34:ASP:OD1	2.52	0.42
39:1n:65:GLN:O	39:1n:68:GLU:HG3	2.19	0.42
39:1n:176:ARG:HE	39:1n:176:ARG:HB2	1.61	0.42
40:1o:57:TYR:CD1	40:1o:57:TYR:N	2.87	0.42
2:1B:175:ILE:HD13	2:1B:175:ILE:HA	1.85	0.42
3:1C:41:GLN:NE2	43:1r:65:PRO:HB2	2.35	0.42
3:1C:155:TYR:O	22:1W:102:HIS:ND1	2.53	0.42
7:1G:315:VAL:CG1	7:1G:340:SER:HB2	2.50	0.42
7:1G:432:ILE:HD11	7:1G:437:HIS:CD2	2.53	0.42
7:1G:601:ARG:NH1	7:1G:605:GLU:HB2	2.35	0.42
8:1H:88:PRO:HG3	8:1H:104:PHE:CD2	2.54	0.42
9:1I:148:LEU:HB3	17:1Q:70:MET:HE1	2.02	0.42
12:1L:101:MET:HG3	12:1L:118:PHE:HE2	1.85	0.42
12:1L:533:MET:O	45:1L:702:3PE:H362	2.20	0.42
14:1N:347:ASN:HB3	29:1d:2:MET:HG3	2.01	0.42
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD22	2.01	0.42
18:1R:87:CYS:SG	18:1R:89:LEU:HG	2.60	0.42
19:1S:44:LYS:O	19:1S:44:LYS:HD3	2.20	0.42
20:1T:36:PHE:HB2	20:1T:37:MET:CE	2.46	0.42
22:1W:29:LYS:HD3	22:1W:29:LYS:HA	1.82	0.42
23:1X:64:GLN:O	23:1X:67:LEU:HB3	2.20	0.42
30:1e:78:ILE:O	30:1e:82:ARG:HB2	2.20	0.42
32:1g:112:CYS:N	41:1p:158:GLN:OE1	2.49	0.42
33:1h:45:VAL:O	33:1h:46:PHE:HD1	2.02	0.42
39:1n:100:GLU:OE2	39:1n:167:TRP:NE1	2.51	0.42
2:1B:87:ILE:HD13	2:1B:114:VAL:HB	2.01	0.42
3:1C:176:TYR:OH	3:1C:181:LYS:HE3	2.20	0.42
4:1D:225:LEU:O	4:1D:229:LEU:HB2	2.20	0.42
5:1E:190:ARG:NH2	6:1F:265:PRO:O	2.53	0.42
6:1F:188:GLU:OE1	6:1F:190:THR:N	2.53	0.42
7:1G:197:GLY:H	7:1G:265:ASP:CG	2.25	0.42
7:1G:568:GLU:OE2	7:1G:590:PRO:HD3	2.20	0.42
11:1K:43:MET:HE3	14:1N:72:MET:SD	2.59	0.42
12:1L:230:HIS:O	12:1L:232:TRP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:366:MET:HB3	12:1L:369:THR:HB	2.01	0.42
12:1L:522:PHE:HA	12:1L:528:TYR:CE1	2.55	0.42
16:1P:222:ASP:OD1	16:1P:222:ASP:N	2.53	0.42
20:1T:75:GLU:HA	20:1T:78:ASP:OD2	2.20	0.42
23:1X:57:GLU:HA	23:1X:60:LYS:HE3	2.02	0.42
25:1Z:22:LYS:HA	25:1Z:22:LYS:HD3	1.90	0.42
25:1Z:77:ALA:HB1	25:1Z:81:ARG:NH2	2.35	0.42
26:1a:48:MET:HE3	26:1a:60:TYR:CG	2.55	0.42
33:1h:48:GLY:HA2	41:1p:55:HIS:NE2	2.34	0.42
40:1o:46:ASN:ND2	40:1o:55:ARG:HH12	2.18	0.42
4:1D:76:CYS:SG	4:1D:406:SER:HB3	2.60	0.41
5:1E:36:LYS:HE3	44:1s:59:SER:HA	2.01	0.41
5:1E:165:THR:H	5:1E:168:ASP:CG	2.26	0.41
6:1F:261:HIS:HE1	6:1F:341:THR:HB	1.83	0.41
6:1F:305:PRO:HG2	6:1F:327:THR:HA	2.02	0.41
6:1F:389:ILE:HG23	6:1F:419:ILE:HG12	2.01	0.41
7:1G:143:GLY:N	7:1G:190:MET:HE1	2.35	0.41
8:1H:203:GLY:O	8:1H:207:LEU:N	2.52	0.41
8:1H:314:ILE:HD12	25:1Z:58:ARG:HD3	2.02	0.41
12:1L:315:VAL:HG11	12:1L:412:THR:HG21	2.00	0.41
12:1L:486:MET:C	12:1L:489:THR:HG1	2.24	0.41
15:1O:96:LEU:O	15:1O:100:LEU:HB2	2.20	0.41
16:1P:2:HIS:HE1	18:1R:22:ASP:OD1	2.03	0.41
18:1R:28:PHE:N	18:1R:28:PHE:HD1	2.18	0.41
19:1S:82:SER:OG	19:1S:84:ASP:OD1	2.35	0.41
22:1W:112:ALA:O	22:1W:114:ARG:NH2	2.53	0.41
25:1Z:103:ASP:OD1	25:1Z:103:ASP:N	2.52	0.41
31:1f:46:ARG:HD2	31:1f:47:GLU:O	2.20	0.41
32:1g:40:LYS:HA	32:1g:40:LYS:HD2	1.61	0.41
34:1i:65:ARG:HG2	34:1i:65:ARG:NH1	2.33	0.41
42:1q:9:ARG:O	42:1q:13:GLN:HG2	2.19	0.41
1:1A:7:LEU:HD23	1:1A:7:LEU:HA	1.89	0.41
2:1B:40:ALA:HB1	8:1H:54:LYS:HB2	2.03	0.41
4:1D:68:LEU:HD12	4:1D:70:GLY:H	1.84	0.41
4:1D:347:HIS:CD2	7:1G:126:ASP:HA	2.54	0.41
5:1E:52:ASP:O	5:1E:56:ARG:N	2.53	0.41
7:1G:147:LYS:HD2	7:1G:702:SER:O	2.20	0.41
7:1G:426:PRO:HD3	7:1G:661:LEU:HD11	2.01	0.41
7:1G:430:GLN:O	7:1G:434:SER:OG	2.38	0.41
7:1G:594:ARG:NH2	22:1W:125:GLY:HA2	2.35	0.41
7:1G:594:ARG:CD	22:1W:126:HIS:HB3	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:667:THR:HB	7:1G:669:LYS:HG2	2.02	0.41
9:1I:42:PHE:HB3	43:1r:7:ILE:HD11	2.03	0.41
10:1J:152:TRP:HZ3	50:1J:201:PC1:H272	1.85	0.41
12:1L:542:LEU:HD23	12:1L:542:LEU:HA	1.82	0.41
13:1M:60:SER:OG	32:1g:83:TYR:OH	2.33	0.41
13:1M:76:MET:HE2	13:1M:230:VAL:HG22	2.00	0.41
13:1M:347:GLY:N	13:1M:414:THR:O	2.53	0.41
13:1M:450:ASN:HB2	50:1M:502:PC1:H221	2.02	0.41
14:1N:2:ASN:OD1	14:1N:4:ILE:HG22	2.19	0.41
14:1N:86:ILE:HG23	14:1N:86:ILE:O	2.21	0.41
15:1O:25:ILE:HD12	15:1O:238:ILE:HD11	2.02	0.41
15:1O:304:TYR:CE2	29:1d:52:PRO:HG3	2.54	0.41
16:1P:198:LYS:C	16:1P:237:LEU:HD11	2.45	0.41
17:1Q:30:ILE:HD12	17:1Q:101:TRP:NE1	2.35	0.41
20:1T:19:LEU:HD12	20:1T:19:LEU:HA	1.83	0.41
20:1T:58:PHE:HD2	20:1T:58:PHE:HA	1.73	0.41
22:1W:63:VAL:O	22:1W:67:PHE:HD2	2.03	0.41
24:1Y:99:THR:O	24:1Y:103:ARG:HG2	2.20	0.41
38:1m:50:TYR:O	39:1n:168:HIS:HE1	2.03	0.41
39:1n:9:LEU:HD23	39:1n:9:LEU:HA	1.74	0.41
1:1A:106:TRP:CD2	45:1A:201:3PE:H231	2.56	0.41
2:1B:48:MET:HE3	2:1B:80:PRO:CA	2.50	0.41
3:1C:12:ARG:NH2	4:1D:124:LYS:HG3	2.35	0.41
3:1C:151:ILE:C	3:1C:151:ILE:HD12	2.45	0.41
4:1D:120:LEU:HD23	4:1D:120:LEU:HA	1.87	0.41
4:1D:149:ASN:ND2	4:1D:371:LYS:HG2	2.35	0.41
4:1D:217:ASN:ND2	43:1r:23:LEU:O	2.51	0.41
4:1D:233:ARG:HH12	50:1H:401:PC1:H31	1.85	0.41
6:1F:82:MET:SD	6:1F:129:MET:SD	3.19	0.41
6:1F:277:LYS:HD2	6:1F:277:LYS:HA	1.89	0.41
6:1F:406:ALA:HB3	48:1F:501:FMN:HM82	2.03	0.41
7:1G:566:TYR:HA	7:1G:569:LYS:HZ2	1.84	0.41
7:1G:646:ASN:HB3	7:1G:650:LYS:HE2	2.02	0.41
8:1H:253:GLU:O	8:1H:256:THR:OG1	2.29	0.41
12:1L:103:PHE:CE2	12:1L:242:PRO:HG3	2.55	0.41
12:1L:183:VAL:HG12	13:1M:382:ILE:HG21	2.02	0.41
12:1L:407:TRP:CE2	37:1l:115:MET:HE2	2.55	0.41
12:1L:504:LEU:HD23	45:1L:704:3PE:O22	2.19	0.41
13:1M:78:MET:HE1	13:1M:439:LEU:HD23	2.02	0.41
13:1M:399:ASN:O	13:1M:403:THR:OG1	2.33	0.41
15:1O:28:ASP:OD2	15:1O:126:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:10:LYS:HA	16:1P:10:LYS:HD3	1.83	0.41
16:1P:283:LYS:O	16:1P:287:VAL:HG13	2.21	0.41
23:1X:46:ARG:HB3	33:1h:141:PRO:HB3	2.01	0.41
27:1b:77:LEU:HD12	27:1b:80:LEU:HD23	2.02	0.41
38:1m:34:GLU:H	38:1m:34:GLU:HG2	1.68	0.41
39:1n:25:HIS:CE1	39:1n:78:PRO:HB3	2.55	0.41
1:1A:75:LEU:HA	1:1A:78:ALA:HB3	2.01	0.41
2:1B:81:ARG:NH1	8:1H:61:LEU:O	2.54	0.41
2:1B:94:ASN:OD1	2:1B:131:SER:HA	2.20	0.41
3:1C:101:PHE:HE1	43:1r:99:PRO:HB3	1.86	0.41
3:1C:151:ILE:HD12	3:1C:152:LEU:HG	2.02	0.41
5:1E:106:THR:HA	5:1E:109:MET:HG3	2.02	0.41
7:1G:107:ILE:HA	9:1I:104:ARG:NH2	2.31	0.41
7:1G:613:TYR:CB	7:1G:618:GLN:HB3	2.51	0.41
8:1H:141:SER:C	8:1H:289:LEU:HD21	2.45	0.41
8:1H:252:PRO:O	8:1H:256:THR:HG23	2.20	0.41
12:1L:384:PRO:O	35:1j:36:ILE:HD12	2.20	0.41
12:1L:475:MET:O	40:1o:51:MET:HE1	2.21	0.41
12:1L:535:ARG:NH1	37:1l:92:SER:O	2.43	0.41
14:1N:41:ILE:N	14:1N:42:PRO:HD2	2.35	0.41
17:1Q:125:ASN:OD1	17:1Q:125:ASN:N	2.50	0.41
17:1Q:126:LYS:HD3	17:1Q:126:LYS:HA	1.67	0.41
18:1R:34:GLU:OE1	42:1q:124:TYR:HA	2.20	0.41
20:1U:54:MET:HE3	20:1U:76:ILE:HG21	2.03	0.41
29:1d:11:LEU:HD11	30:1e:3:PHE:HB3	2.02	0.41
30:1e:70:LYS:NZ	30:1e:74:ARG:HB2	2.35	0.41
32:1g:66:PHE:CD1	33:1h:28:TYR:HE2	2.38	0.41
37:1l:158:ILE:HD11	40:1o:99:LYS:C	2.45	0.41
40:1o:60:HIS:HD1	40:1o:60:HIS:H	1.67	0.41
42:1q:44:TYR:HE2	42:1q:83:PRO:HB3	1.85	0.41
43:1r:8:GLN:O	43:1r:12:ASN:ND2	2.54	0.41
4:1D:100:LEU:HD12	4:1D:118:TYR:CD2	2.55	0.41
4:1D:112:MET:SD	4:1D:194:ILE:HG12	2.61	0.41
4:1D:234:ILE:HA	4:1D:237:ASN:ND2	2.35	0.41
7:1G:198:ASN:CG	7:1G:262:TRP:HB3	2.46	0.41
7:1G:200:ILE:HD13	7:1G:210:SER:HB3	2.01	0.41
7:1G:285:ARG:CG	7:1G:291:LEU:HA	2.50	0.41
7:1G:344:CYS:HB2	7:1G:510:GLY:O	2.21	0.41
7:1G:577:GLU:OE2	7:1G:577:GLU:HA	2.21	0.41
7:1G:592:LEU:HD22	16:1P:6:ILE:HG23	2.02	0.41
8:1H:74:ALA:HB3	8:1H:75:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:31:VAL:O	9:1I:35:GLY:N	2.53	0.41
9:1I:69:ARG:NH1	9:1I:155:LEU:HD12	2.36	0.41
11:1K:55:LEU:HD12	11:1K:55:LEU:HA	1.77	0.41
12:1L:487:LYS:NZ	35:1j:49:GLY:HA2	2.35	0.41
13:1M:73:LEU:HA	13:1M:76:MET:SD	2.60	0.41
14:1N:275:SER:HB2	24:1Y:136:ALA:HB3	2.03	0.41
15:1O:14:THR:HG21	15:1O:116:LEU:HG	2.01	0.41
16:1P:83:LYS:HE2	16:1P:83:LYS:HB3	1.82	0.41
16:1P:133:SER:O	16:1P:167:LYS:HA	2.19	0.41
16:1P:144:ARG:O	16:1P:148:SER:OG	2.38	0.41
16:1P:157:ARG:NH2	16:1P:225:GLY:O	2.45	0.41
17:1Q:23:THR:HG23	17:1Q:25:VAL:H	1.85	0.41
19:1S:19:ARG:O	19:1S:65:TRP:N	2.39	0.41
20:1T:8:LEU:O	20:1T:11:ILE:HB	2.20	0.41
20:1U:78:ASP:HB3	34:1i:15:ARG:CZ	2.50	0.41
21:1V:72:GLN:NE2	43:1r:99:PRO:HB2	2.36	0.41
25:1Z:5:LYS:HE2	25:1Z:5:LYS:HA	2.01	0.41
53:1a:101:CDL:H552	53:1a:101:CDL:H741	2.03	0.41
37:1l:5:THR:HG23	37:1l:7:ASP:OD1	2.20	0.41
37:1l:128:VAL:HG11	40:1o:94:TYR:OH	2.19	0.41
2:1B:69:MET:HE1	2:1B:76:PHE:N	2.35	0.41
4:1D:144:ILE:HD13	4:1D:144:ILE:HA	1.88	0.41
5:1E:99:HIS:H	5:1E:157:ASN:HA	1.85	0.41
5:1E:105:THR:OG1	5:1E:106:THR:N	2.54	0.41
6:1F:298:ILE:HG13	6:1F:306:LEU:HD13	2.02	0.41
6:1F:317:MET:HA	6:1F:322:LEU:HD21	2.02	0.41
7:1G:478:ARG:HE	7:1G:483:VAL:HB	1.86	0.41
7:1G:503:LEU:CD1	7:1G:509:PRO:HB3	2.48	0.41
8:1H:149:ILE:HG23	8:1H:181:LEU:HD22	2.03	0.41
8:1H:216:ALA:O	8:1H:220:PHE:HB3	2.21	0.41
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.20	0.41
12:1L:129:MET:O	12:1L:133:THR:OG1	2.35	0.41
12:1L:548:SER:HA	12:1L:552:LEU:HB3	2.03	0.41
45:1L:703:3PE:H2	45:1L:703:3PE:H221	1.50	0.41
13:1M:204:MET:HE3	13:1M:204:MET:HB3	1.78	0.41
14:1N:173:THR:O	14:1N:227:THR:OG1	2.38	0.41
17:1Q:69:LEU:HD12	17:1Q:69:LEU:HA	1.71	0.41
20:1T:52:MET:HE3	22:1W:40:TYR:HD2	1.85	0.41
22:1W:75:ASP:O	22:1W:79:VAL:HG12	2.21	0.41
25:1Z:98:MET:HG2	25:1Z:104:TRP:CE2	2.55	0.41
29:1d:115:GLU:HG2	29:1d:115:GLU:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:55:THR:O	31:1f:56:TRP:C	2.64	0.41
33:1h:114:MET:HE1	33:1h:121:PRO:HD2	2.02	0.41
35:1j:60:THR:HG1	35:1j:63:GLU:CD	2.27	0.41
39:1n:40:ALA:O	39:1n:44:ARG:N	2.44	0.41
40:1o:71:ASP:HB3	41:1p:22:GLN:HG3	2.03	0.41
6:1F:32:ARG:HG3	6:1F:34:LYS:HG2	2.03	0.41
6:1F:215:VAL:O	6:1F:218:CYS:HB2	2.21	0.41
6:1F:247:ARG:N	6:1F:250:ASN:O	2.54	0.41
7:1G:644:GLN:OE1	7:1G:644:GLN:N	2.52	0.41
8:1H:142:TYR:CZ	8:1H:289:LEU:HB2	2.56	0.41
8:1H:293:PHE:O	8:1H:297:THR:OG1	2.32	0.41
9:1I:79:ALA:HB2	9:1I:106:THR:HG22	2.02	0.41
12:1L:95:PHE:CE1	12:1L:456:ARG:HG2	2.56	0.41
13:1M:1:FME:O	13:1M:5:ILE:HD12	2.20	0.41
13:1M:16:TRP:CH2	45:1N:401:3PE:H241	2.55	0.41
13:1M:442:LEU:HD11	32:1g:70:LEU:HD21	2.03	0.41
14:1N:304:MET:HB2	14:1N:304:MET:HE2	1.82	0.41
15:1O:58:TYR:O	15:1O:62:THR:HG23	2.21	0.41
15:1O:169:VAL:HG11	15:1O:214:MET:HE1	2.02	0.41
16:1P:30:LEU:HD21	16:1P:94:LEU:HB2	2.02	0.41
16:1P:165:ILE:HG23	16:1P:227:THR:HG23	2.02	0.41
17:1Q:35:VAL:HG21	17:1Q:101:TRP:HB3	2.02	0.41
20:1T:83:LYS:NZ	20:1T:84:LYS:HB3	2.33	0.41
20:1U:35:HIS:NE2	20:1U:38:LYS:HD3	2.35	0.41
21:1V:80:ILE:H	21:1V:80:ILE:HG12	1.70	0.41
23:1X:100:ARG:HA	23:1X:100:ARG:HD3	1.90	0.41
23:1X:166:LEU:HG	23:1X:167:PHE:HD2	1.85	0.41
25:1Z:87:LEU:HD23	25:1Z:87:LEU:HA	1.78	0.41
27:1b:62:MET:N	27:1b:62:MET:SD	2.94	0.41
28:1c:1:LYS:HD3	28:1c:3:TYR:HD2	1.86	0.41
31:1f:48:LEU:HD21	31:1f:53:GLU:C	2.45	0.41
50:1f:101:PC1:H3I1	33:1h:39:GLY:HA3	2.02	0.41
33:1h:24:LEU:O	33:1h:28:TYR:HB3	2.21	0.41
38:1m:119:LYS:HA	38:1m:119:LYS:HD2	1.89	0.41
39:1n:107:HIS:CD2	39:1n:108:PRO:HD2	2.56	0.41
41:1p:48:ARG:O	41:1p:52:GLU:HG2	2.21	0.41
42:1q:72:ASP:OD2	42:1q:72:ASP:C	2.64	0.41
2:1B:47:PRO:HA	2:1B:85:VAL:O	2.21	0.41
2:1B:59:MET:HG3	2:1B:116:MET:HE1	2.03	0.41
2:1B:113:VAL:HG11	2:1B:140:VAL:HG12	2.02	0.41
3:1C:46:ASN:OD1	3:1C:46:ASN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:86:PHE:HB2	6:1F:200:GLN:NE2	2.36	0.41
6:1F:199:LYS:HD2	6:1F:200:GLN:H	1.85	0.41
7:1G:14:ASP:OD1	7:1G:81:THR:N	2.48	0.41
8:1H:127:TYR:OH	8:1H:208:VAL:HG23	2.21	0.41
8:1H:197:PRO:HG2	8:1H:198:PHE:CD1	2.56	0.41
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.55	0.41
12:1L:500:LEU:HD12	12:1L:501:ALA:H	1.86	0.41
45:1L:704:3PE:H222	45:1L:704:3PE:O31	2.21	0.41
13:1M:210:TYR:HB2	13:1M:268:GLY:HA3	2.02	0.41
13:1M:411:LEU:HA	13:1M:411:LEU:HD12	1.82	0.41
16:1P:173:GLY:N	16:1P:176:ASP:HB3	2.36	0.41
20:1T:14:ARG:O	20:1T:18:VAL:HG13	2.20	0.41
20:1T:85:ASP:OD1	20:1T:85:ASP:N	2.54	0.41
20:1U:51:ILE:HD13	20:1U:62:ILE:HD11	2.02	0.41
21:1V:25:ILE:O	21:1V:29:LYS:HD2	2.20	0.41
21:1V:76:ILE:N	21:1V:76:ILE:HD13	2.36	0.41
24:1Y:119:LEU:O	24:1Y:123:LEU:N	2.46	0.41
36:1k:35:LEU:HD11	36:1k:42:ASP:N	2.35	0.41
39:1n:52:ASN:N	39:1n:52:ASN:OD1	2.54	0.41
42:1q:32:ASP:OD2	42:1q:34:ARG:NH2	2.54	0.41
1:1A:72:LEU:HD11	8:1H:148:ILE:HD12	2.03	0.41
2:1B:54:CYS:O	4:1D:189:MET:HE1	2.21	0.41
3:1C:51:PHE:HB3	21:1V:111:TRP:CZ2	2.56	0.41
3:1C:84:PRO:HB3	17:1Q:95:PHE:CE1	2.56	0.41
3:1C:127:ALA:O	3:1C:128:ASN:C	2.64	0.41
3:1C:136:ASP:OD1	3:1C:150:ARG:HA	2.21	0.41
3:1C:149:ARG:HA	22:1W:88:MET:HE1	2.03	0.41
4:1D:162:GLY:HA3	8:1H:279:ARG:HB3	2.02	0.41
4:1D:389:CYS:O	4:1D:389:CYS:SG	2.79	0.41
5:1E:205:PRO:HA	5:1E:206:PRO:HD3	1.96	0.41
6:1F:89:ARG:HB3	6:1F:218:CYS:SG	2.61	0.41
6:1F:93:LEU:HB3	6:1F:134:ALA:HA	2.03	0.41
6:1F:145:GLU:OE1	6:1F:145:GLU:N	2.48	0.41
6:1F:224:ASN:O	6:1F:228:VAL:HG23	2.21	0.41
7:1G:203:CYS:HB3	49:1G:804:K:K	2.14	0.41
7:1G:227:SER:O	7:1G:228:ILE:HD13	2.21	0.41
7:1G:285:ARG:HB3	42:1q:144:TYR:N	2.36	0.41
7:1G:328:LEU:HD13	7:1G:502:ALA:HA	2.02	0.41
7:1G:433:ALA:HB1	7:1G:472:ASN:ND2	2.35	0.41
7:1G:460:ARG:HG2	7:1G:461:SER:H	1.86	0.41
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	2.02	0.41
50:1H:401:PC1:H331	9:1I:27:TRP:CZ2	2.56	0.41
9:1I:99:ARG:HB2	9:1I:103:SER:O	2.21	0.41
10:1J:59:ILE:CD1	11:1K:64:LEU:HD22	2.51	0.41
10:1J:119:PHE:CD1	11:1K:1:FME:HB2	2.55	0.41
12:1L:28:LYS:HD2	12:1L:30:ASN:H	1.85	0.41
12:1L:367:PRO:O	12:1L:371:THR:OG1	2.30	0.41
12:1L:373:LEU:HD12	12:1L:373:LEU:HA	1.87	0.41
12:1L:528:TYR:CG	37:1I:101:MET:HE1	2.56	0.41
12:1L:543:SER:OG	12:1L:547:LYS:NZ	2.52	0.41
12:1L:544:MET:O	12:1L:548:SER:OG	2.23	0.41
12:1L:558:LEU:HD23	12:1L:558:LEU:HA	1.96	0.41
45:1L:703:3PE:H371	45:1L:703:3PE:C23	2.50	0.41
13:1M:116:ILE:HD13	13:1M:164:LEU:HD22	2.03	0.41
13:1M:116:ILE:O	13:1M:120:ILE:HD12	2.21	0.41
13:1M:250:LEU:HD23	13:1M:250:LEU:HA	1.84	0.41
13:1M:277:LEU:O	37:1I:88:ARG:NH2	2.54	0.41
13:1M:286:ILE:O	13:1M:289:SER:OG	2.24	0.41
13:1M:360:LEU:HD23	13:1M:411:LEU:HD21	2.03	0.41
14:1N:221:HIS:CD2	14:1N:323:MET:HE3	2.55	0.41
16:1P:178:PHE:CD1	16:1P:178:PHE:N	2.87	0.41
16:1P:294:LEU:HD11	16:1P:297:LEU:HD12	2.02	0.41
16:1P:297:LEU:HD23	16:1P:297:LEU:HA	1.88	0.41
20:1T:70:LEU:HD11	20:1T:79:TYR:HD2	1.85	0.41
21:1V:63:ASP:OD1	21:1V:65:LYS:HE3	2.20	0.41
22:1W:52:LEU:HD23	22:1W:52:LEU:HA	1.76	0.41
24:1Y:120:THR:HA	24:1Y:123:LEU:HB2	2.02	0.41
26:1a:2:TRP:HH2	53:1a:101:CDL:H751	1.86	0.41
27:1b:59:ASP:OD1	27:1b:59:ASP:N	2.52	0.41
29:1d:31:LEU:HD21	29:1d:69:VAL:HG13	2.03	0.41
33:1h:7:ARG:NH2	34:1i:27:LEU:H	2.19	0.41
40:1o:38:MET:HE3	40:1o:57:TYR:HA	2.02	0.41
40:1o:105:ARG:O	40:1o:109:GLN:OE1	2.38	0.41
41:1p:126:LYS:HE3	41:1p:126:LYS:HB3	1.81	0.41
42:1q:95:ASP:H	43:1r:34:THR:HG23	1.86	0.41
43:1r:104:GLU:N	43:1r:104:GLU:CD	2.78	0.41
2:1B:126:TYR:N	2:1B:126:TYR:CD2	2.89	0.41
4:1D:30:PRO:HA	4:1D:31:PRO:HD3	1.99	0.41
4:1D:124:LYS:HB2	4:1D:124:LYS:HE3	1.65	0.41
4:1D:161:ILE:HA	4:1D:238:ARG:NH2	2.36	0.41
4:1D:184:VAL:HG23	4:1D:185:SER:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:92:TYR:CE2	6:1F:133:ALA:HB3	2.56	0.41
6:1F:123:LEU:HD12	6:1F:124:VAL:HG13	2.01	0.41
7:1G:58:GLU:HG3	7:1G:86:SER:OG	2.21	0.41
7:1G:88:LYS:HE2	7:1G:88:LYS:HB2	1.62	0.41
7:1G:373:GLU:H	7:1G:373:GLU:CD	2.24	0.41
11:1K:73:LEU:HD22	14:1N:38:LEU:HD12	2.03	0.41
45:1L:704:3PE:H231	45:1L:704:3PE:H321	2.01	0.41
13:1M:12:LEU:HB3	13:1M:13:PRO:HD3	2.01	0.41
15:1O:105:LEU:HA	15:1O:128:ILE:HG21	2.03	0.41
18:1R:10:LYS:HB3	18:1R:10:LYS:HE3	1.69	0.41
19:1S:24:GLN:CB	19:1S:25:ARG:NH1	2.84	0.41
23:1X:139:ASN:OD1	23:1X:139:ASN:N	2.54	0.41
26:1a:61:HIS:ND1	26:1a:61:HIS:O	2.53	0.41
53:1a:101:CDL:H312	53:1a:101:CDL:OB9	2.21	0.41
29:1d:5:ARG:O	29:1d:8:ARG:HB2	2.21	0.41
41:1p:167:LYS:HD2	41:1p:171:GLU:OE1	2.21	0.41
42:1q:31:ASN:HD22	42:1q:31:ASN:HA	1.68	0.41
4:1D:99:ALA:HA	4:1D:102:TYR:CD2	2.54	0.40
4:1D:124:LYS:HD2	4:1D:363:THR:HG21	2.03	0.40
4:1D:171:PHE:HA	4:1D:174:ARG:HG3	2.03	0.40
5:1E:110:LEU:HD22	6:1F:261:HIS:CE1	2.56	0.40
5:1E:186:PRO:C	5:1E:187:ARG:HD2	2.46	0.40
7:1G:278:ARG:HA	7:1G:278:ARG:HD2	1.85	0.40
7:1G:374:ALA:HA	7:1G:448:LYS:HB3	2.03	0.40
8:1H:234:MET:O	8:1H:238:THR:OG1	2.28	0.40
9:1I:107:THR:O	42:1q:129:THR:HG23	2.20	0.40
12:1L:534:HIS:HB3	45:1L:702:3PE:H31	2.02	0.40
12:1L:550:SER:O	12:1L:554:ASP:HB3	2.21	0.40
13:1M:116:ILE:HD13	13:1M:116:ILE:HA	1.81	0.40
13:1M:254:THR:O	13:1M:258:ALA:N	2.54	0.40
14:1N:186:HIS:O	14:1N:190:MET:HG2	2.21	0.40
16:1P:46:ILE:HG23	18:1R:26:VAL:HG21	2.02	0.40
16:1P:140:LYS:H	16:1P:140:LYS:HG3	1.57	0.40
19:1S:86:VAL:O	19:1S:90:LEU:HG	2.21	0.40
21:1V:17:GLU:O	21:1V:19:PRO:HD3	2.21	0.40
23:1X:78:ALA:O	23:1X:82:THR:HG23	2.21	0.40
45:1Y:201:3PE:H252	45:1Y:201:3PE:H221	1.95	0.40
37:1l:101:MET:HA	37:1l:101:MET:HE3	2.03	0.40
39:1n:97:LYS:HZ3	39:1n:173:PRO:HB2	1.87	0.40
41:1p:145:LEU:HD11	41:1p:154:CYS:HA	2.02	0.40
4:1D:170:MET:N	4:1D:170:MET:SD	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:148:CYS:SG	6:1F:103:GLY:N	2.84	0.40
6:1F:150:GLN:O	6:1F:153:ILE:HG22	2.21	0.40
6:1F:232:PRO:HB2	6:1F:236:ARG:NH2	2.36	0.40
6:1F:348:ALA:HB2	6:1F:376:MET:SD	2.62	0.40
48:1F:501:FMN:H1'2	48:1F:501:FMN:H4'	1.85	0.40
7:1G:285:ARG:NH2	42:1q:144:TYR:HD1	2.18	0.40
8:1H:142:TYR:CD1	8:1H:289:LEU:HD13	2.56	0.40
8:1H:261:LEU:HD23	8:1H:261:LEU:HA	1.89	0.40
10:1J:153:LEU:HD23	10:1J:153:LEU:HA	1.89	0.40
13:1M:371:PRO:HG2	13:1M:448:THR:HG21	2.03	0.40
14:1N:48:PHE:CD1	14:1N:48:PHE:O	2.74	0.40
14:1N:95:MET:HE3	14:1N:148:SER:O	2.22	0.40
14:1N:151:PRO:HG2	24:1Y:137:GLU:OE1	2.21	0.40
14:1N:191:THR:HA	14:1N:194:LEU:HB2	2.02	0.40
15:1O:59:ALA:O	15:1O:62:THR:OG1	2.30	0.40
16:1P:48:PRO:HB3	16:1P:73:TRP:CG	2.57	0.40
16:1P:136:ASN:HD21	16:1P:291:ASP:HA	1.85	0.40
16:1P:318:LEU:HD23	16:1P:318:LEU:O	2.21	0.40
17:1Q:57:MET:HE1	17:1Q:101:TRP:HZ3	1.86	0.40
20:1U:15:VAL:O	20:1U:19:LEU:HD12	2.21	0.40
22:1W:62:LYS:HD3	22:1W:107:PHE:CD2	2.56	0.40
25:1Z:51:MET:SD	25:1Z:55:ARG:NE	2.94	0.40
25:1Z:86:MET:HE2	25:1Z:86:MET:HB2	1.92	0.40
37:1l:47:TYR:OH	37:1l:77:ILE:O	2.22	0.40
40:1o:30:PHE:CD2	40:1o:33:ARG:HD2	2.57	0.40
40:1o:46:ASN:ND2	41:1p:122:GLN:HE21	2.19	0.40
1:1A:87:MET:C	1:1A:87:MET:SD	3.04	0.40
45:1A:201:3PE:H2D1	8:1H:302:MET:HE1	2.03	0.40
3:1C:70:ALA:HB1	3:1C:72:PHE:HD1	1.86	0.40
3:1C:72:PHE:CE2	3:1C:105:ILE:HG13	2.56	0.40
3:1C:155:TYR:HD2	22:1W:98:LYS:HA	1.86	0.40
5:1E:101:GLN:OE1	5:1E:101:GLN:HA	2.21	0.40
6:1F:52:GLY:O	6:1F:56:ILE:HD12	2.21	0.40
7:1G:287:GLU:CD	7:1G:287:GLU:H	2.29	0.40
7:1G:424:ASP:O	7:1G:660:PRO:HA	2.22	0.40
8:1H:4:ILE:H	8:1H:4:ILE:HG13	1.37	0.40
8:1H:141:SER:OG	8:1H:290:TRP:NE1	2.53	0.40
8:1H:219:PRO:HA	8:1H:222:MET:HG2	2.02	0.40
8:1H:307:LEU:HB3	8:1H:308:PRO:HD3	2.03	0.40
8:1H:315:PRO:HB3	25:1Z:54:ASN:HD21	1.86	0.40
10:1J:123:GLY:O	10:1J:126:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:34:GLU:O	11:1K:37:MET:HG3	2.21	0.40
13:1M:119:TYR:CD1	13:1M:160:LEU:HD23	2.57	0.40
15:1O:132:PHE:CD1	15:1O:132:PHE:C	2.99	0.40
16:1P:6:ILE:HA	16:1P:7:PRO:HD3	1.91	0.40
21:1V:22:ARG:O	21:1V:22:ARG:NH1	2.54	0.40
22:1W:63:VAL:HA	22:1W:66:MET:HE3	2.04	0.40
23:1X:67:LEU:O	23:1X:71:ARG:N	2.53	0.40
25:1Z:30:LEU:HB3	25:1Z:34:SER:OG	2.22	0.40
25:1Z:72:MET:N	25:1Z:73:PRO:HD2	2.36	0.40
37:1l:98:TRP:HA	37:1l:101:MET:HB2	2.02	0.40
38:1m:42:LEU:HD23	38:1m:42:LEU:HA	1.89	0.40
42:1q:137:TRP:CD1	42:1q:138:VAL:H	2.39	0.40
1:1A:98:LEU:HD12	1:1A:98:LEU:HA	1.84	0.40
4:1D:139:VAL:HG23	4:1D:278:TYR:HE1	1.86	0.40
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.57	0.40
6:1F:22:PHE:HB2	6:1F:25:LEU:HB2	2.02	0.40
6:1F:42:TRP:CE3	6:1F:161:LEU:HD13	2.57	0.40
6:1F:108:ARG:HE	6:1F:108:ARG:HB3	1.71	0.40
7:1G:354:ALA:HB2	7:1G:648:LEU:HB3	2.04	0.40
7:1G:378:LEU:HD12	7:1G:409:ILE:HD11	2.03	0.40
9:1I:160:LYS:HD2	9:1I:161:TRP:CD1	2.56	0.40
12:1L:48:LEU:HA	12:1L:48:LEU:HD12	1.78	0.40
13:1M:1:FME:HE3	13:1M:111:THR:HG21	2.03	0.40
14:1N:144:GLN:HE21	30:1e:2:PHE:N	2.20	0.40
14:1N:230:LEU:HD12	14:1N:230:LEU:HA	1.76	0.40
14:1N:248:LEU:HD11	14:1N:296:LEU:HB3	2.02	0.40
16:1P:238:LEU:HD12	16:1P:238:LEU:HA	1.90	0.40
22:1W:39:TRP:O	22:1W:43:VAL:HG23	2.22	0.40
23:1X:54:ARG:HA	23:1X:54:ARG:HD3	1.81	0.40
23:1X:77:CYS:HB3	23:1X:80:PRO:HG2	2.02	0.40
26:1a:18:ILE:N	26:1a:19:PRO:HD2	2.36	0.40
30:1e:87:LYS:HE2	30:1e:87:LYS:HB2	1.80	0.40
32:1g:55:LEU:O	32:1g:59:ARG:HG3	2.21	0.40
32:1g:113:PHE:N	41:1p:158:GLN:OE1	2.53	0.40
38:1m:48:LEU:HD23	38:1m:48:LEU:HA	1.90	0.40
39:1n:82:PRO:HB3	39:1n:89:SER:H	1.86	0.40
1:1A:97:LEU:HD13	1:1A:97:LEU:HA	1.94	0.40
4:1D:260:LEU:HB3	4:1D:265:ILE:HB	2.03	0.40
4:1D:284:ASP:O	4:1D:306:GLN:HG3	2.22	0.40
4:1D:322:GLU:CD	43:1r:44:PRO:HD3	2.46	0.40
6:1F:115:PRO:O	6:1F:119:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:136:ILE:HD11	6:1F:177:VAL:HG22	2.03	0.40
6:1F:248:GLU:C	6:1F:250:ASN:H	2.30	0.40
6:1F:300:GLY:HA2	6:1F:333:ALA:N	2.36	0.40
7:1G:460:ARG:NH2	7:1G:657:LEU:HB3	2.36	0.40
7:1G:474:ALA:O	7:1G:478:ARG:HB2	2.22	0.40
8:1H:55:LEU:HD23	8:1H:55:LEU:HA	1.89	0.40
8:1H:272:TRP:CZ2	9:1I:38:LEU:HG	2.57	0.40
12:1L:293:ILE:CD1	12:1L:294:THR:HG23	2.50	0.40
13:1M:121:LEU:H	13:1M:121:LEU:HG	1.75	0.40
13:1M:135:ARG:HE	45:1N:401:3PE:H362	1.87	0.40
13:1M:438:ALA:O	13:1M:442:LEU:HG	2.21	0.40
14:1N:183:SER:HB2	14:1N:208:TYR:OH	2.21	0.40
14:1N:278:MET:HB2	14:1N:279:PRO:HD3	2.03	0.40
16:1P:27:THR:O	16:1P:27:THR:OG1	2.37	0.40
16:1P:319:ARG:HA	16:1P:322:ARG:HD3	2.04	0.40
19:1S:13:LEU:H	19:1S:13:LEU:HG	1.75	0.40
23:1X:82:THR:O	23:1X:86:THR:OG1	2.26	0.40
30:1e:13:LEU:HD12	30:1e:13:LEU:HA	1.85	0.40
30:1e:49:ILE:H	30:1e:49:ILE:HG12	1.73	0.40
37:1l:116:PHE:O	37:1l:116:PHE:HD1	2.04	0.40
39:1n:113:MET:HG2	39:1n:114:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	83/115 (72%)	78 (94%)	3 (4%)	2 (2%)	4	29
2	1B	153/258 (59%)	140 (92%)	13 (8%)	0	100	100
3	1C	207/264 (78%)	192 (93%)	15 (7%)	0	100	100
4	1D	414/476 (87%)	380 (92%)	34 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	1E	212/249 (85%)	193 (91%)	19 (9%)	0	100	100
6	1F	430/464 (93%)	397 (92%)	33 (8%)	0	100	100
7	1G	697/727 (96%)	620 (89%)	71 (10%)	6 (1%)	14	45
8	1H	316/318 (99%)	290 (92%)	24 (8%)	2 (1%)	21	52
9	1I	174/239 (73%)	164 (94%)	10 (6%)	0	100	100
10	1J	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	21	52
11	1K	96/98 (98%)	90 (94%)	6 (6%)	0	100	100
12	1L	604/606 (100%)	557 (92%)	44 (7%)	3 (0%)	24	56
13	1M	457/459 (100%)	436 (95%)	20 (4%)	1 (0%)	43	72
14	1N	345/347 (99%)	326 (94%)	19 (6%)	0	100	100
15	1O	318/357 (89%)	288 (91%)	30 (9%)	0	100	100
16	1P	340/377 (90%)	304 (89%)	35 (10%)	1 (0%)	36	65
17	1Q	127/175 (73%)	115 (91%)	12 (9%)	0	100	100
18	1R	94/123 (76%)	83 (88%)	10 (11%)	1 (1%)	11	42
19	1S	85/99 (86%)	77 (91%)	8 (9%)	0	100	100
20	1T	83/156 (53%)	76 (92%)	7 (8%)	0	100	100
20	1U	84/156 (54%)	79 (94%)	5 (6%)	0	100	100
21	1V	113/116 (97%)	99 (88%)	14 (12%)	0	100	100
22	1W	113/128 (88%)	106 (94%)	6 (5%)	1 (1%)	14	45
23	1X	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
24	1Y	137/141 (97%)	129 (94%)	8 (6%)	0	100	100
25	1Z	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
26	1a	68/70 (97%)	63 (93%)	5 (7%)	0	100	100
27	1b	81/84 (96%)	77 (95%)	4 (5%)	0	100	100
28	1c	47/76 (62%)	45 (96%)	2 (4%)	0	100	100
29	1d	117/123 (95%)	109 (93%)	8 (7%)	0	100	100
30	1e	97/106 (92%)	94 (97%)	3 (3%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	8 (14%)	0	100	100
32	1g	98/154 (64%)	89 (91%)	8 (8%)	1 (1%)	12	43
33	1h	136/189 (72%)	132 (97%)	4 (3%)	0	100	100
34	1i	124/128 (97%)	113 (91%)	11 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	1j	69/105 (66%)	63 (91%)	5 (7%)	1 (1%)	9	37
36	1k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	1l	154/186 (83%)	141 (92%)	13 (8%)	0	100	100
38	1m	126/129 (98%)	116 (92%)	10 (8%)	0	100	100
39	1n	170/179 (95%)	163 (96%)	7 (4%)	0	100	100
40	1o	120/137 (88%)	117 (98%)	3 (2%)	0	100	100
41	1p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	131 (92%)	11 (8%)	1 (1%)	18	50
43	1r	90/114 (79%)	82 (91%)	8 (9%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	8151/9744 (84%)	7525 (92%)	605 (7%)	21 (0%)	37	65

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	109	LYS
7	1G	652	VAL
7	1G	671	PHE
8	1H	92	PRO
12	1L	464	ALA
13	1M	85	SER
16	1P	222	ASP
18	1R	79	THR
32	1g	24	ILE
1	1A	75	LEU
8	1H	213	VAL
10	1J	116	ILE
12	1L	549	ALA
7	1G	166	ILE
7	1G	256	GLU
7	1G	72	PRO
12	1L	159	HIS
42	1q	134	ILE
7	1G	367	THR
35	1j	50	HIS
22	1W	96	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	75/99 (76%)	73 (97%)	2 (3%)	39	59
2	1B	131/212 (62%)	129 (98%)	2 (2%)	57	68
3	1C	190/227 (84%)	187 (98%)	3 (2%)	55	68
4	1D	364/405 (90%)	362 (100%)	2 (0%)	81	80
5	1E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	344 (99%)	2 (1%)	78	79
7	1G	588/610 (96%)	584 (99%)	4 (1%)	76	77
8	1H	274/274 (100%)	267 (97%)	7 (3%)	40	60
9	1I	151/201 (75%)	149 (99%)	2 (1%)	61	71
10	1J	140/140 (100%)	139 (99%)	1 (1%)	76	77
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	535 (99%)	4 (1%)	76	77
13	1M	408/408 (100%)	405 (99%)	3 (1%)	76	77
14	1N	310/310 (100%)	309 (100%)	1 (0%)	86	83
15	1O	283/307 (92%)	281 (99%)	2 (1%)	76	77
16	1P	296/323 (92%)	294 (99%)	2 (1%)	76	77
17	1Q	117/152 (77%)	117 (100%)	0	100	100
18	1R	79/97 (81%)	78 (99%)	1 (1%)	61	71
19	1S	77/82 (94%)	76 (99%)	1 (1%)	61	71
20	1T	79/133 (59%)	76 (96%)	3 (4%)	29	53
20	1U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	99 (99%)	1 (1%)	68	74
22	1W	107/112 (96%)	106 (99%)	1 (1%)	70	75
23	1X	153/154 (99%)	150 (98%)	3 (2%)	48	64
24	1Y	101/102 (99%)	101 (100%)	0	100	100
25	1Z	123/124 (99%)	123 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	1a	58/58 (100%)	58 (100%)	0	100	100
27	1b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	107/109 (98%)	107 (100%)	0	100	100
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%)	61 (97%)	2 (3%)	34	56
37	1l	141/161 (88%)	141 (100%)	0	100	100
38	1m	113/114 (99%)	112 (99%)	1 (1%)	70	75
39	1n	156/160 (98%)	156 (100%)	0	100	100
40	1o	110/120 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	153 (99%)	1 (1%)	78	79
42	1q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	85 (100%)	0	100	100
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7188/8272 (87%)	7135 (99%)	53 (1%)	73	77

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	65	PHE
1	1A	97	LEU
2	1B	68	ASP
2	1B	156	LEU
3	1C	11	ILE
3	1C	20	LYS
3	1C	183	VAL
4	1D	4	TRP
4	1D	376	VAL
6	1F	31	TRP
6	1F	149	LEU

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Mol	Chain	Res	Type
7	1G	77	TRP
7	1G	283	MET
7	1G	525	LEU
7	1G	636	VAL
8	1H	32	GLN
8	1H	33	LEU
8	1H	143	GLU
8	1H	145	THR
8	1H	213	VAL
8	1H	284	GLN
8	1H	300	LEU
9	1I	92	ILE
9	1I	141	THR
10	1J	17	PHE
12	1L	66	TRP
12	1L	163	ASP
12	1L	459	ILE
12	1L	471	ASN
13	1M	86	LYS
13	1M	439	LEU
13	1M	455	LEU
14	1N	164	ILE
15	1O	96	LEU
15	1O	270	LEU
16	1P	140	LYS
16	1P	258	LEU
18	1R	43	LEU
19	1S	87	THR
20	1T	15	VAL
20	1T	58	PHE
20	1T	66	ASP
21	1V	94	LEU
22	1W	126	HIS
23	1X	93	LEU
23	1X	107	ASP
23	1X	144	ARG
30	1e	6	GLN
34	1i	47	ASN
36	1k	28	LEU
36	1k	29	GLU
38	1m	126	ILE
41	1p	62	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (81) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	162	GLN
3	1C	38	GLN
3	1C	67	HIS
3	1C	69	ASN
3	1C	95	ASN
3	1C	211	GLN
4	1D	27	HIS
4	1D	34	ASN
4	1D	150	HIS
5	1E	55	GLN
5	1E	91	ASN
6	1F	37	GLN
6	1F	116	HIS
7	1G	182	GLN
7	1G	237	ASN
7	1G	255	HIS
7	1G	499	GLN
7	1G	517	ASN
7	1G	682	GLN
8	1H	138	GLN
8	1H	284	GLN
9	1I	150	ASN
9	1I	156	ASN
11	1K	94	ASN
12	1L	23	ASN
12	1L	248	HIS
12	1L	296	ASN
12	1L	321	GLN
12	1L	471	ASN
12	1L	506	ASN
12	1L	579	ASN
13	1M	44	GLN
13	1M	103	GLN
14	1N	36	ASN
14	1N	134	GLN
14	1N	152	ASN
14	1N	174	GLN
14	1N	235	ASN
15	1O	50	HIS
15	1O	204	ASN
15	1O	265	ASN

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Mol	Chain	Res	Type
16	1P	2	HIS
16	1P	3	HIS
16	1P	180	ASN
16	1P	203	GLN
16	1P	216	ASN
17	1Q	6	GLN
17	1Q	46	GLN
17	1Q	50	ASN
17	1Q	81	ASN
18	1R	16	GLN
18	1R	36	ASN
19	1S	24	GLN
19	1S	80	ASN
21	1V	70	GLN
21	1V	85	ASN
22	1W	26	ASN
22	1W	51	GLN
22	1W	102	HIS
23	1X	150	ASN
24	1Y	133	GLN
27	1b	45	ASN
29	1d	61	GLN
29	1d	117	HIS
30	1e	97	HIS
34	1i	44	GLN
37	1l	28	ASN
37	1l	55	GLN
38	1m	78	ASN
39	1n	65	GLN
40	1o	46	ASN
40	1o	75	ASN
41	1p	55	HIS
41	1p	58	ASN
41	1p	103	ASN
41	1p	122	GLN
41	1p	123	ASN
43	1r	12	ASN
43	1r	24	GLN
44	1s	40	ASN
44	1s	75	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	$\# Z > 2$
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	1.01	1 (12%)
10	FME	1J	1	10	8,9,10	0.55	0	8,9,11	0.92	1 (12%)
14	FME	1N	1	14	8,9,10	0.54	0	8,9,11	0.91	1 (12%)
1	FME	1A	1	25,1	8,9,10	0.54	0	8,9,11	0.96	1 (12%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.98	1 (12%)
8	FME	1H	1	8	8,9,10	0.65	0	8,9,11	1.02	1 (12%)
34	SAC	1i	1	-	7,8,9	0.56	0	7,9,11	1.17	1 (14%)
11	FME	1K	1	14,30,11	8,9,10	0.56	0	8,9,11	0.96	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
12	FME	1L	1	12	-	0/7/9/11	-
10	FME	1J	1	10	-	2/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
1	FME	1A	1	25,1	-	0/7/9/11	-
13	FME	1M	1	13	-	1/7/9/11	-
8	FME	1H	1	8	-	1/7/9/11	-
34	SAC	1i	1	-	-	2/7/8/10	-
11	FME	1K	1	14,30,11	-	1/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-3.03	116.97	124.77
11	1K	1	FME	O-C-CA	-2.67	117.92	124.77
8	1H	1	FME	O-C-CA	-2.65	117.95	124.77
12	1L	1	FME	O-C-CA	-2.63	118.02	124.77
10	1J	1	FME	O-C-CA	-2.58	118.13	124.77
13	1M	1	FME	O-C-CA	-2.51	118.32	124.77
14	1N	1	FME	O-C-CA	-2.48	118.39	124.77
1	1A	1	FME	O-C-CA	-2.47	118.43	124.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
10	1J	1	FME	N-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
10	1J	1	FME	C-CA-CB-CG
34	1i	1	SAC	CB-CA-N-C1A
34	1i	1	SAC	C-CA-N-C1A
13	1M	1	FME	C-CA-CB-CG

There are no ring outliers.

7 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	1L	1	FME	2	0
14	1N	1	FME	1	0
1	1A	1	FME	2	0
13	1M	1	FME	3	0
8	1H	1	FME	1	0
34	1i	1	SAC	2	0
11	1K	1	FME	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
46	SF4	1F	502	6	0,12,12	-	-	-		
52	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.48	0
48	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.64	1 (2%)
46	SF4	1B	201	2	0,12,12	-	-	-		
47	FES	1G	803	7	0,4,4	-	-	-		
46	SF4	1I	202	9	0,12,12	-	-	-		
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.39	0
50	PC1	1J	201	10	34,34,53	0.32	0	40,42,61	0.32	0
46	SF4	1G	801	7	0,12,12	-	-	-		
45	3PE	1L	704	-	41,41,50	0.31	0	44,46,55	1.30	5 (11%)
51	MYR	1L	701	-	13,14,15	0.29	0	12,13,15	0.29	0
53	CDL	1a	101	-	60,60,99	0.33	0	66,72,111	0.42	0
47	FES	1E	301	5	0,4,4	-	-	-		
58	EHZ	1W	201	-	31,36,37	0.20	0	36,44,47	1.16	1 (2%)
45	3PE	1L	703	12	30,30,50	0.37	0	33,35,55	0.59	0
50	PC1	1f	101	31	45,45,53	0.28	0	51,53,61	0.34	0
53	CDL	1N	402	14	76,76,99	0.30	0	82,88,111	0.37	0
50	PC1	1M	502	13	43,43,53	0.29	0	49,51,61	0.44	0
46	SF4	1G	802	7	0,12,12	-	-	-		
46	SF4	1I	201	9	0,12,12	-	-	-		
45	3PE	1N	401	-	50,50,50	0.28	0	53,55,55	0.40	0
45	3PE	1Y	201	-	50,50,50	0.27	0	53,55,55	0.43	0
54	GTP	1O	401	55	33,34,34	0.60	0	50,54,54	0.61	0
50	PC1	1H	401	-	53,53,53	0.27	0	59,61,61	0.32	0
45	3PE	1L	702	-	45,45,50	0.30	0	48,50,55	0.32	0
56	NDP	1P	501	-	51,52,52	0.51	0	71,80,80	0.78	1 (1%)
50	PC1	1I	203	9	43,43,53	0.29	0	49,51,61	0.39	0
58	EHZ	1n	201	39	31,36,37	0.18	0	36,44,47	1.31	2 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	SF4	1F	502	6	-	-	0/6/5/5
52	PGT	1M	501	-	-	22/55/55/55	-
48	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
46	SF4	1B	201	2	-	-	0/6/5/5
47	FES	1G	803	7	-	-	0/1/1/1
46	SF4	1I	202	9	-	-	0/6/5/5
45	3PE	1A	201	-	-	3/50/50/54	-
50	PC1	1J	201	10	-	5/38/38/57	-
46	SF4	1G	801	7	-	-	0/6/5/5
45	3PE	1L	704	-	-	7/45/45/54	-
51	MYR	1L	701	-	-	2/12/12/13	-
53	CDL	1a	101	-	-	10/71/71/110	-
47	FES	1E	301	5	-	-	0/1/1/1
58	EHZ	1W	201	-	-	6/42/44/45	-
45	3PE	1L	703	12	-	7/34/34/54	-
50	PC1	1f	101	31	-	6/49/49/57	-
53	CDL	1N	402	14	-	9/87/87/110	-
50	PC1	1M	502	13	-	7/47/47/57	-
46	SF4	1G	802	7	-	-	0/6/5/5
46	SF4	1I	201	9	-	-	0/6/5/5
45	3PE	1N	401	-	-	8/54/54/54	-
45	3PE	1Y	201	-	-	8/54/54/54	-
54	GTP	1O	401	55	-	3/22/38/38	0/3/3/3
50	PC1	1H	401	-	-	5/57/57/57	-
45	3PE	1L	702	-	-	2/49/49/54	-
56	NDP	1P	501	-	-	10/34/77/77	0/5/5/5
50	PC1	1I	203	9	-	5/47/47/57	-
58	EHZ	1n	201	39	-	15/42/44/45	-

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	1W	201	EHZ	C10-S1-C9	6.49	121.03	101.84
58	1n	201	EHZ	C10-S1-C9	6.45	120.90	101.84
45	1L	704	3PE	O21-C21-C22	6.44	125.41	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1P	501	NDP	P2B-O2B-C2B	-4.62	111.09	123.43
58	1n	201	EHZ	C14-C13-C12	3.04	117.46	112.39
45	1L	704	3PE	O21-C21-O22	-2.80	117.16	123.70
45	1L	704	3PE	C2-O21-C21	2.62	124.07	117.80
45	1L	704	3PE	O21-C2-C3	2.23	116.34	108.34
45	1L	704	3PE	O21-C2-C1	2.07	115.77	108.34
48	1F	501	FMN	C4-N3-C2	-2.07	121.97	125.64

There are no chirality outliers.

All (142) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	C1-O11-P-O14
45	1L	703	3PE	O32-C31-O31-C3
45	1L	703	3PE	C32-C31-O31-C3
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2
45	1L	704	3PE	C1-O11-P-O14
45	1L	704	3PE	O22-C21-O21-C2
45	1L	704	3PE	C22-C21-O21-C2
45	1N	401	3PE	C1-O11-P-O14
45	1Y	201	3PE	C1-O11-P-O14
50	1I	203	PC1	C11-O13-P-O14
50	1I	203	PC1	C11-O13-P-O11
50	1J	201	PC1	C1-O11-P-O14
50	1J	201	PC1	C1-O11-P-O13
50	1M	502	PC1	C1-O11-P-O14
50	1f	101	PC1	O32-C31-O31-C3
50	1f	101	PC1	C32-C31-O31-C3
51	1L	701	MYR	O1-C1-C2-C3
52	1M	501	PGT	O31-C31-O2-C2
52	1M	501	PGT	C1-O3P-P-O1P
52	1M	501	PGT	C4-O4P-P-O3P
52	1M	501	PGT	C5-C4-O4P-P
52	1M	501	PGT	C4-C5-C6-O6
52	1M	501	PGT	O5-C5-C6-O6
52	1M	501	PGT	O11-C11-O3-C3
52	1M	501	PGT	C12-C11-O3-C3
53	1a	101	CDL	CA3-OA5-PA1-OA3
53	1a	101	CDL	CB3-OB5-PB2-OB3
53	1a	101	CDL	CB4-CB3-OB5-PB2
56	1P	501	NDP	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
56	1P	501	NDP	C5B-O5B-PA-O2A
56	1P	501	NDP	C4B-C5B-O5B-PA
56	1P	501	NDP	O4D-C1D-N1N-C6N
58	1W	201	EHZ	C16-C17-C20-O6
58	1W	201	EHZ	C18-C17-C20-O6
58	1W	201	EHZ	C19-C17-C20-O6
58	1W	201	EHZ	O2-C9-S1-C10
58	1W	201	EHZ	C8-C9-S1-C10
58	1n	201	EHZ	S1-C10-C11-N1
58	1n	201	EHZ	N2-C15-C16-C17
58	1n	201	EHZ	N2-C15-C16-O5
58	1n	201	EHZ	O4-C15-C16-C17
58	1n	201	EHZ	O4-C15-C16-O5
58	1n	201	EHZ	C15-C16-C17-C18
58	1n	201	EHZ	C15-C16-C17-C19
58	1n	201	EHZ	C15-C16-C17-C20
58	1n	201	EHZ	O2-C9-S1-C10
58	1n	201	EHZ	C8-C9-S1-C10
52	1M	501	PGT	C32-C31-O2-C2
45	1Y	201	3PE	C2-C1-O11-P
58	1n	201	EHZ	C13-C14-N2-C15
53	1N	402	CDL	OA6-CA4-CA6-OA8
52	1M	501	PGT	C15-C16-C17-C18
52	1M	501	PGT	C14-C15-C16-C17
50	1f	101	PC1	C35-C36-C37-C38
52	1M	501	PGT	C40-C41-C42-C43
56	1P	501	NDP	O4D-C4D-C5D-O5D
56	1P	501	NDP	C3D-C4D-C5D-O5D
52	1M	501	PGT	C34-C35-C36-C37
50	1I	203	PC1	O21-C2-C3-O31
52	1M	501	PGT	C44-C45-C46-C47
52	1M	501	PGT	C22-C23-C24-C25
56	1P	501	NDP	O4B-C4B-C5B-O5B
45	1Y	201	3PE	C35-C36-C37-C38
50	1I	203	PC1	C1-C2-C3-O31
50	1H	401	PC1	C24-C25-C26-C27
45	1L	704	3PE	O11-C1-C2-O21
50	1M	502	PC1	O11-C1-C2-C3
53	1N	402	CDL	CA3-CA4-CA6-OA8
45	1Y	201	3PE	C3C-C3D-C3E-C3F
53	1a	101	CDL	CA4-CA3-OA5-PA1
45	1N	401	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
45	1A	201	3PE	O21-C2-C3-O31
53	1N	402	CDL	C75-C76-C77-C78
52	1M	501	PGT	C21-C22-C23-C24
53	1N	402	CDL	OA5-CA3-CA4-CA6
50	1I	203	PC1	C32-C33-C34-C35
45	1Y	201	3PE	O11-C1-C2-O21
50	1M	502	PC1	O11-C1-C2-O21
45	1N	401	3PE	C2-C3-O31-C31
58	1n	201	EHZ	C2-C1-C21-C22
45	1Y	201	3PE	C12-C11-O13-P
50	1H	401	PC1	O21-C2-C3-O31
50	1J	201	PC1	O21-C2-C3-O31
53	1a	101	CDL	OB6-CB4-CB6-OB8
50	1J	201	PC1	O13-C11-C12-N
53	1N	402	CDL	C32-C33-C34-C35
48	1F	501	FMN	N10-C1'-C2'-O2'
52	1M	501	PGT	C33-C34-C35-C36
50	1H	401	PC1	C1-C2-C3-O31
53	1N	402	CDL	C55-C56-C57-C58
45	1N	401	3PE	C34-C35-C36-C37
50	1M	502	PC1	C1-O11-P-O12
50	1M	502	PC1	C1-O11-P-O13
50	1f	101	PC1	C11-O13-P-O14
52	1M	501	PGT	C4-O4P-P-O1P
53	1a	101	CDL	CB2-OB2-PB2-OB3
56	1P	501	NDP	C5B-O5B-PA-O3
58	1n	201	EHZ	O5-C16-C17-C20
45	1L	703	3PE	C31-C32-C33-C34
45	1N	401	3PE	C2-C1-O11-P
53	1a	101	CDL	C52-C51-CB5-OB6
45	1L	704	3PE	C1-C2-C3-O31
54	1O	401	GTP	PG-O3B-PB-O1B
50	1H	401	PC1	O31-C31-C32-C33
53	1N	402	CDL	CB2-C1-CA2-OA2
45	1Y	201	3PE	O11-C1-C2-C3
45	1L	702	3PE	C33-C34-C35-C36
52	1M	501	PGT	O2-C2-C3-O3
45	1A	201	3PE	C32-C33-C34-C35
45	1L	704	3PE	C1-C2-O21-C21
45	1N	401	3PE	C3A-C3B-C3C-C3D
50	1M	502	PC1	C25-C26-C27-C28
52	1M	501	PGT	C2-C1-O3P-P

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Mol	Chain	Res	Type	Atoms
53	1N	402	CDL	OA5-CA3-CA4-OA6
58	1n	201	EHZ	C12-C13-C14-N2
53	1N	402	CDL	C53-C54-C55-C56
54	1O	401	GTP	C4'-C5'-O5'-PA
45	1Y	201	3PE	C24-C25-C26-C27
53	1a	101	CDL	CB2-C1-CA2-OA2
45	1A	201	3PE	C1-C2-C3-O31
53	1a	101	CDL	CB3-CB4-CB6-OB8
50	1M	502	PC1	C31-C32-C33-C34
45	1N	401	3PE	C39-C3A-C3B-C3C
45	1L	702	3PE	C37-C38-C39-C3A
54	1O	401	GTP	PG-O3B-PB-O2B
56	1P	501	NDP	PN-O3-PA-O2A
52	1M	501	PGT	C19-C20-C21-C22
45	1N	401	3PE	O11-C1-C2-O21
50	1f	101	PC1	C3C-C3D-C3E-C3F
50	1J	201	PC1	C1-C2-C3-O31
52	1M	501	PGT	C1-C2-C3-O3
45	1L	703	3PE	C32-C33-C34-C35
48	1F	501	FMN	N10-C1'-C2'-C3'
45	1L	704	3PE	C22-C23-C24-C25
51	1L	701	MYR	C5-C6-C7-C8
50	1H	401	PC1	C3E-C3F-C3G-C3H
50	1f	101	PC1	C2-C1-O11-P
53	1a	101	CDL	C12-C13-C14-C15
58	1n	201	EHZ	C4-C5-C6-C7
58	1W	201	EHZ	C21-C22-C23-C24
56	1P	501	NDP	PN-O3-PA-O1A

There are no ring outliers.

22 monomers are involved in 82 short contacts:

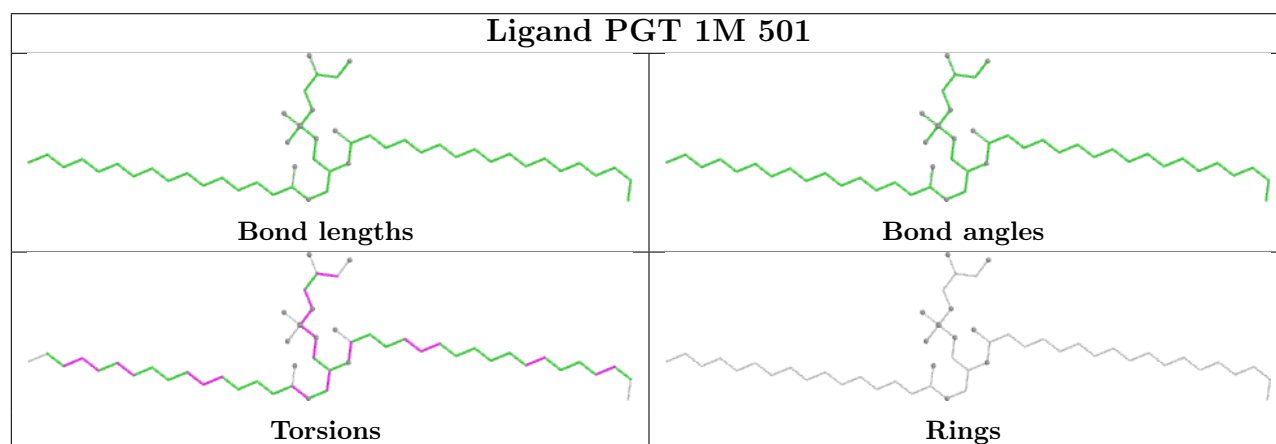
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1F	502	SF4	1	0
52	1M	501	PGT	8	0
48	1F	501	FMN	4	0
46	1B	201	SF4	2	0
45	1A	201	3PE	4	0
50	1J	201	PC1	2	0
46	1G	801	SF4	1	0
45	1L	704	3PE	6	0
51	1L	701	MYR	2	0

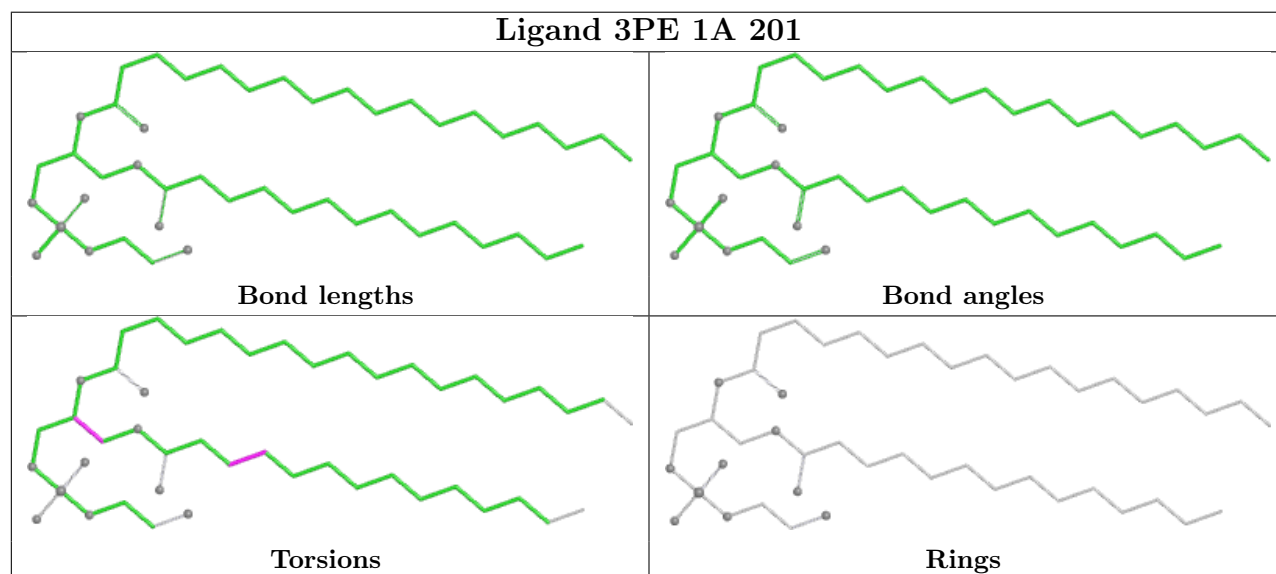
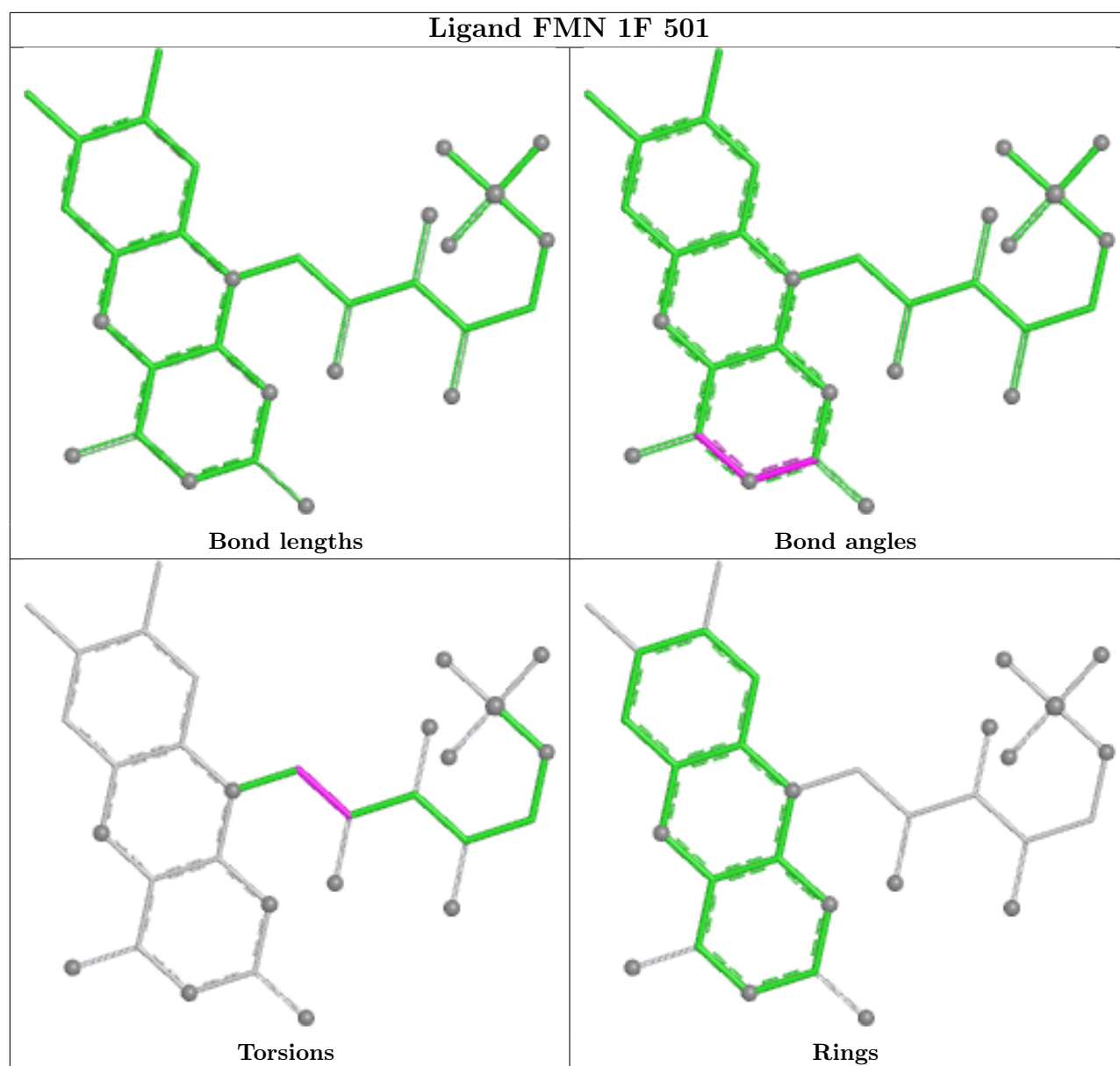
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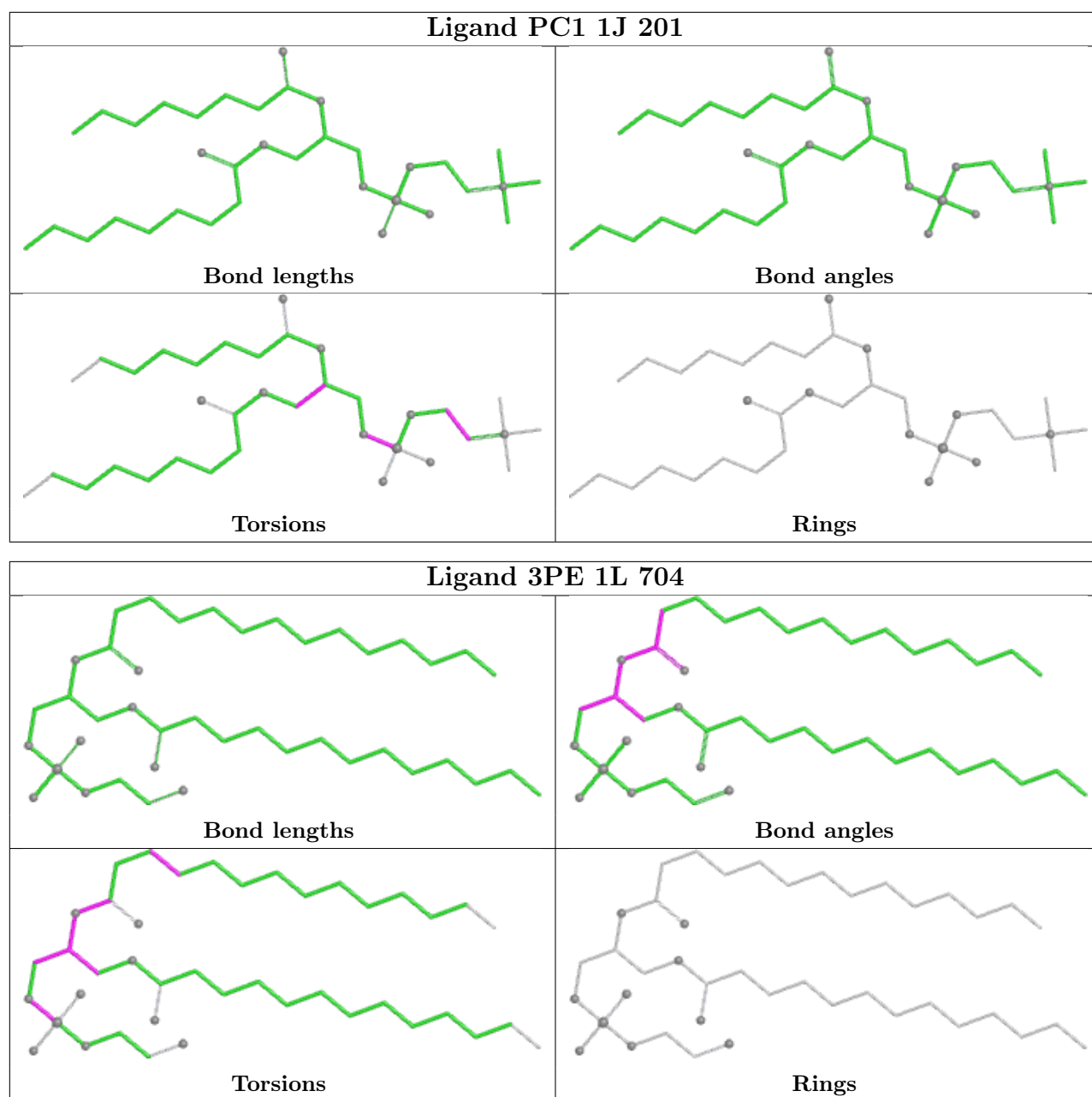
Continued from previous page...

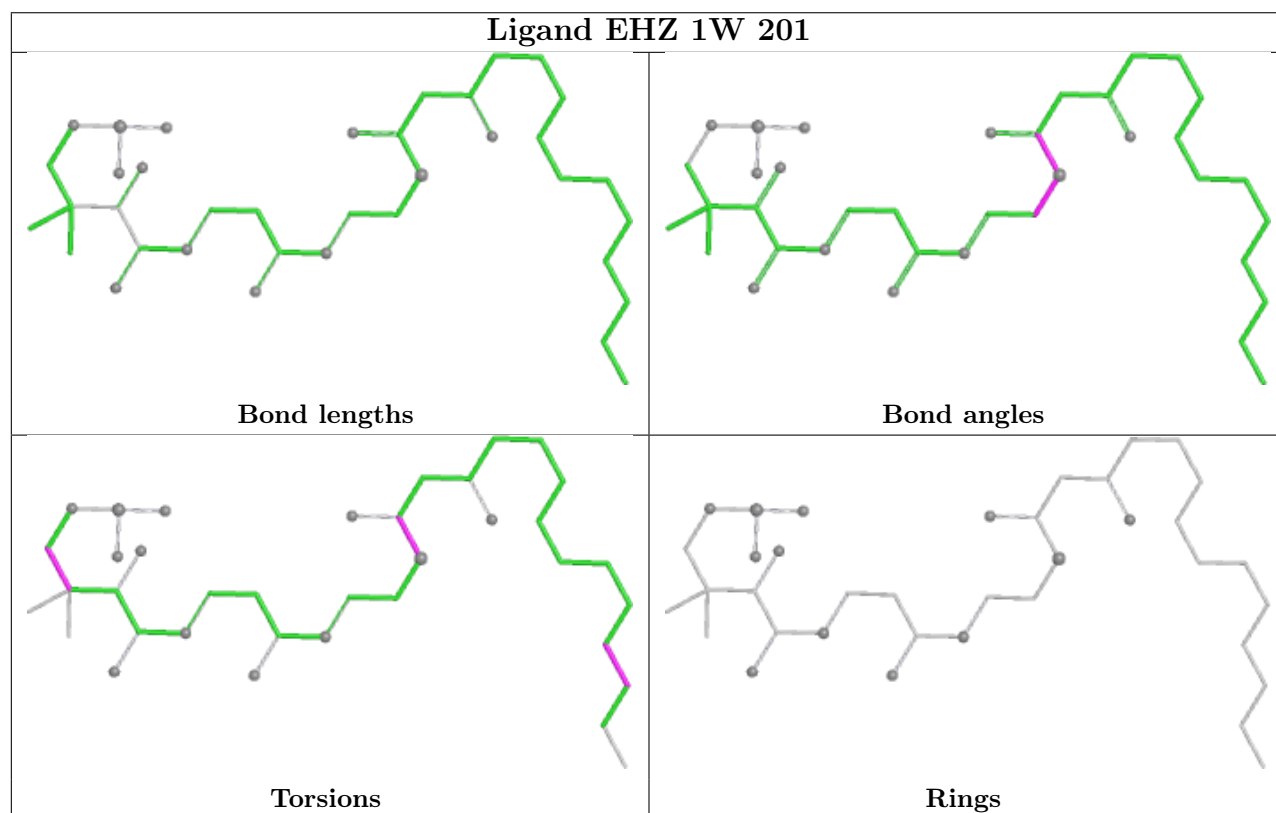
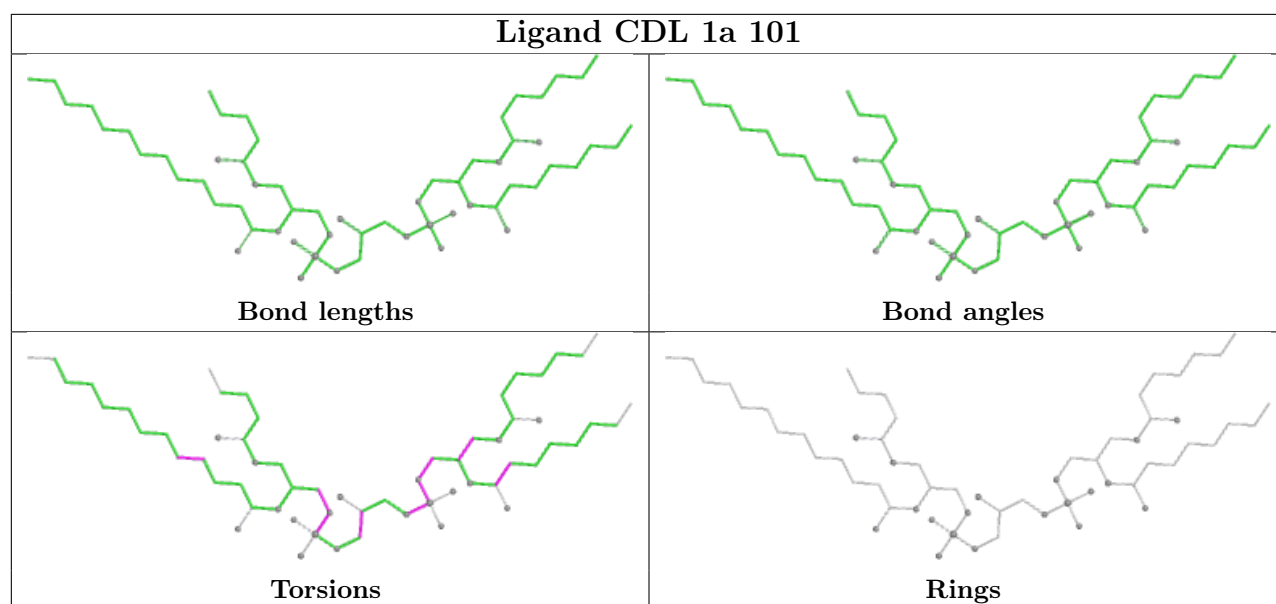
Mol	Chain	Res	Type	Clashes	Symm-Clashes
53	1a	101	CDL	4	0
45	1L	703	3PE	6	0
50	1f	101	PC1	6	0
53	1N	402	CDL	2	0
50	1M	502	PC1	2	0
46	1I	201	SF4	2	0
45	1N	401	3PE	6	0
45	1Y	201	3PE	1	0
54	1O	401	GTP	3	0
50	1H	401	PC1	7	0
45	1L	702	3PE	6	0
56	1P	501	NDP	5	0
50	1I	203	PC1	2	0

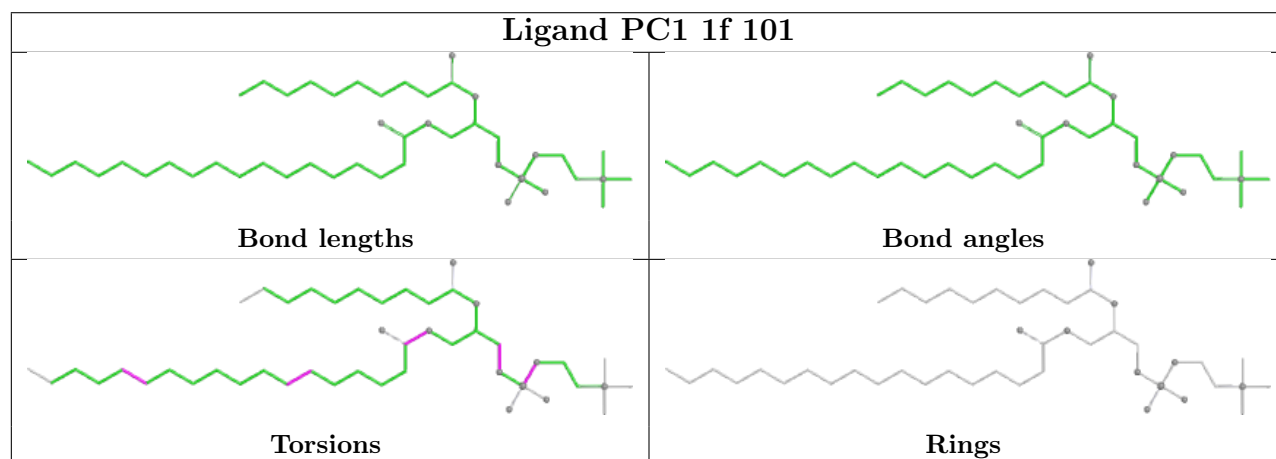
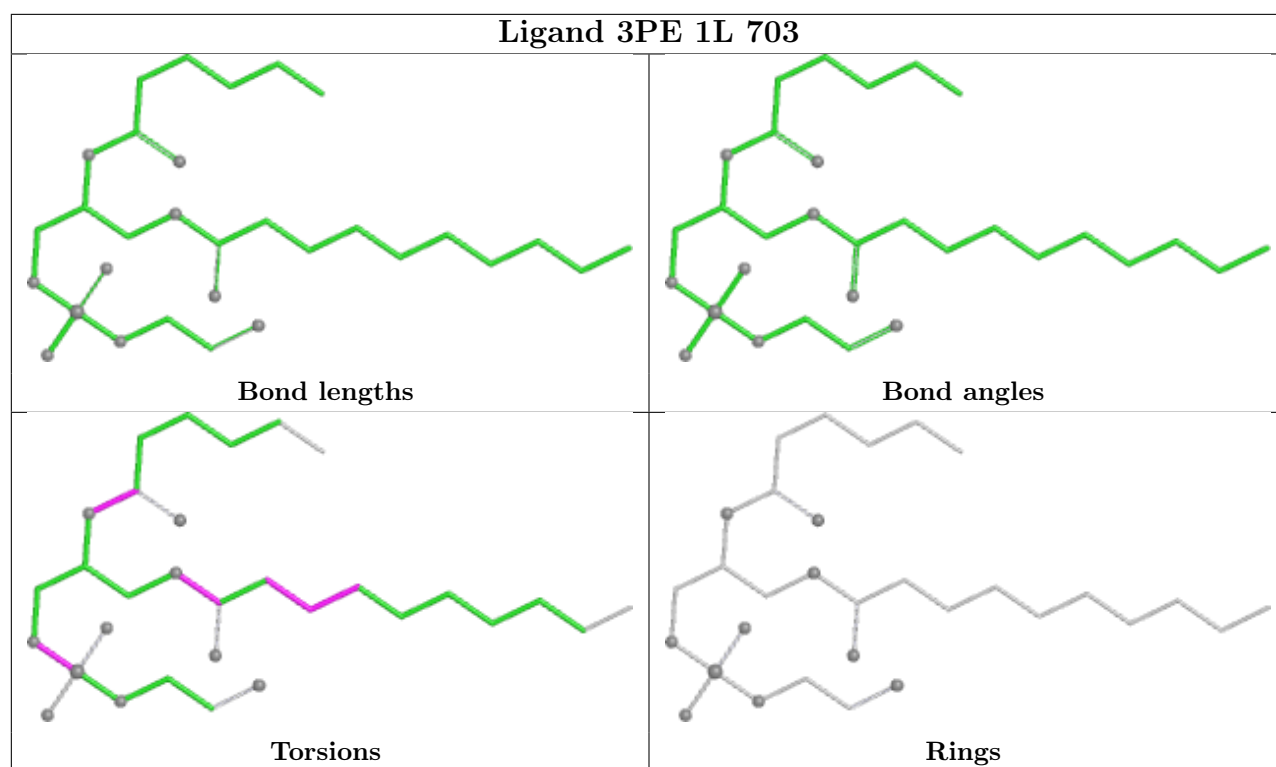
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

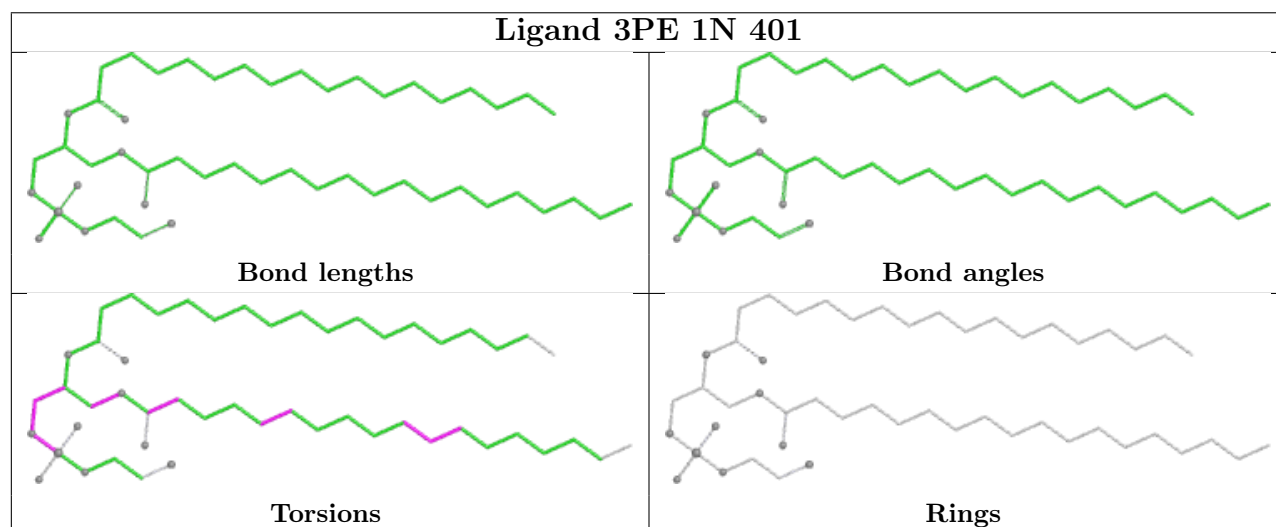
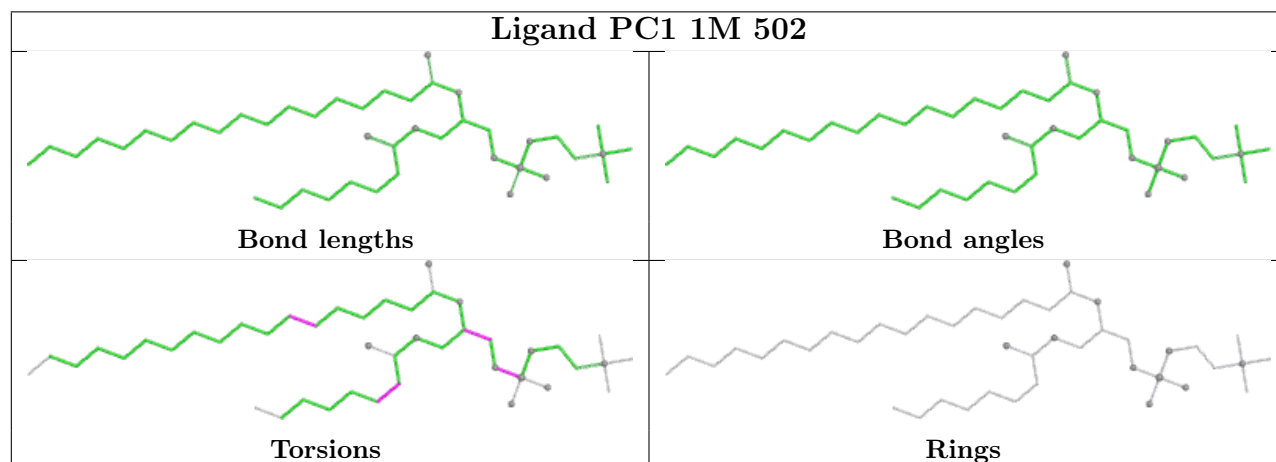
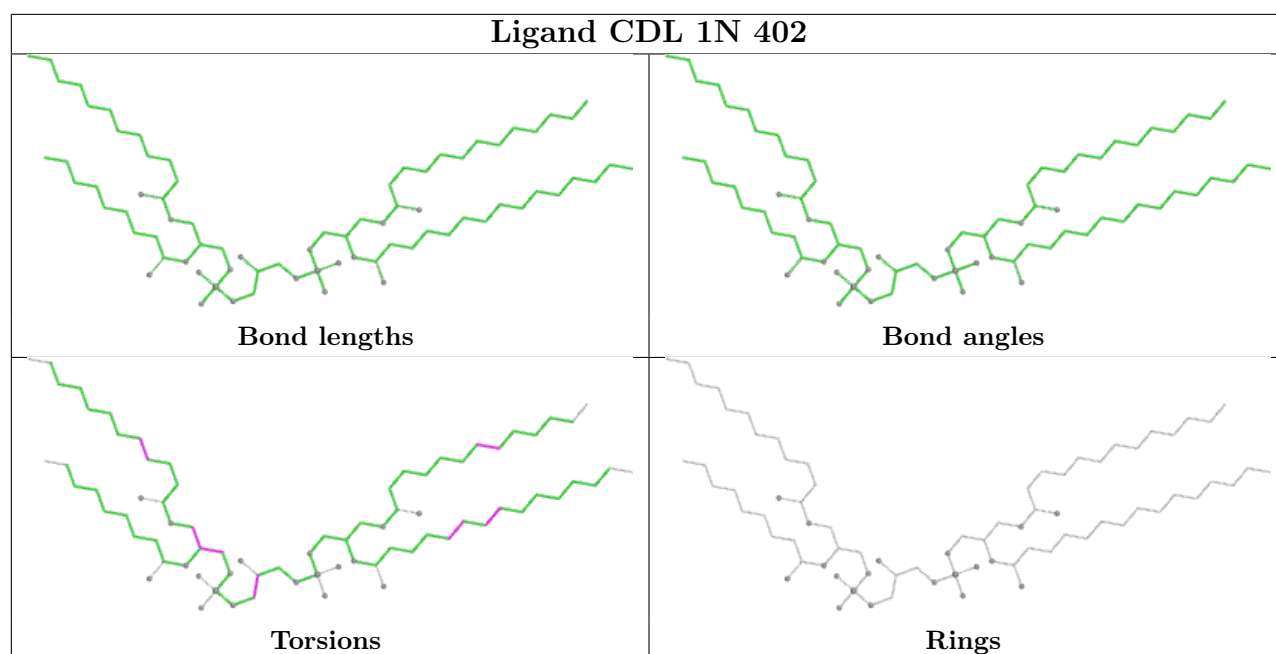


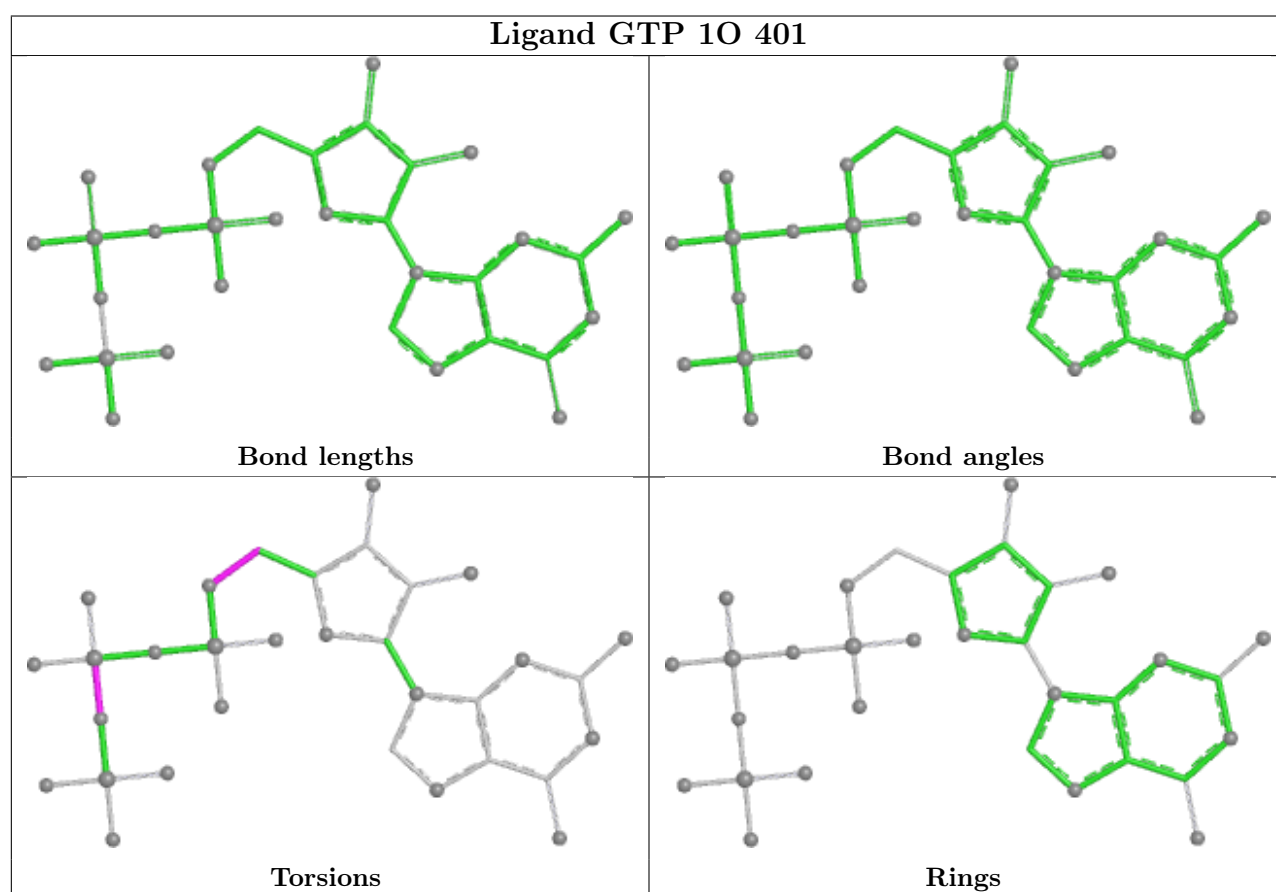
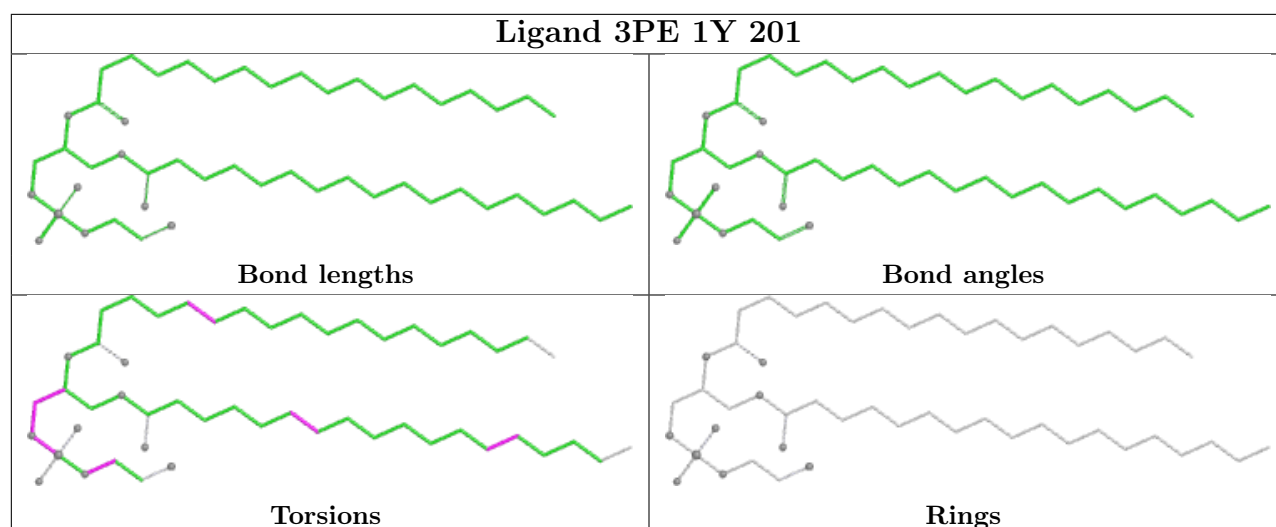


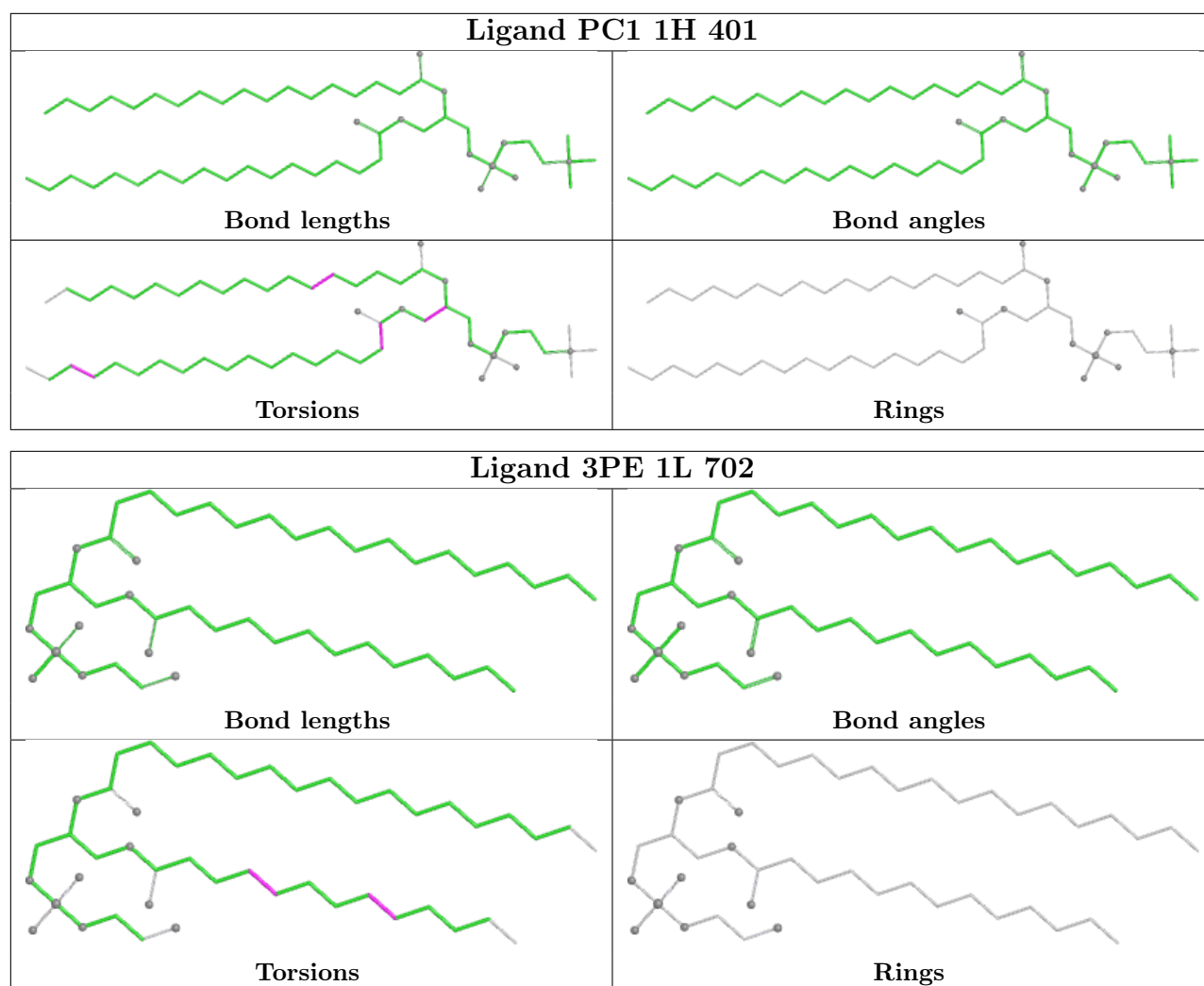


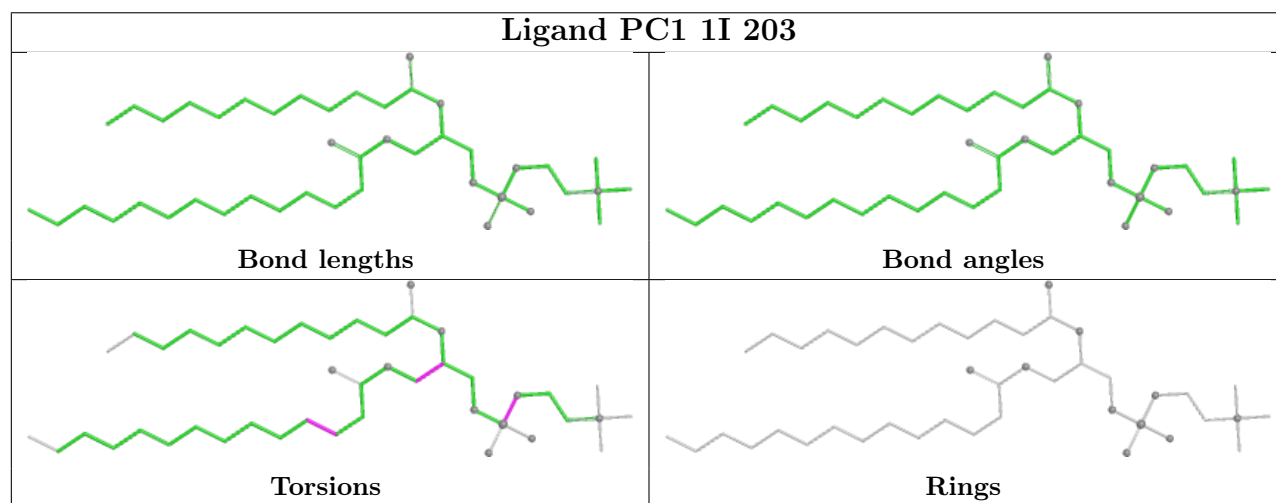
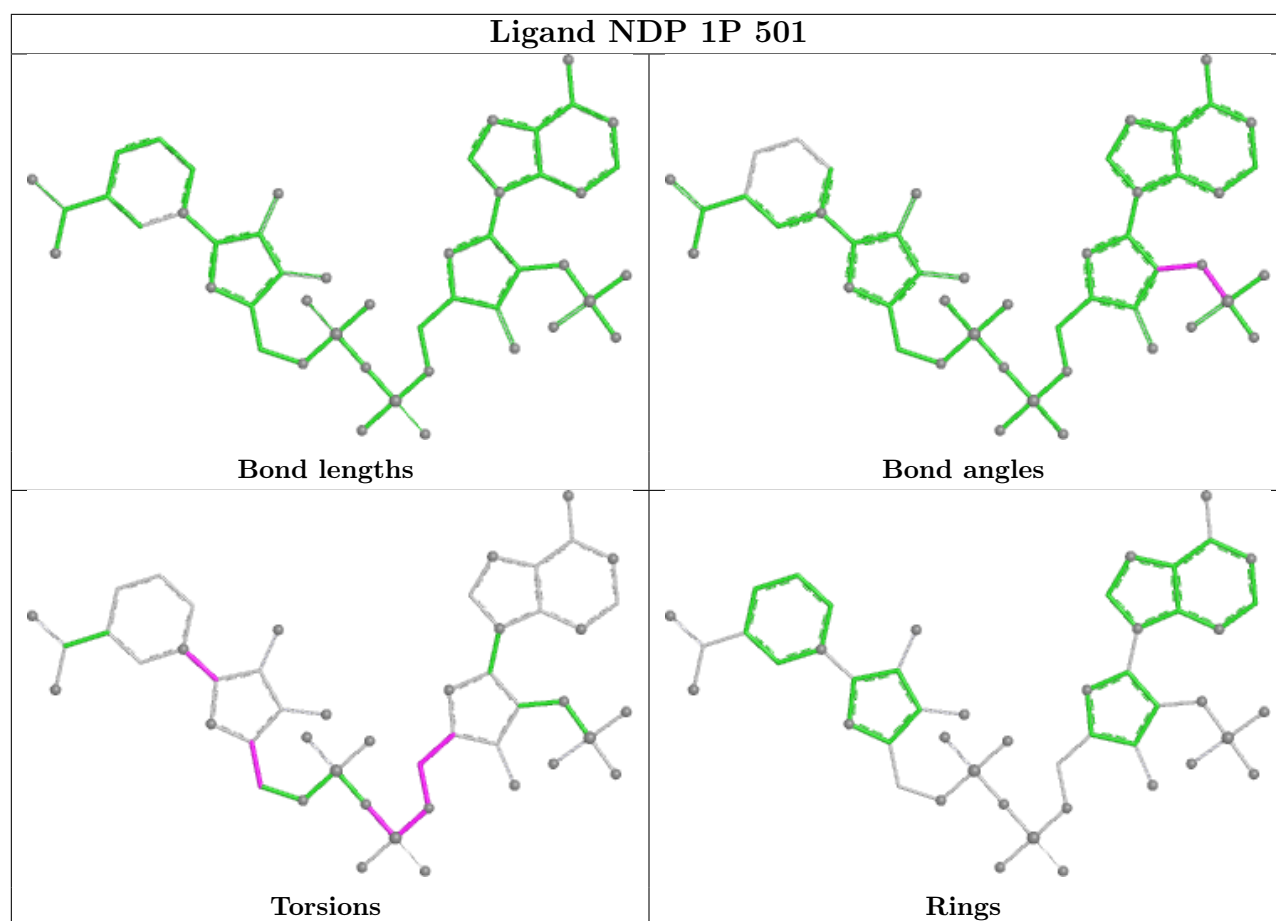


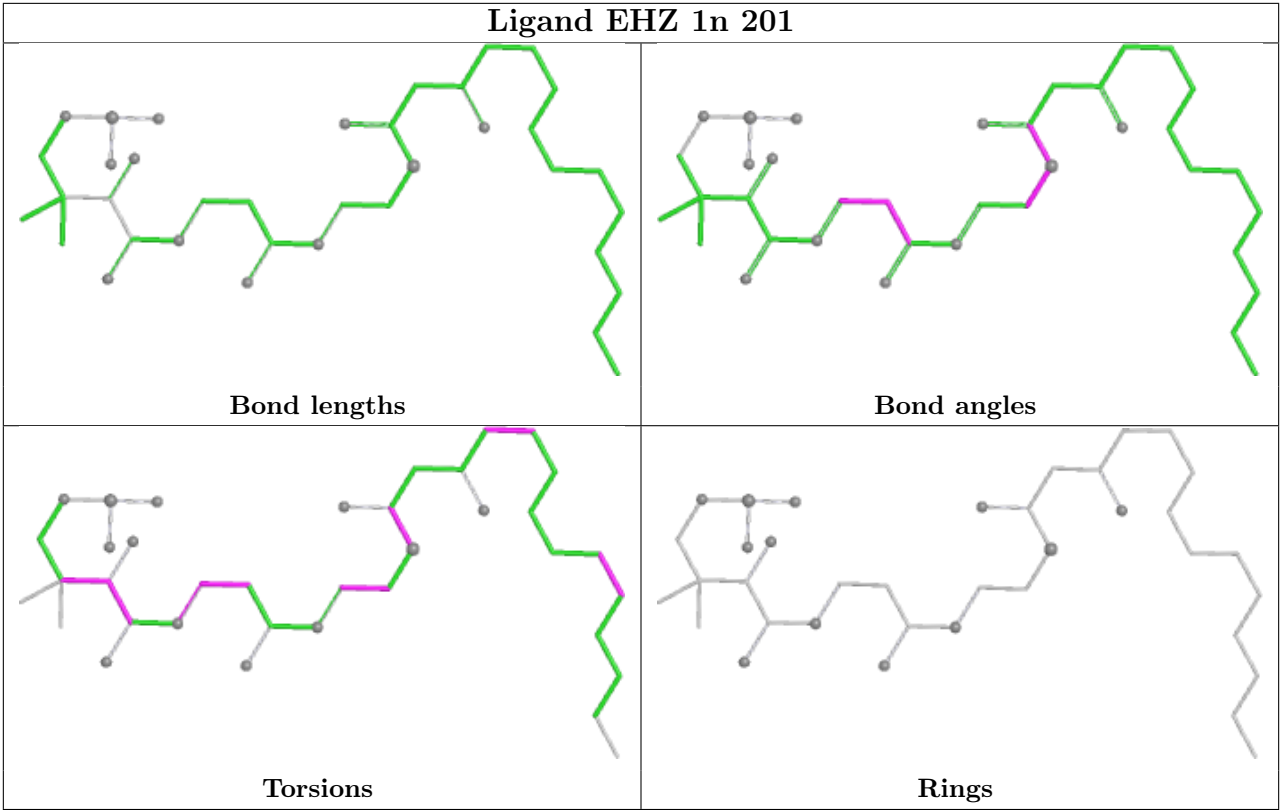












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	3.33
1	1r	1:ALA	C	2:SER	N	2.79

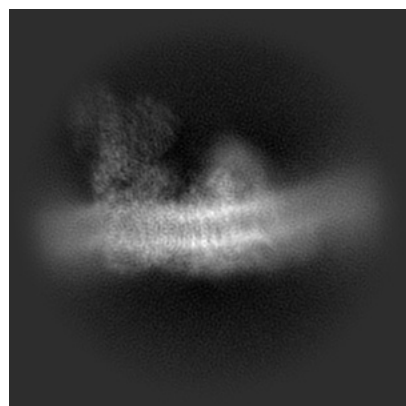
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42170. These allow visual inspection of the internal detail of the map and identification of artifacts.

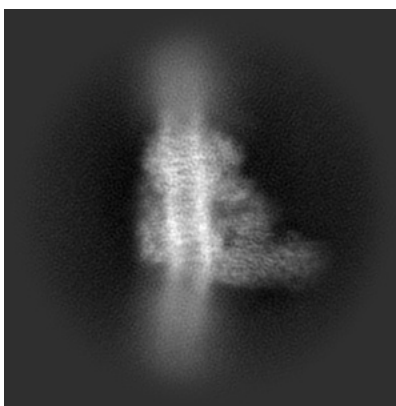
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

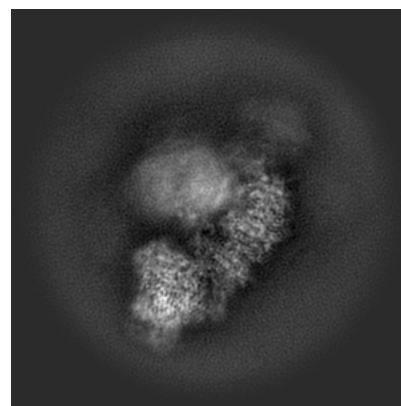
6.1.1 Primary map



X

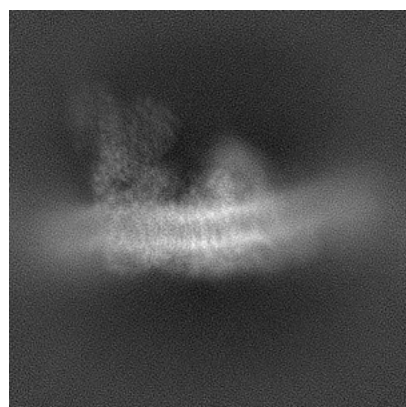


Y

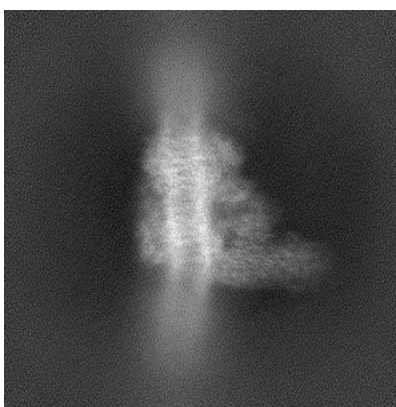


Z

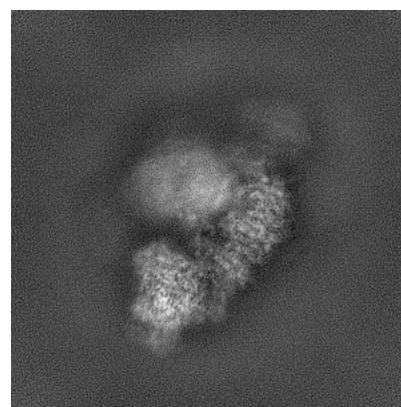
6.1.2 Raw map



X



Y

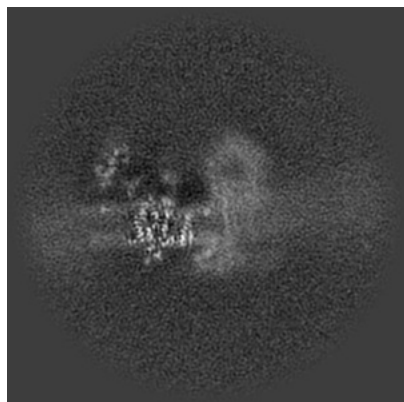


Z

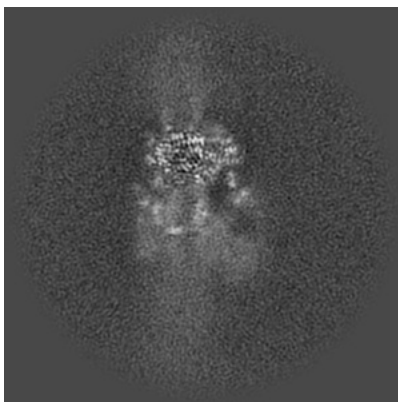
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

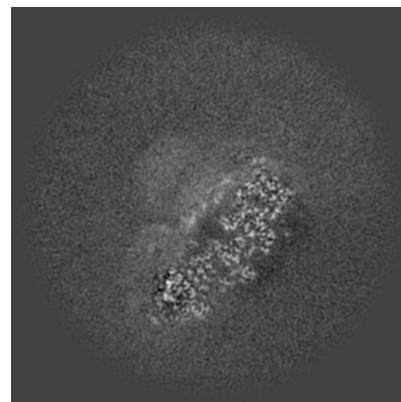
6.2.1 Primary map



X Index: 160



Y Index: 160

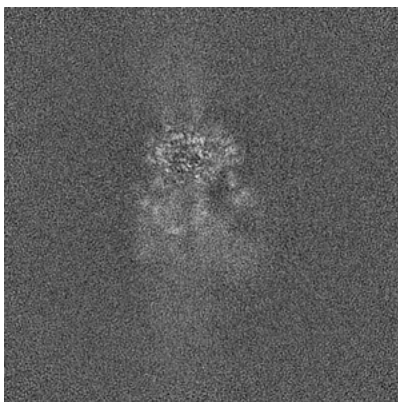


Z Index: 160

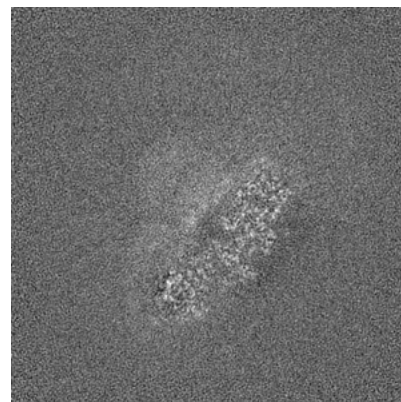
6.2.2 Raw map



X Index: 160



Y Index: 160

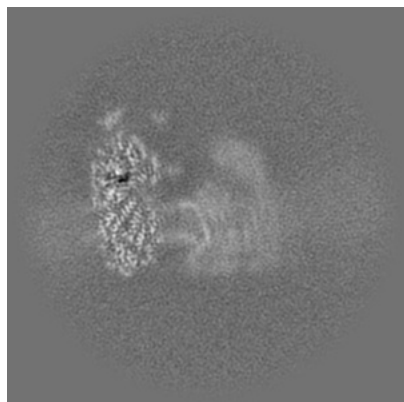


Z Index: 160

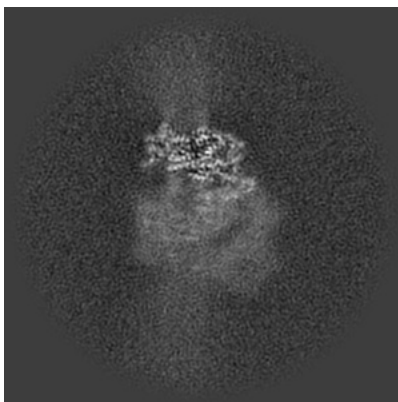
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

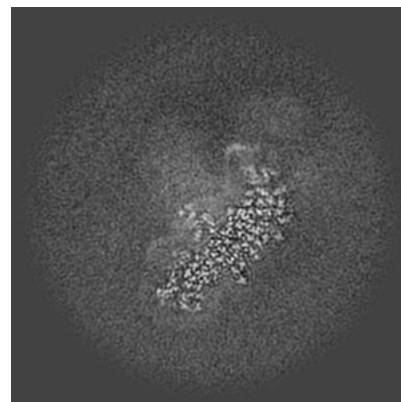
6.3.1 Primary map



X Index: 140

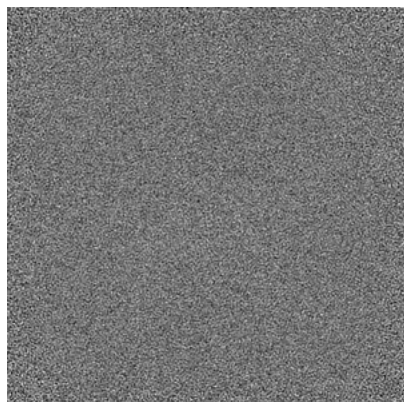


Y Index: 172

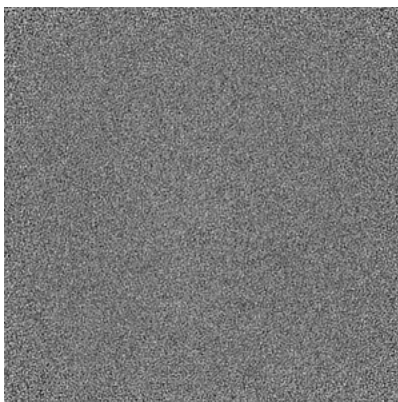


Z Index: 134

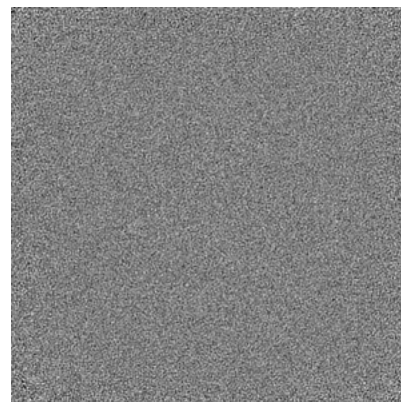
6.3.2 Raw map



X Index: 0



Y Index: 0

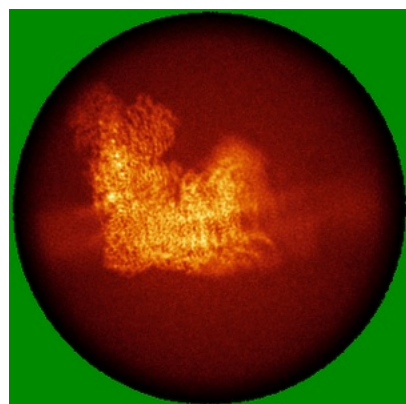


Z Index: 0

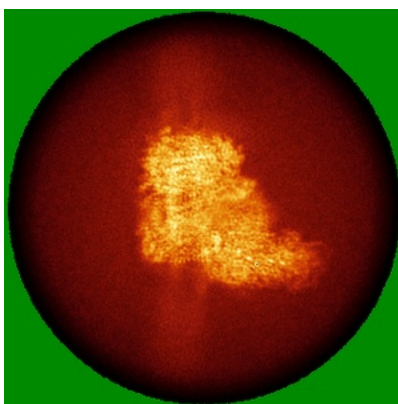
The images above show the largest variance slices of the map in three orthogonal directions.

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

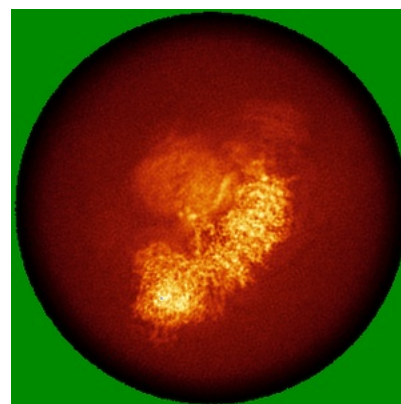
6.4.1 Primary map



X

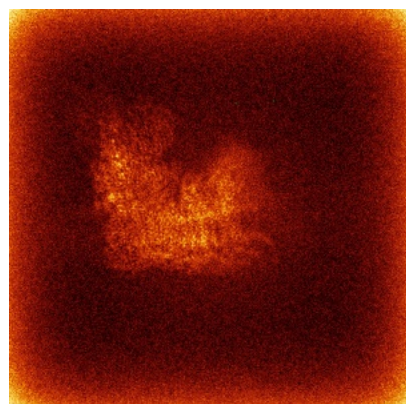


Y

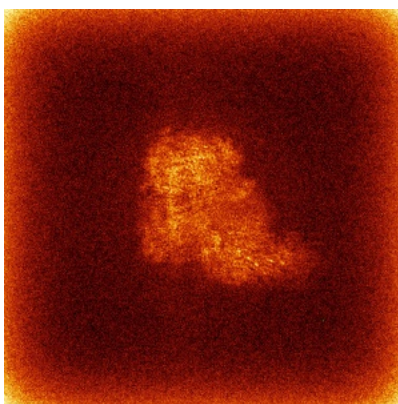


Z

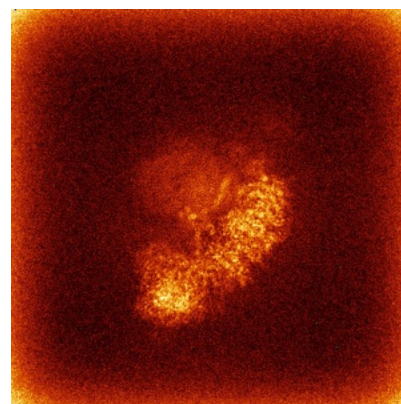
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

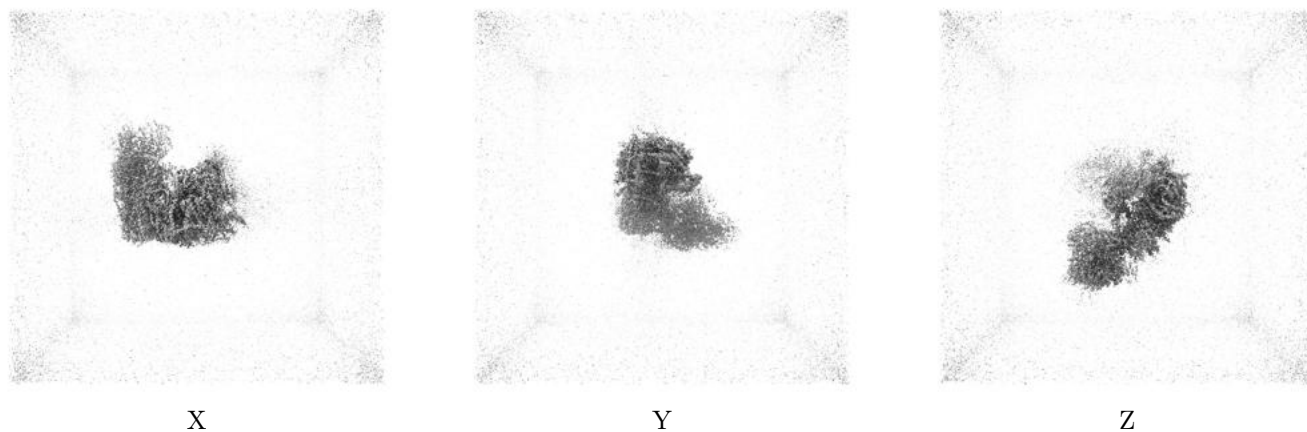
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

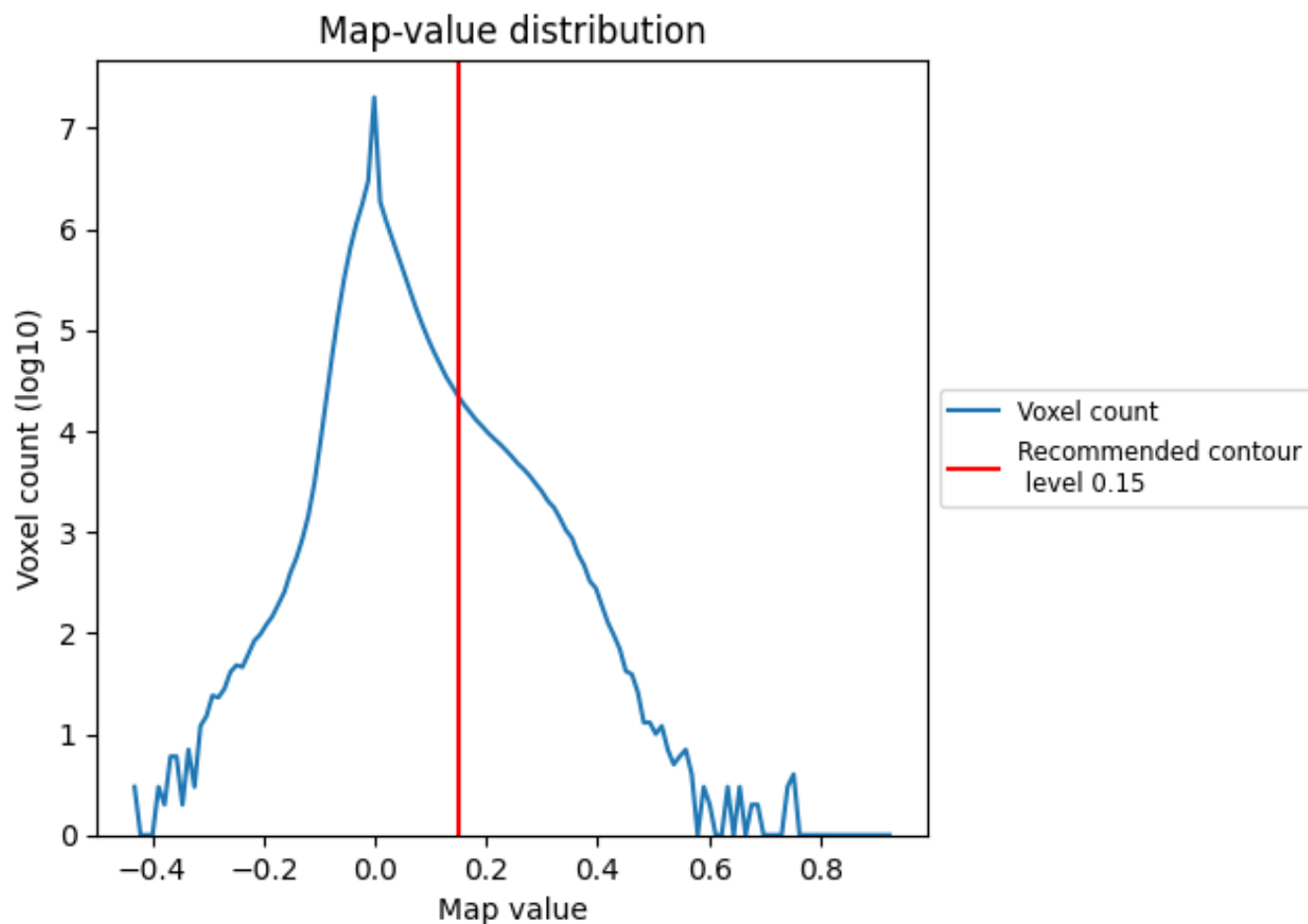
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

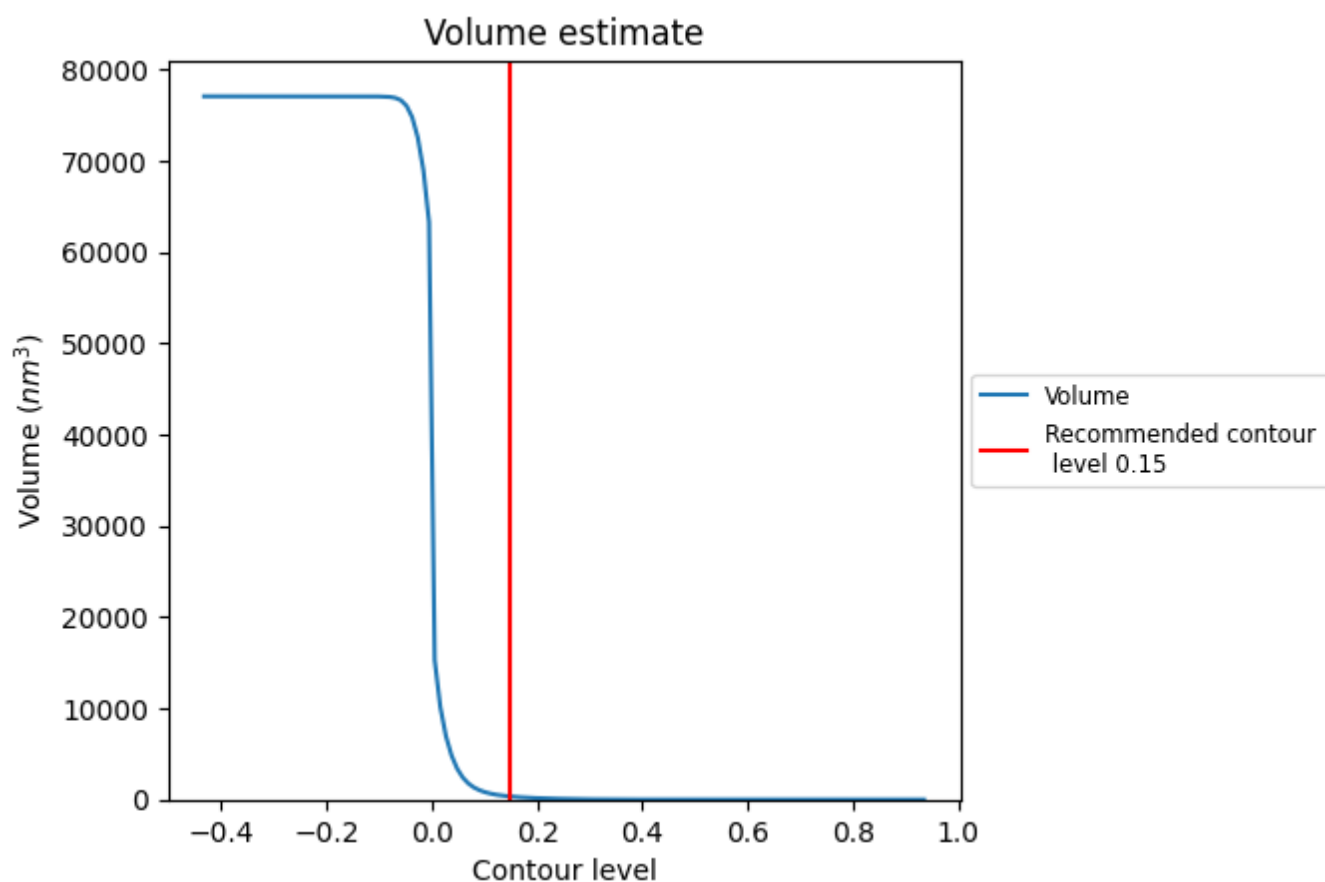
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

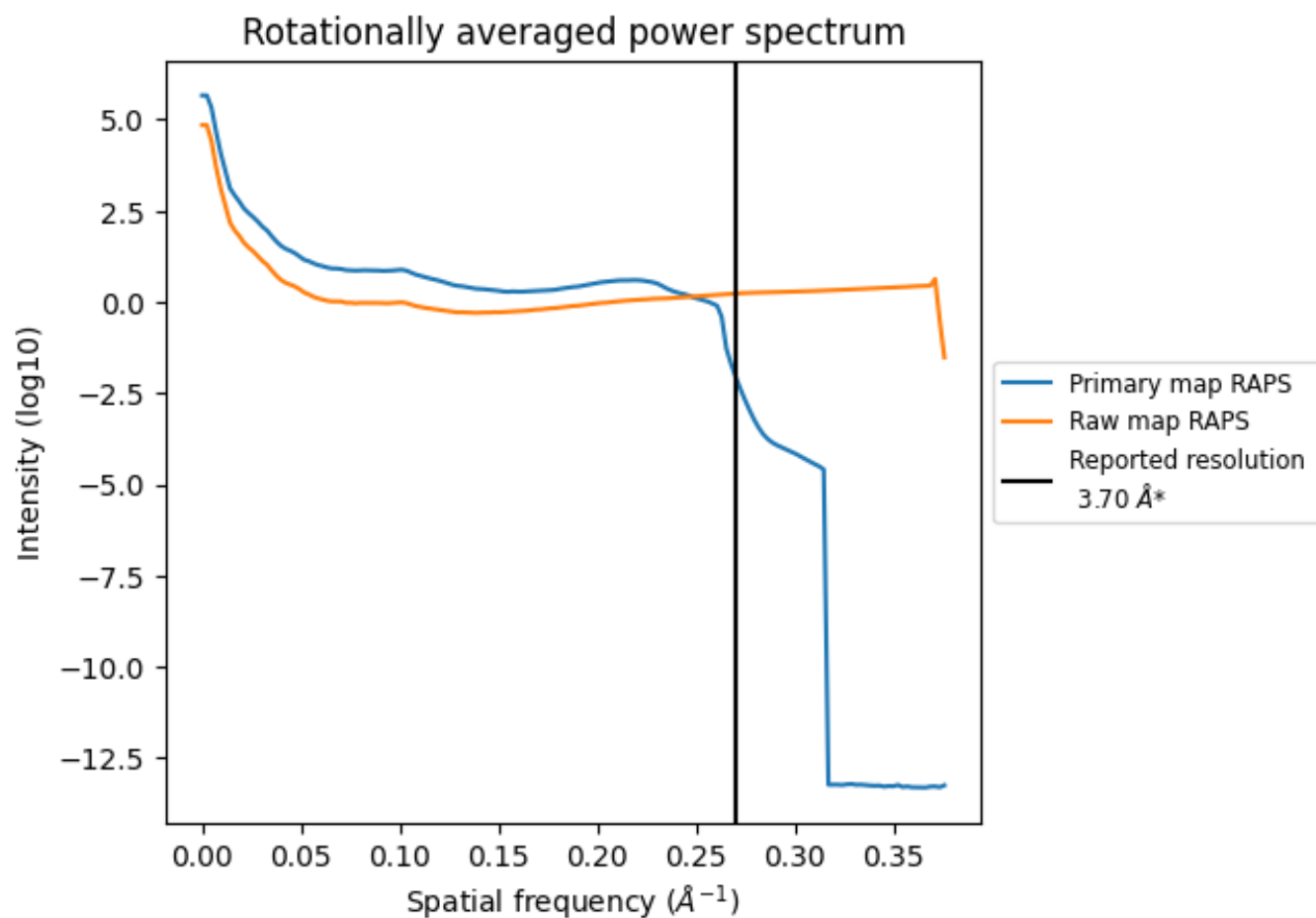
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 337 nm³; this corresponds to an approximate mass of 304 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 ⓘ

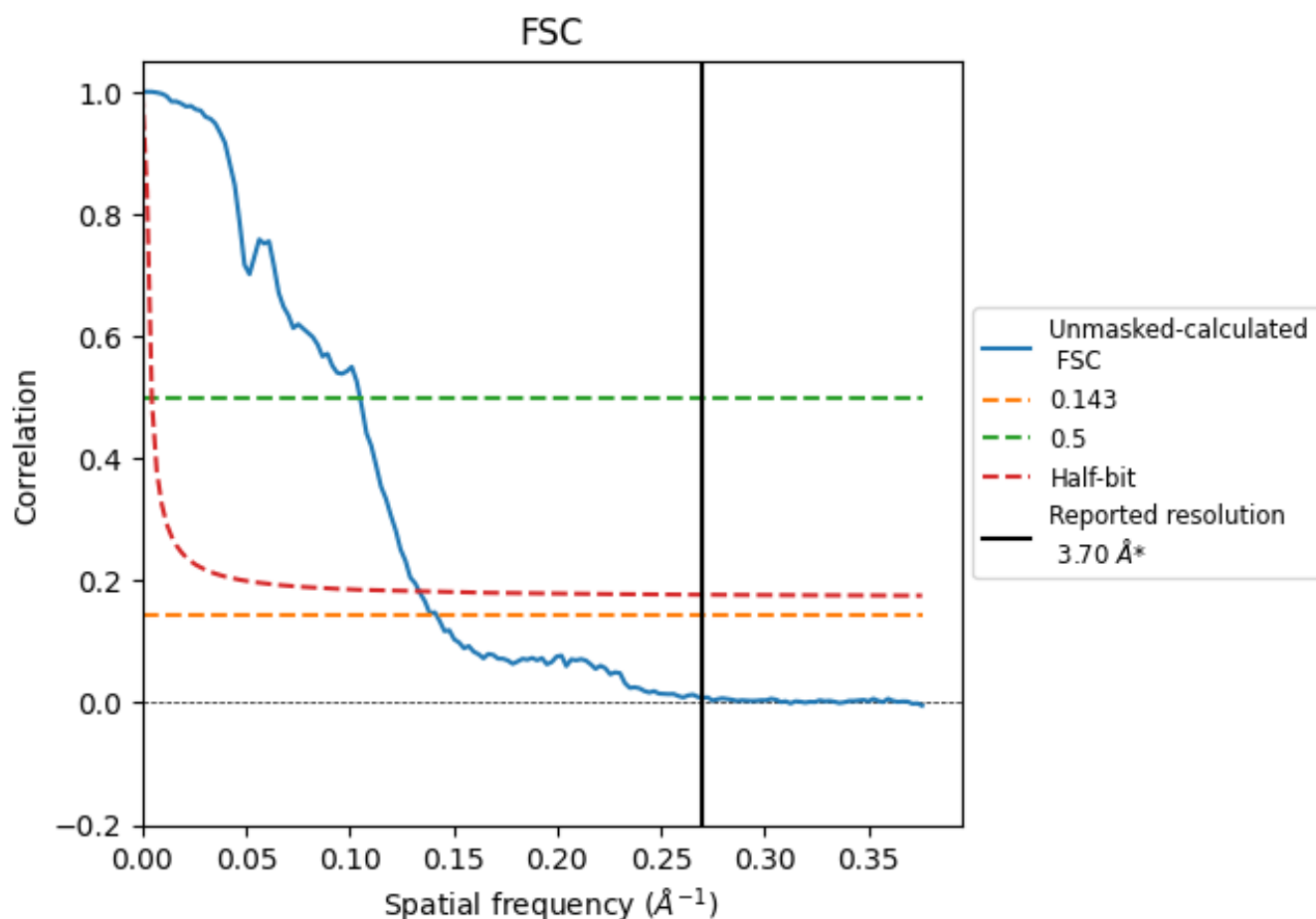


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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](#)

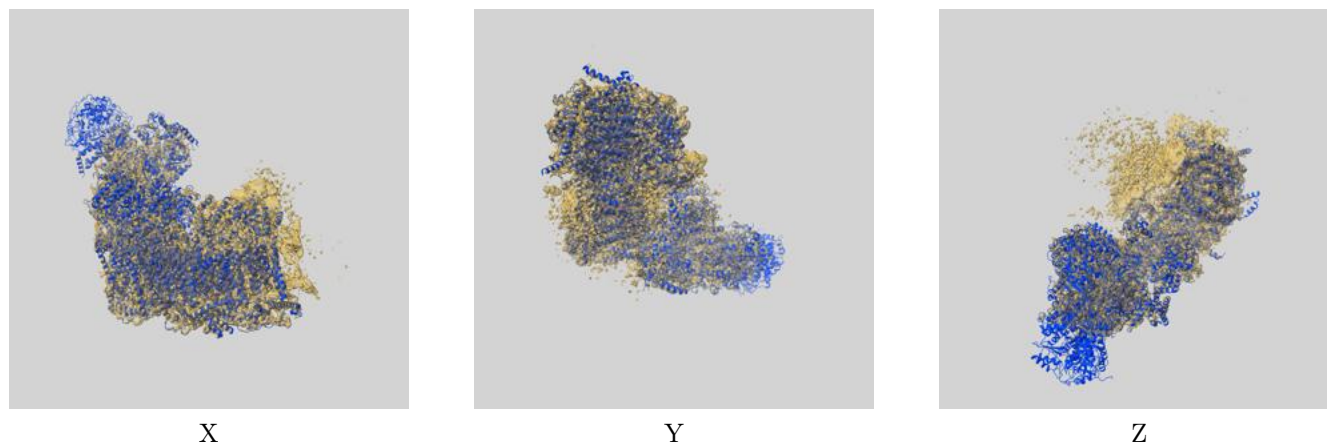
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.05	9.53	7.49

*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 7.05 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

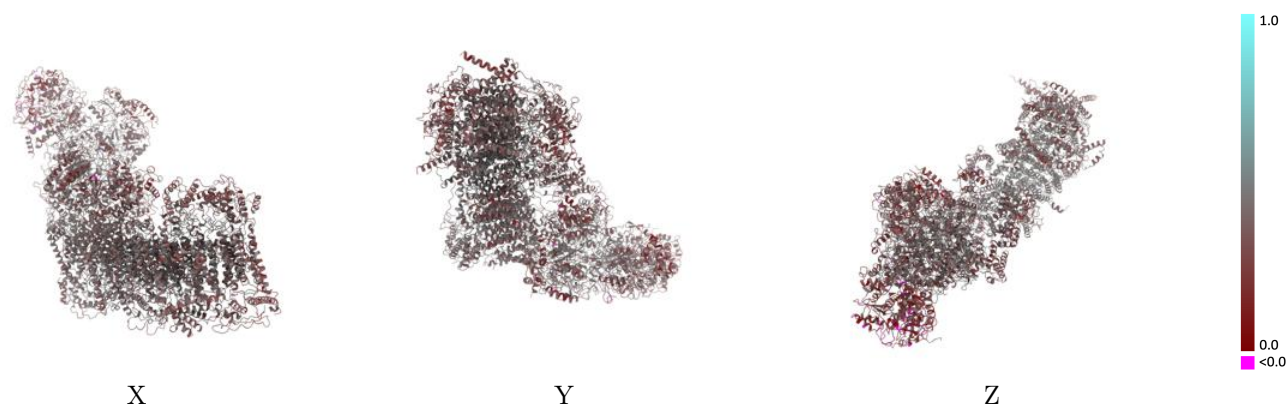
This section contains information regarding the fit between EMDB map EMD-42170 and PDB model 8UET. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



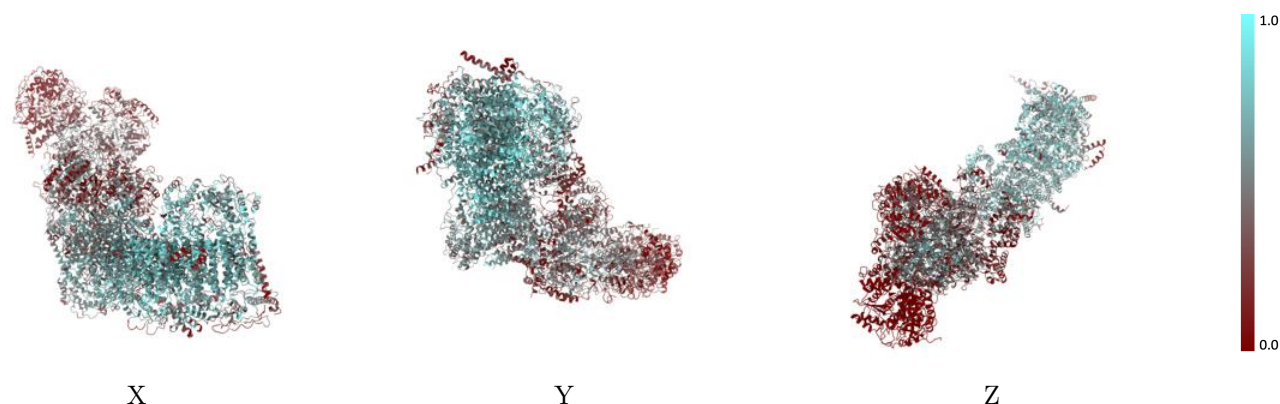
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



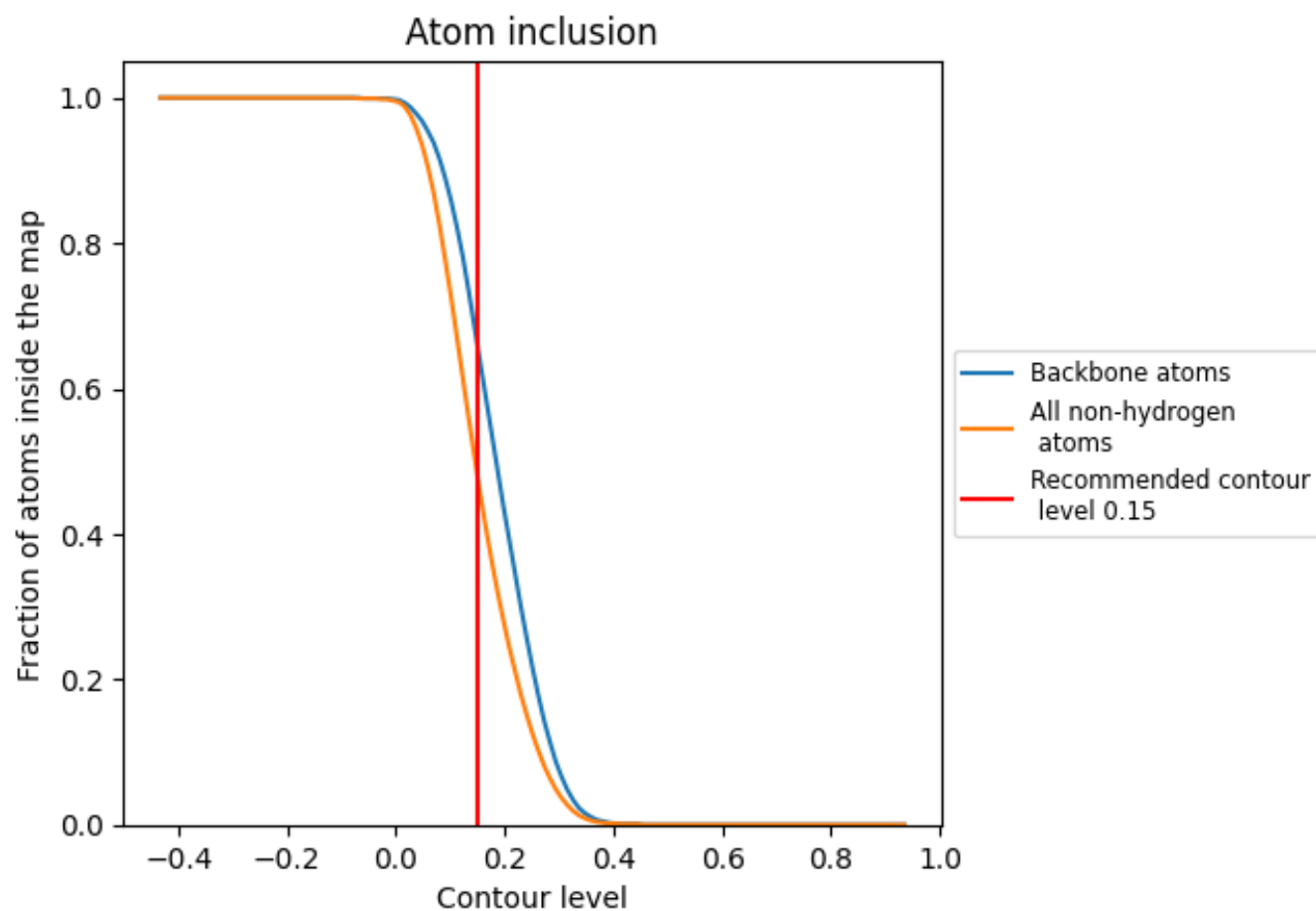
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 48% 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	 0.4800	 0.3770
1A	 0.4830	 0.4010
1B	 0.5470	 0.4180
1C	 0.3960	 0.4030
1D	 0.4800	 0.3900
1E	 0.0280	 0.2870
1F	 0.0360	 0.2590
1G	 0.2840	 0.3580
1H	 0.6170	 0.4070
1I	 0.5820	 0.4160
1J	 0.5090	 0.3870
1K	 0.6140	 0.4060
1L	 0.7190	 0.4070
1M	 0.7590	 0.4370
1N	 0.6800	 0.4280
1O	 0.3880	 0.3560
1P	 0.2990	 0.3370
1Q	 0.3150	 0.3830
1R	 0.2950	 0.4120
1S	 0.1410	 0.2900
1T	 0.2340	 0.2780
1U	 0.6150	 0.3370
1V	 0.2060	 0.3380
1W	 0.3060	 0.3340
1X	 0.5480	 0.4050
1Y	 0.6740	 0.3790
1Z	 0.5480	 0.4150
1a	 0.6110	 0.4090
1b	 0.5370	 0.4110
1c	 0.4680	 0.3690
1d	 0.6670	 0.4240
1e	 0.5960	 0.4280
1f	 0.4620	 0.3840
1g	 0.6020	 0.3950
1h	 0.6730	 0.4090



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Chain	Atom inclusion	Q-score
1i	 0.3890	 0.3470
1j	 0.5240	 0.3740
1k	 0.5120	 0.3590
1l	 0.6540	 0.3980
1m	 0.7090	 0.3890
1n	 0.6720	 0.3670
1o	 0.5030	 0.3170
1p	 0.6070	 0.3830
1q	 0.4470	 0.4090
1r	 0.3790	 0.4020
1s	 0.0000	 0.2520