



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 07:49 PM UTC

PDB ID : 8UEX / pdb_00008uex
EMDB ID : EMD-42174
Title : In-situ complex I, Deactive class06
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

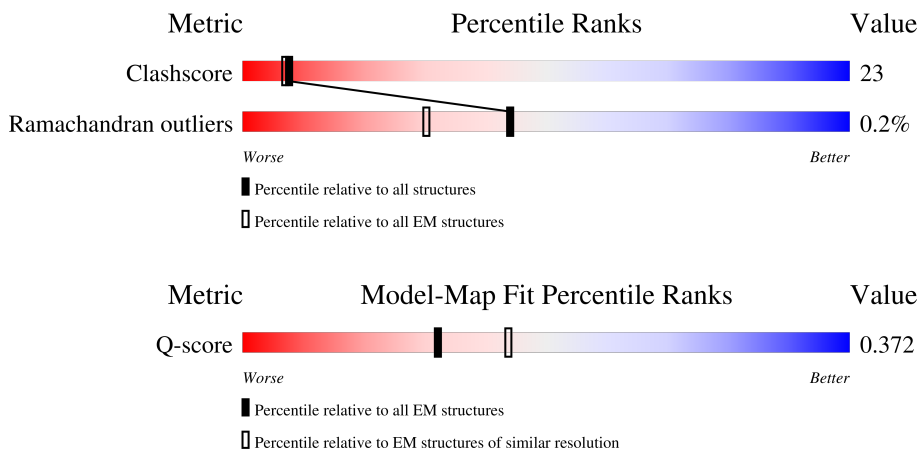
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 3.90 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	-
Q-score	-	25397	8855 (3.40 - 4.40)

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	
5	1E	249	

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Mol	Chain	Length	Quality of chain
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	
29	1d	123	

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Mol	Chain	Length	Quality of chain
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	1F	502	-	-	X	-
48	FES	1E	301	-	-	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	88	Total	C	N	O	S	0	0
			707	484	101	117	5		

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	1D	418	Total	C	N	O	S	0	0
			3369	2155	574	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	0	0
			1062	691	182	189		

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

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

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

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

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

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

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

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

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

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

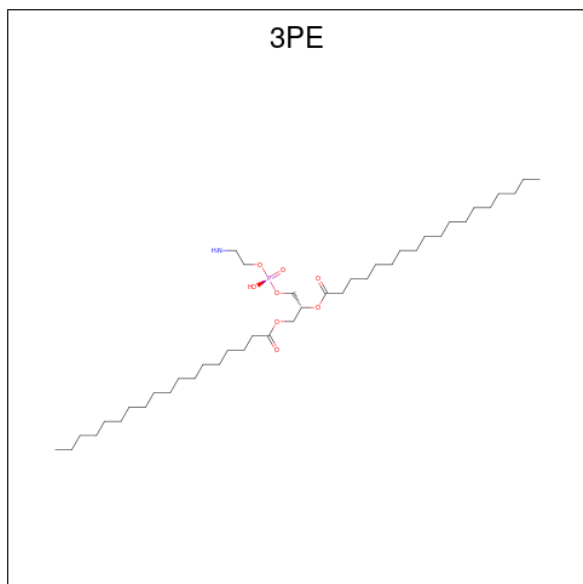
There is a discrepancy between the modelled and reference sequences:

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

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

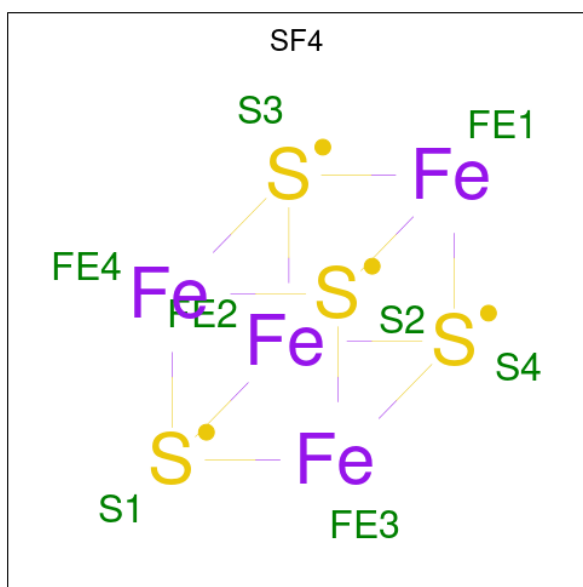
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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



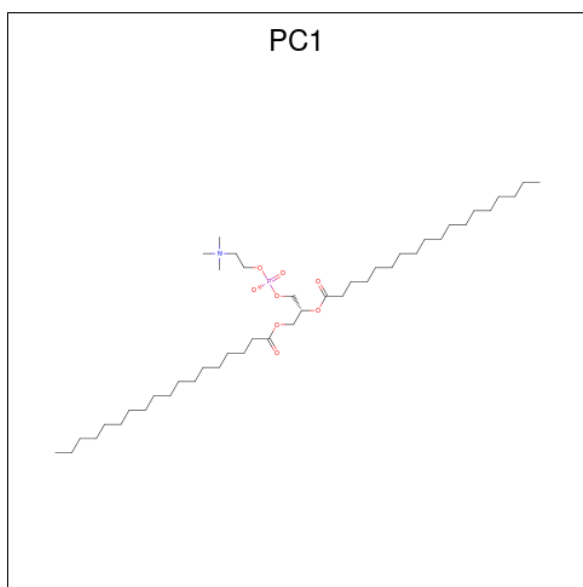
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



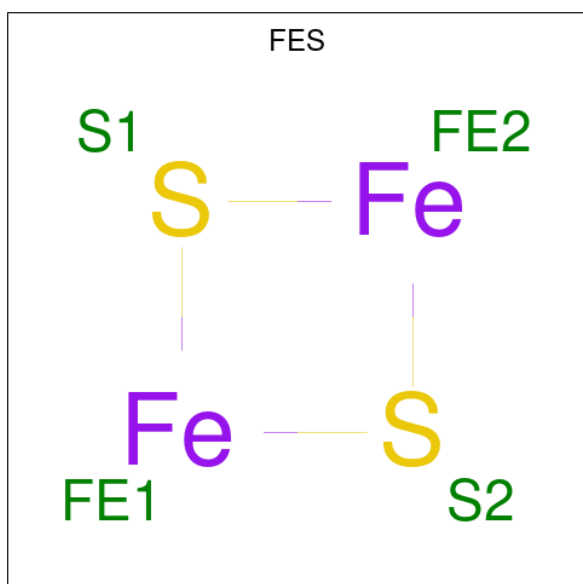
Mol	Chain	Residues	Atoms			AltConf
46	1B	1	Total	Fe	S	0
			8	4	4	
46	1F	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$).



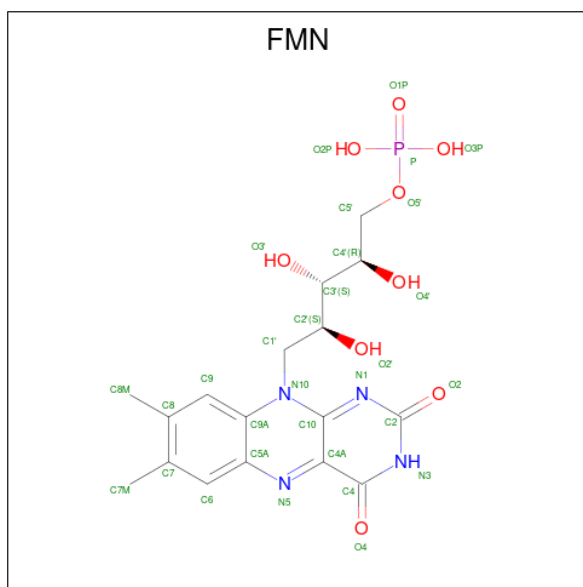
Mol	Chain	Residues	Atoms					AltConf
47	1D	1	Total	C	N	O	P	0
			54	44	1	8	1	
47	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
47	1M	1	Total	C	N	O	P	0
			44	34	1	8	1	
47	1h	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



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

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

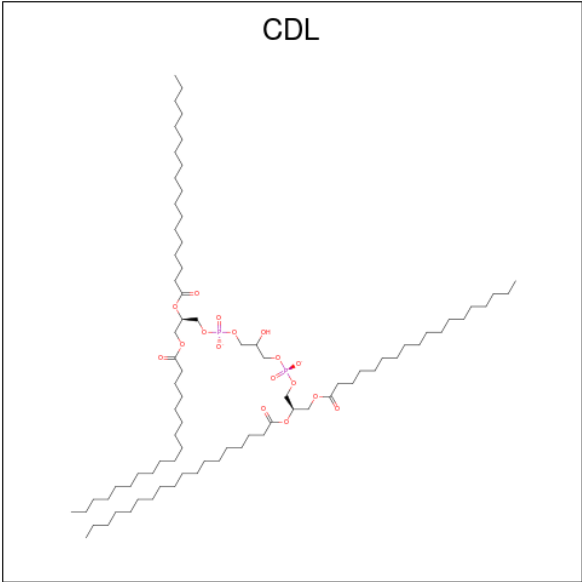


Mol	Chain	Residues	Atoms					AltConf
49	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

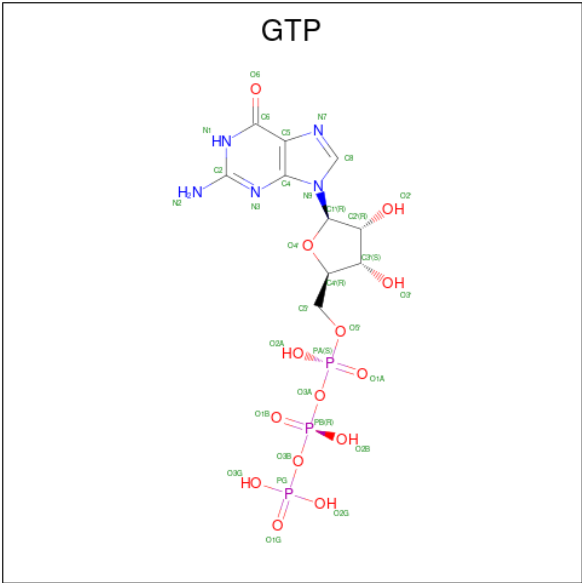
Mol	Chain	Residues	Atoms		AltConf
50	1G	1	Total	K	0
			1	1	

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



Mol	Chain	Residues	Atoms				AltConf
51	1N	1	Total	C	O	P	0
			77	58	17	2	
51	1r	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

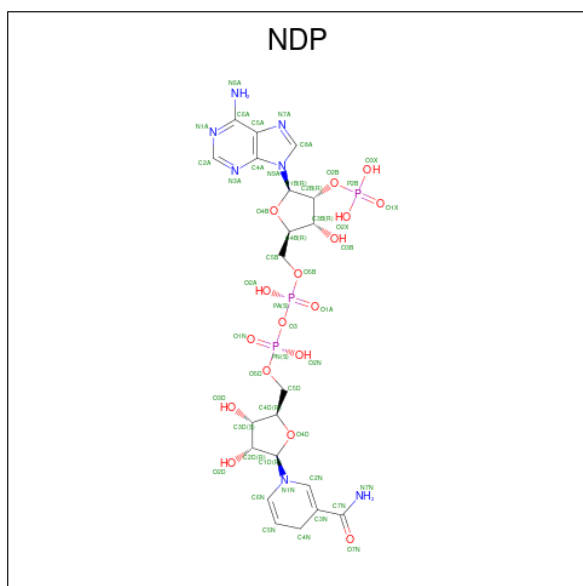


Mol	Chain	Residues	Atoms					AltConf
52	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	1O	1	Total	Mg	0
			1	1	

- Molecule 54 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).

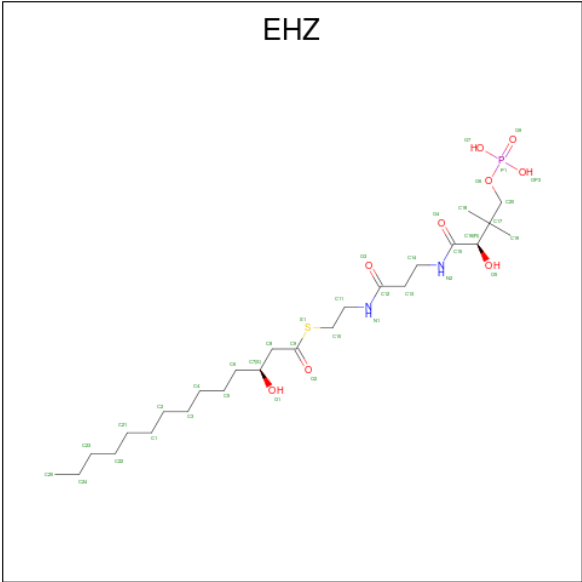


Mol	Chain	Residues	Atoms					AltConf
54	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

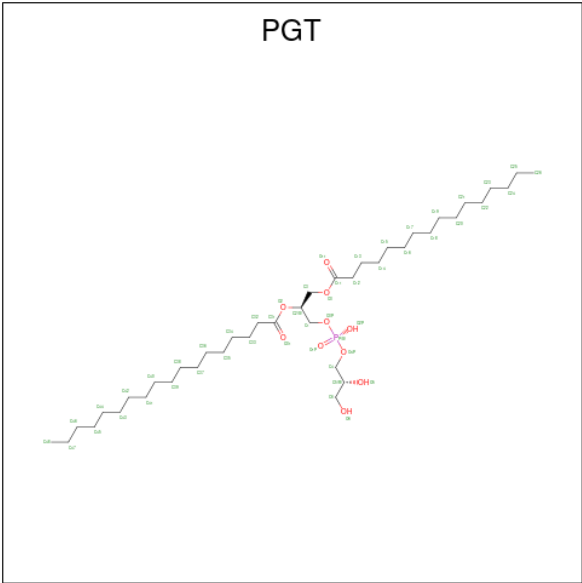
Mol	Chain	Residues	Atoms		AltConf
55	1R	1	Total	Zn	0
			1	1	

- Molecule 56 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: $C_{25}H_{49}N_2O_9PS$).



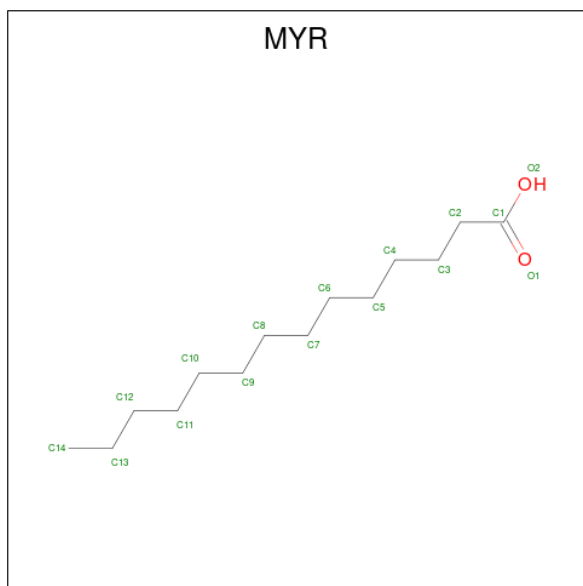
Mol	Chain	Residues	Atoms						AltConf
56	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 57 is (1S)-2-{{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: C₄₀H₇₉O₁₀P).

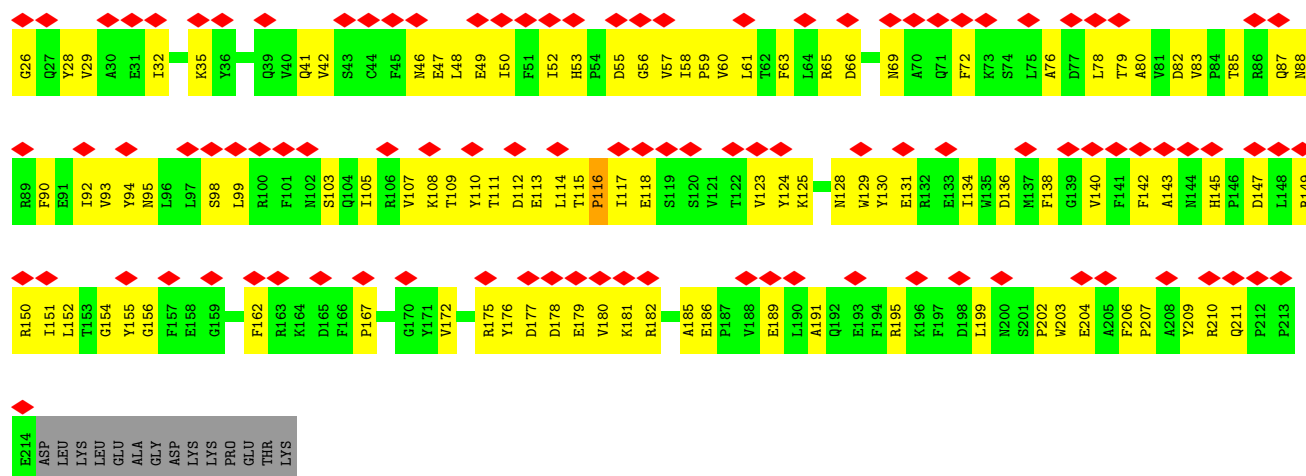


Mol	Chain	Residues	Atoms				AltConf
57	1Y	1	Total	C	O	P	0
			51	40	10	1	

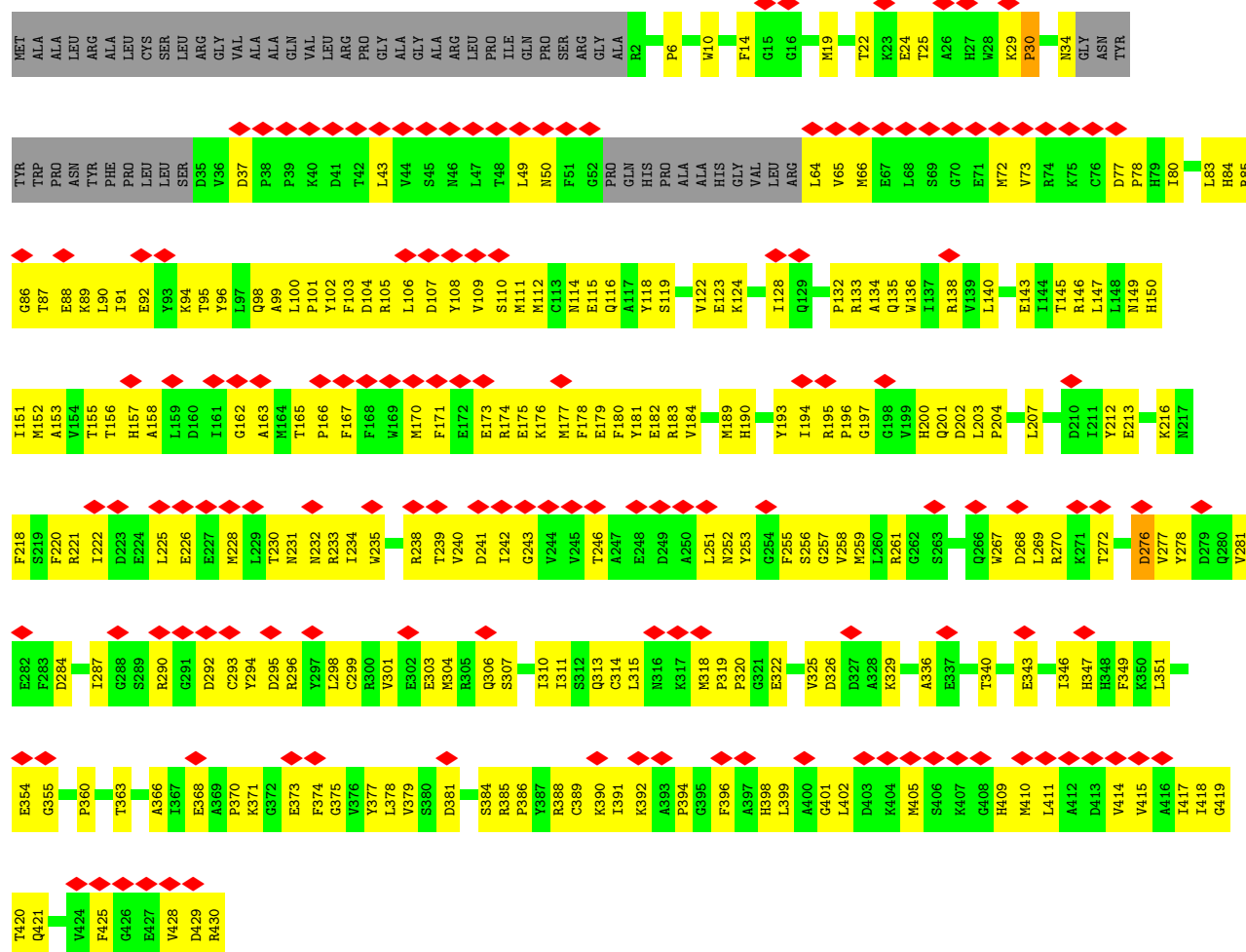
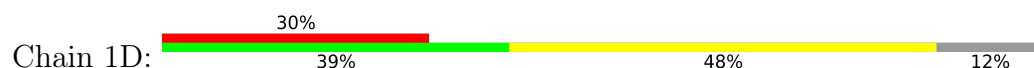
- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).



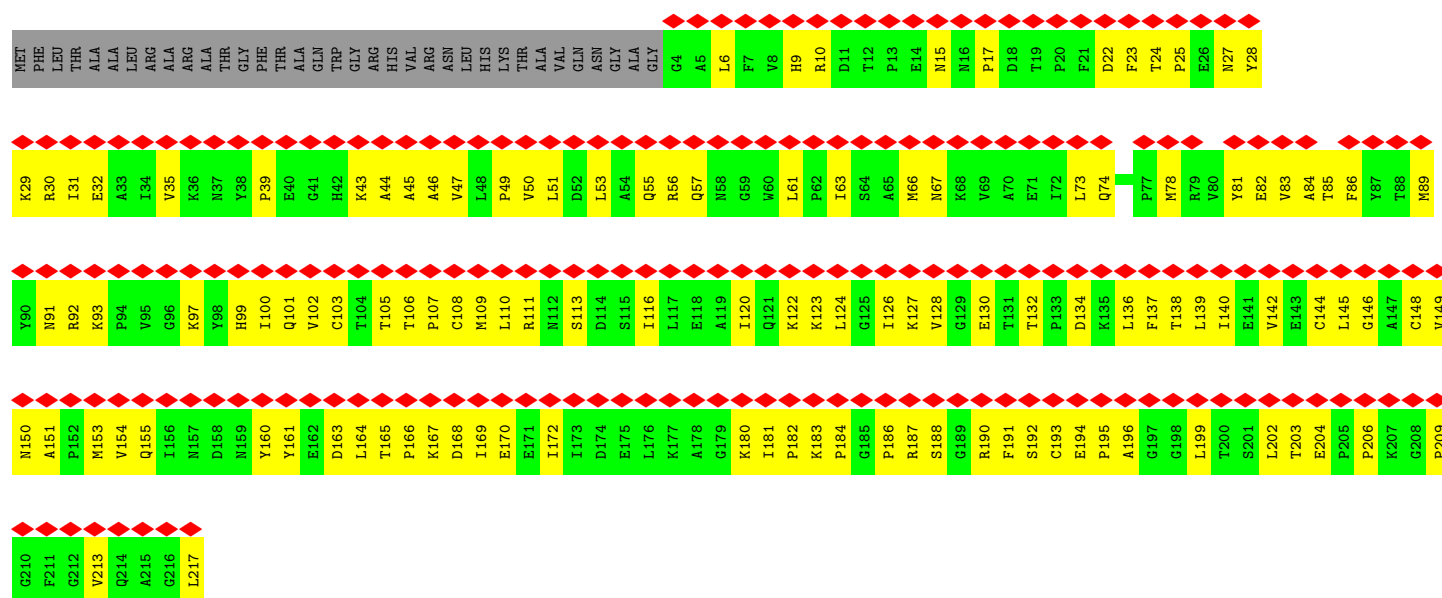
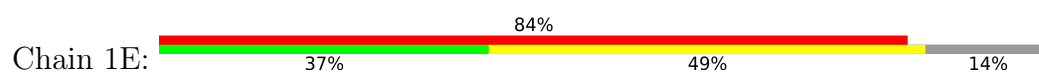
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
58	1l	1	15	14	1	0



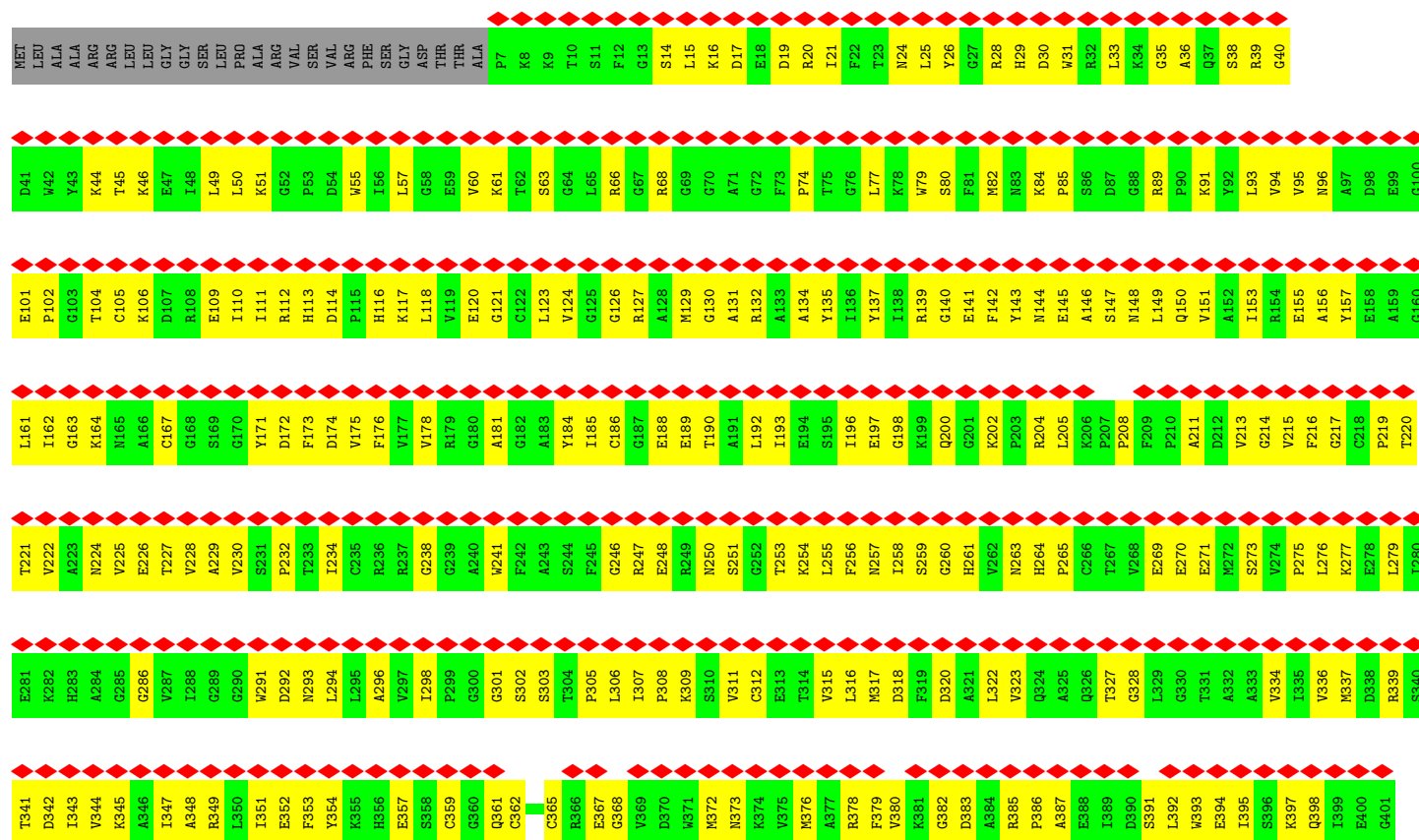
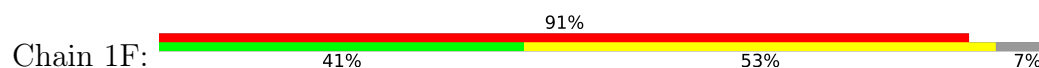
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

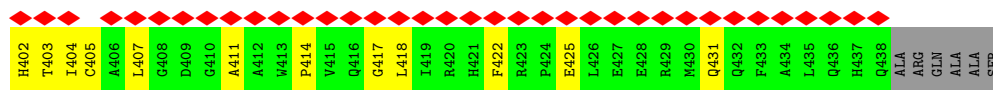


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

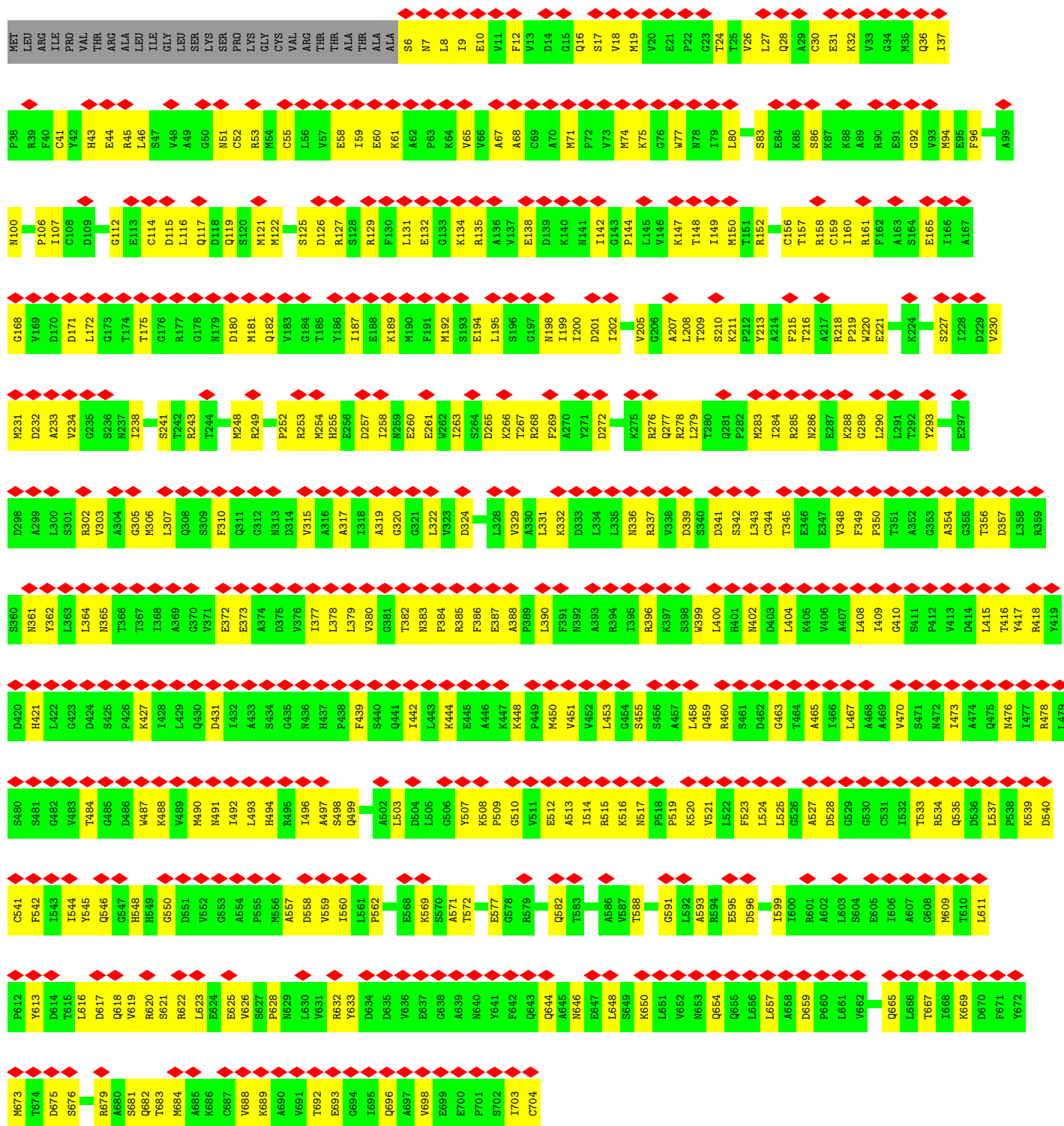


• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

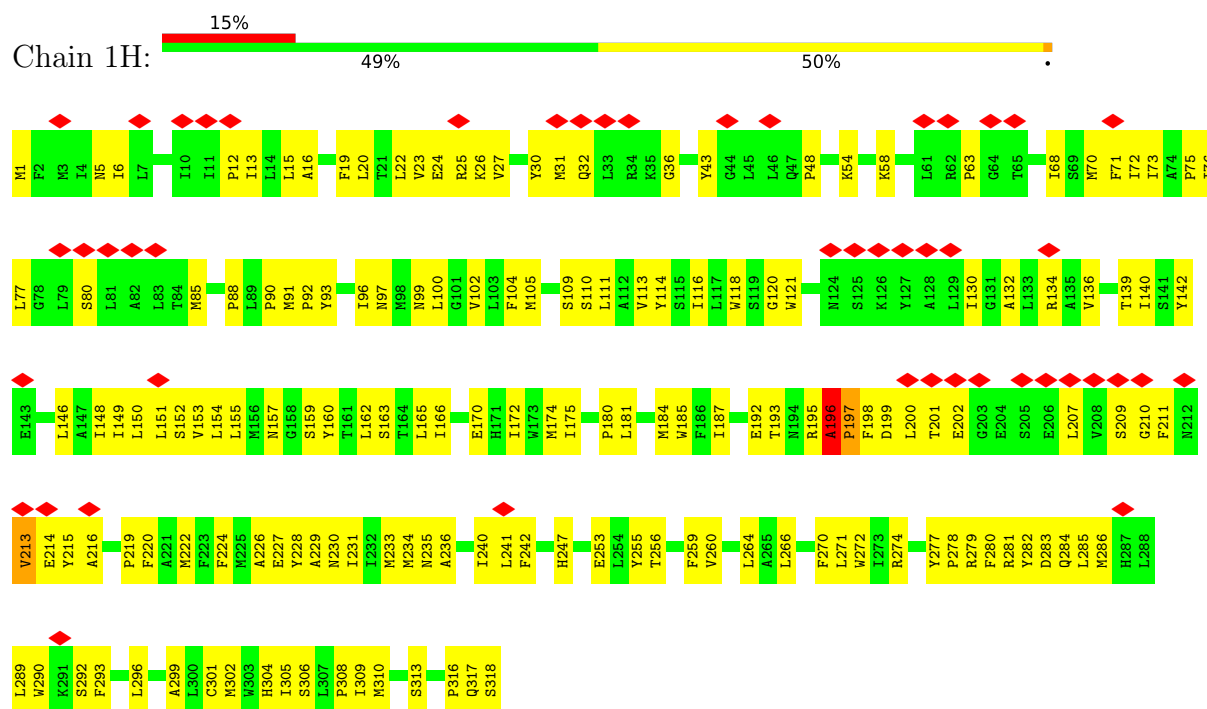




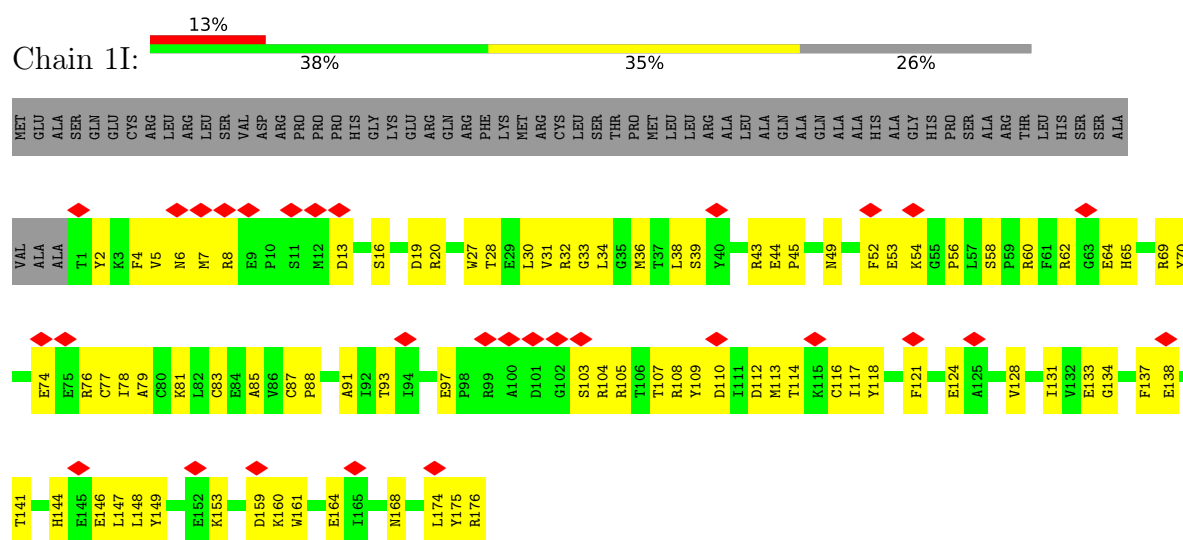
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



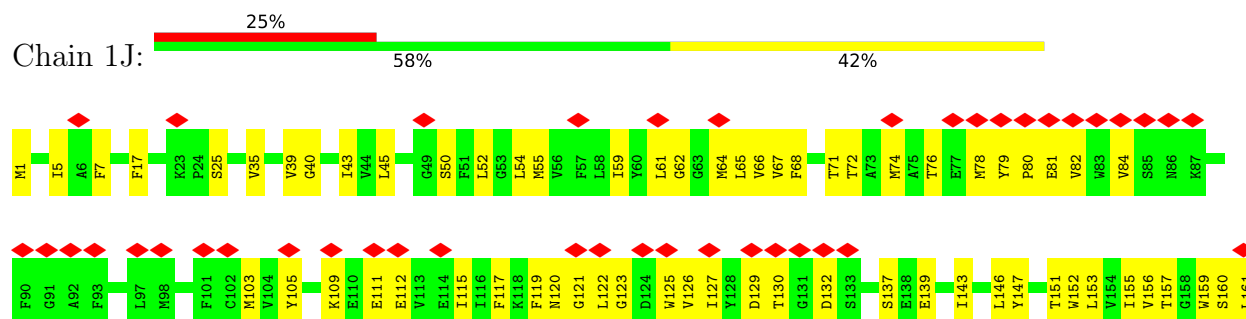
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



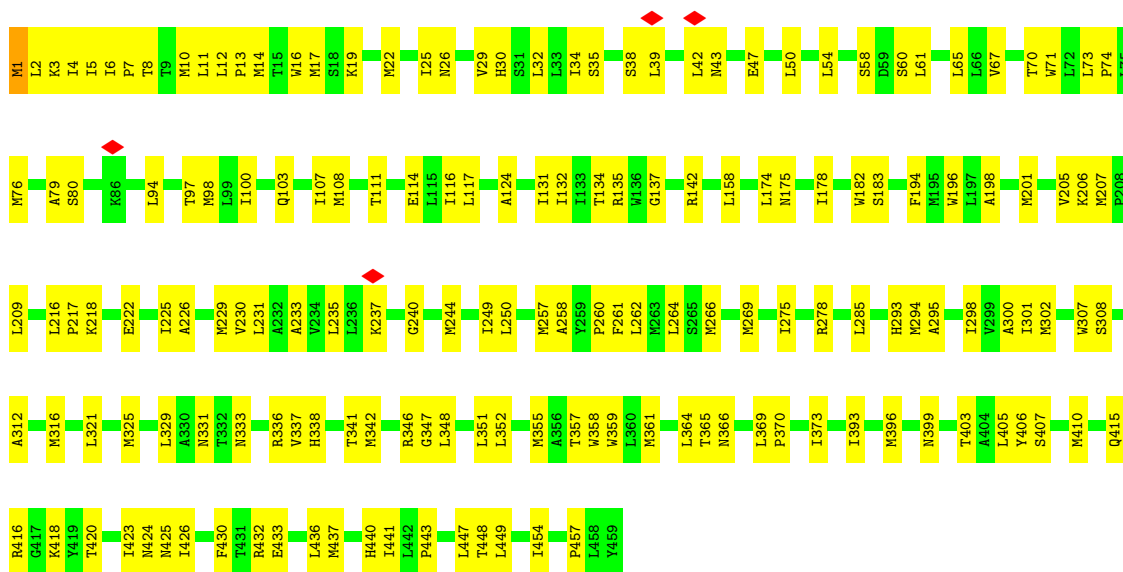
• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



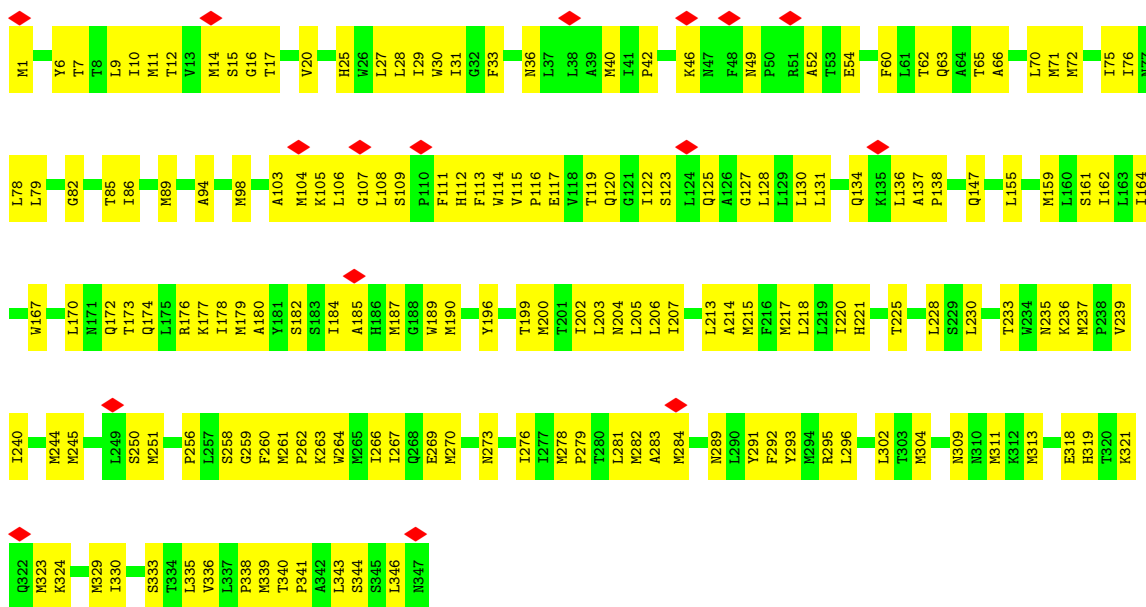
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



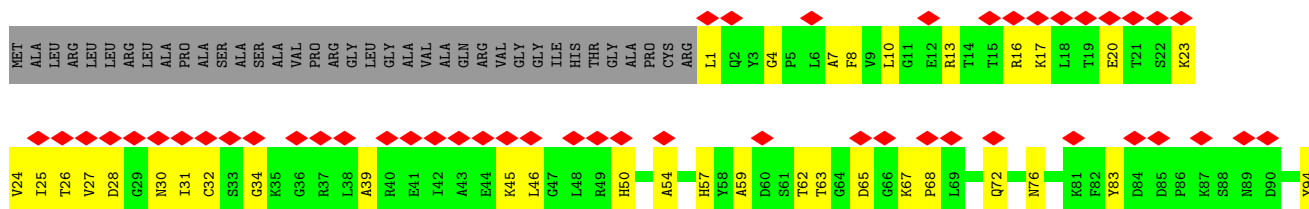


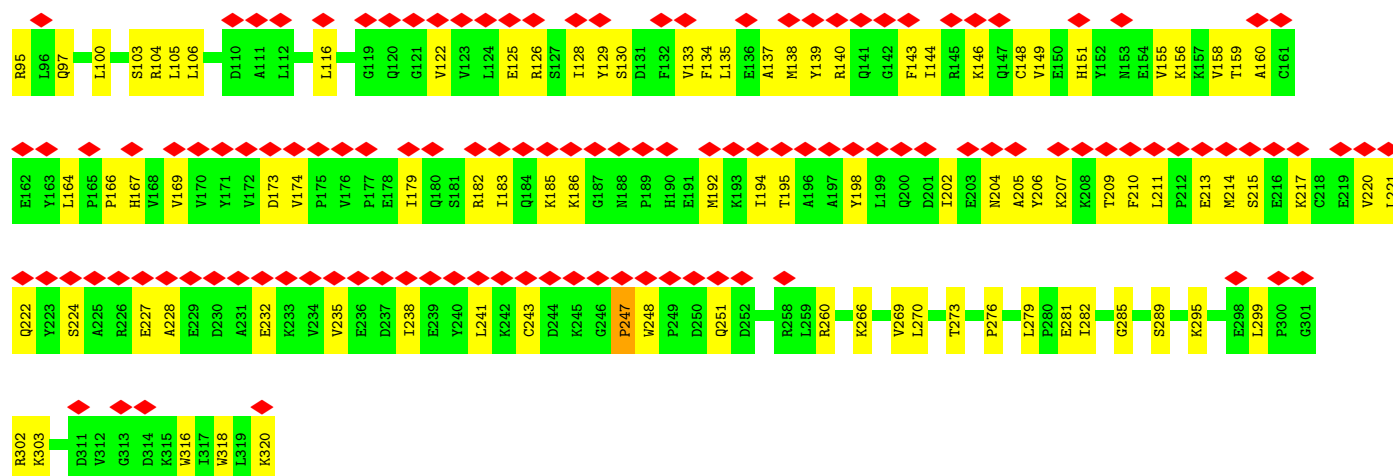


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

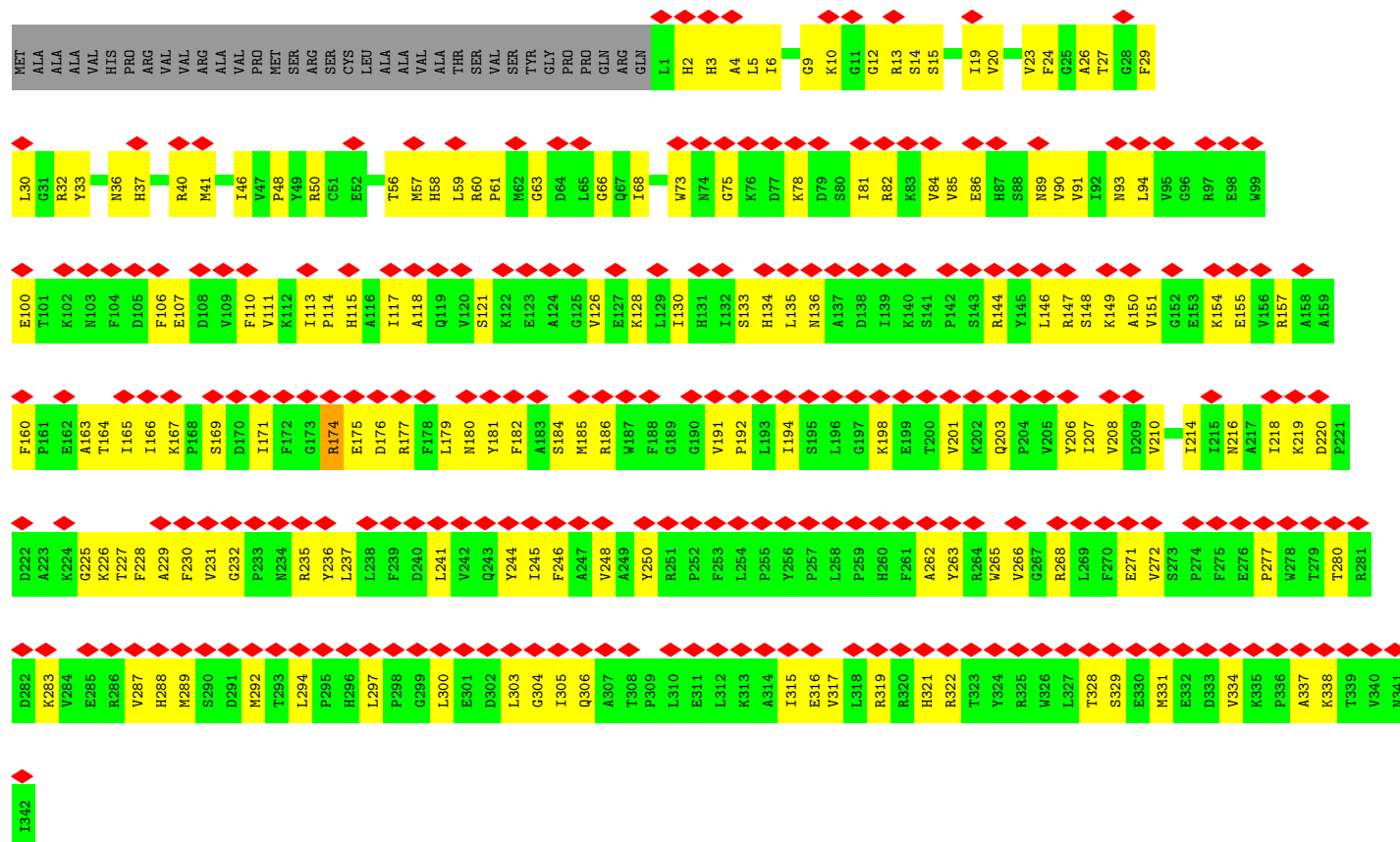


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



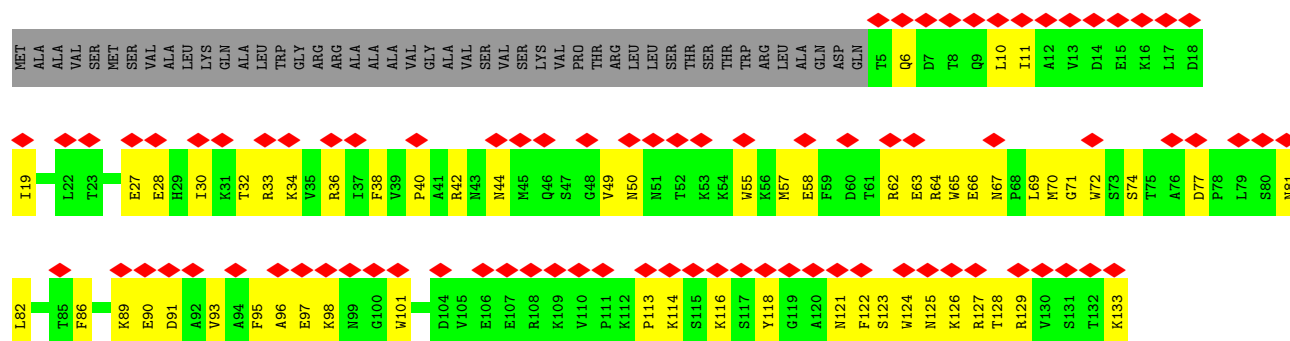


• Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

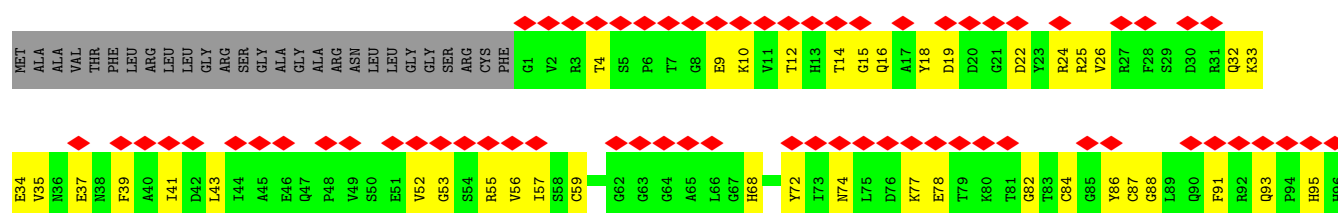


• Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

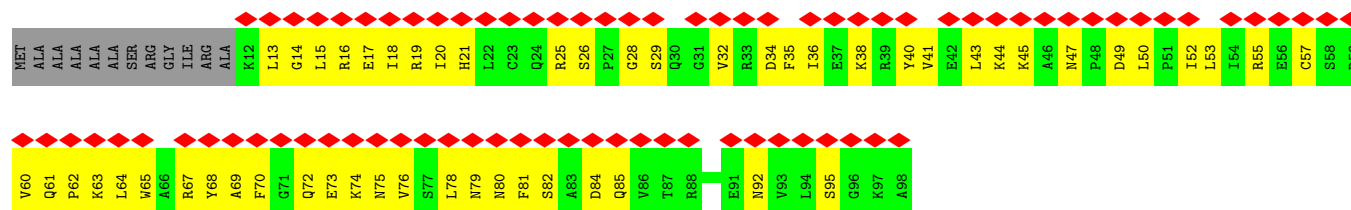
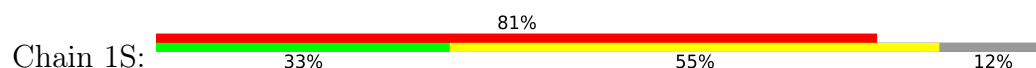




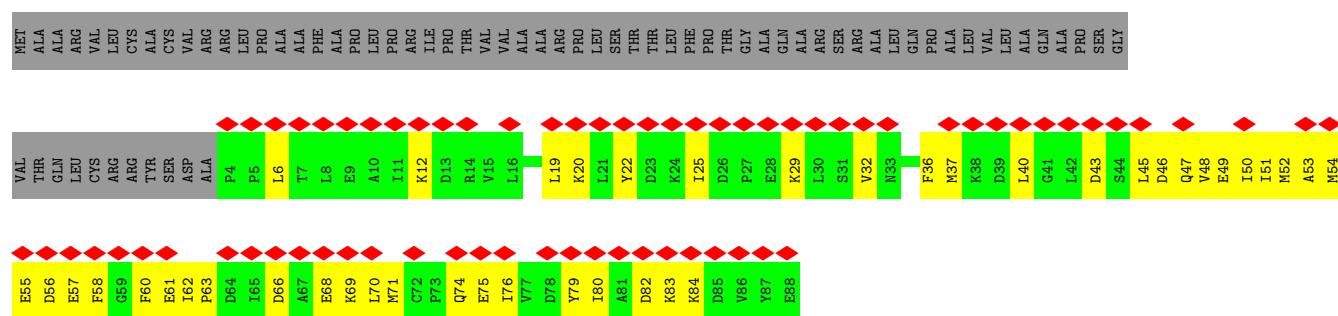
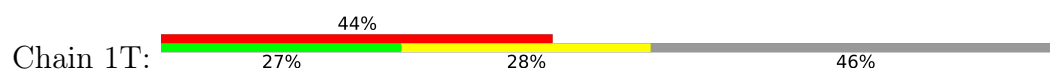
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



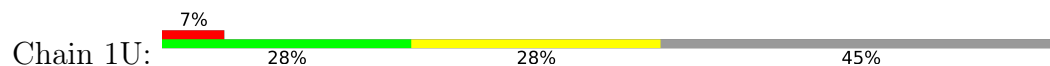
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

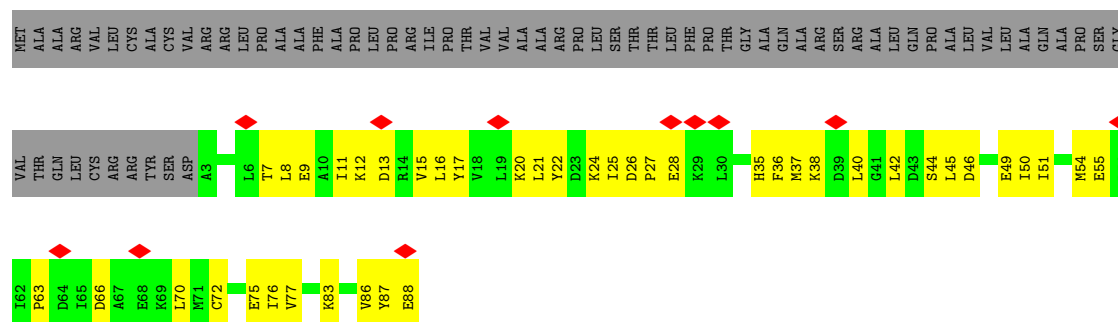


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

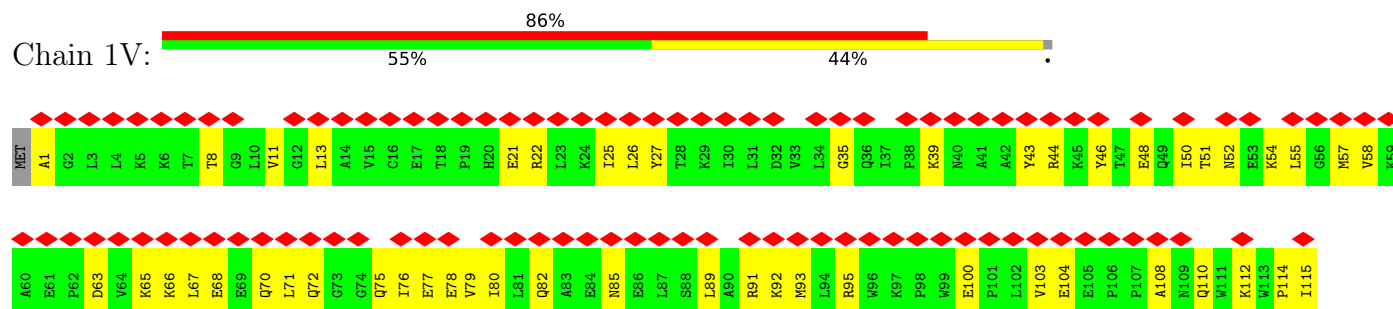


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

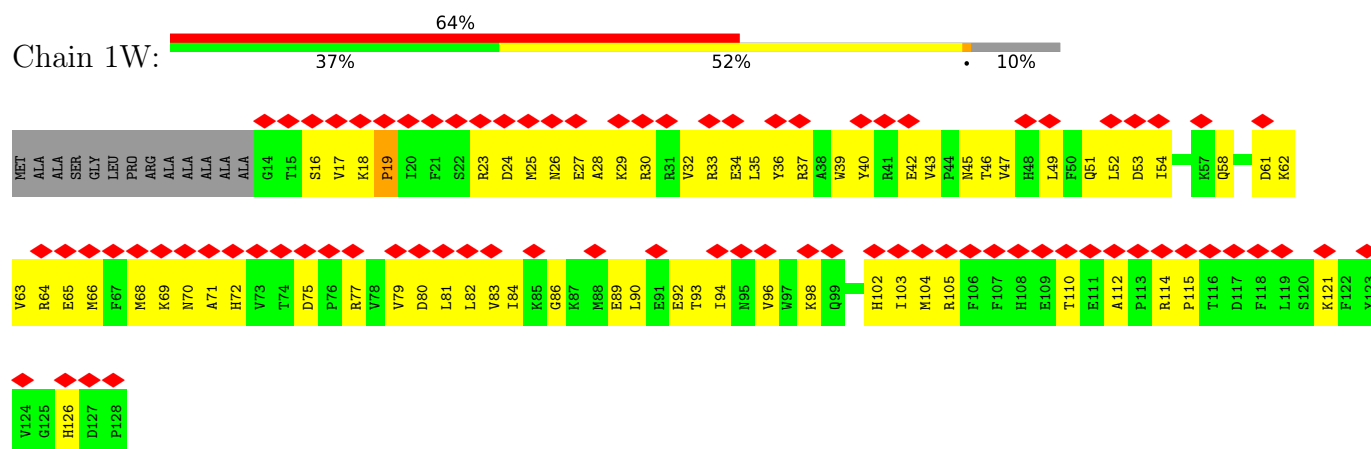




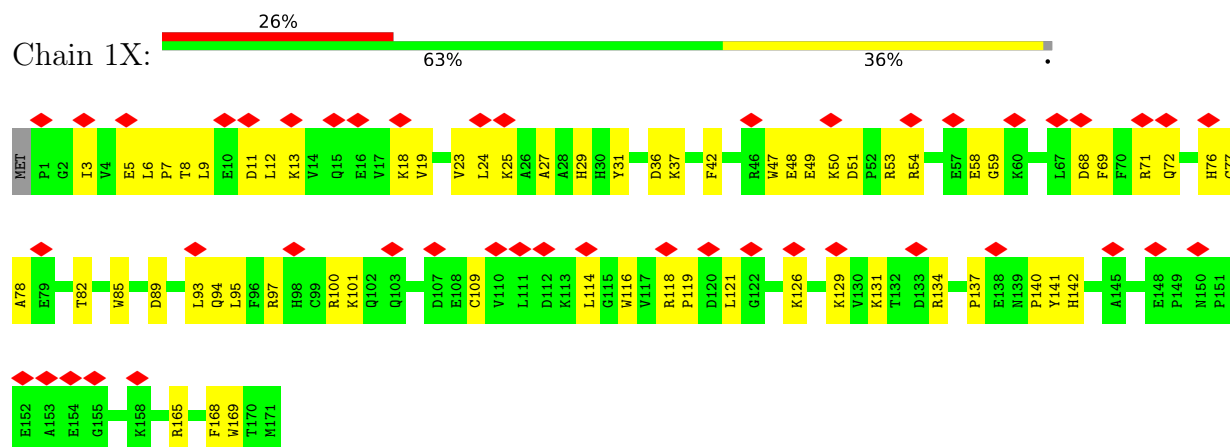
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



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

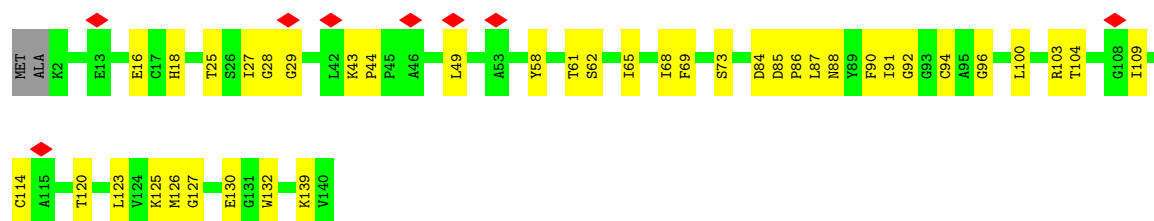


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



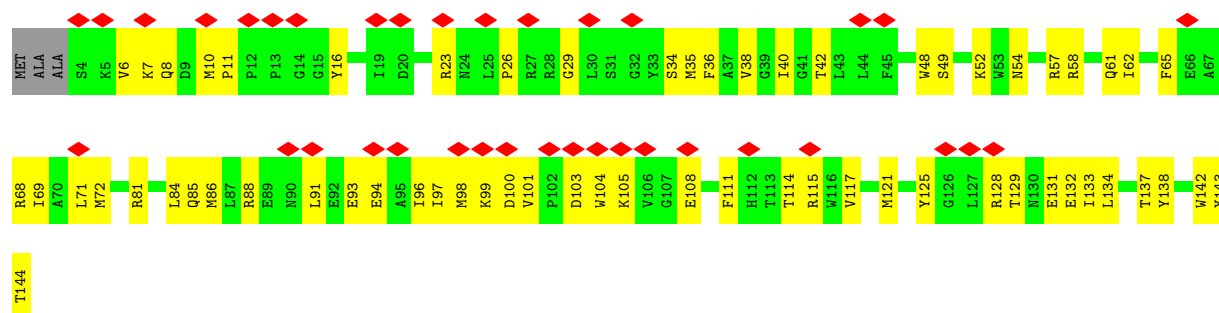
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain 1Y: 



- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13

Chain 1Z: 



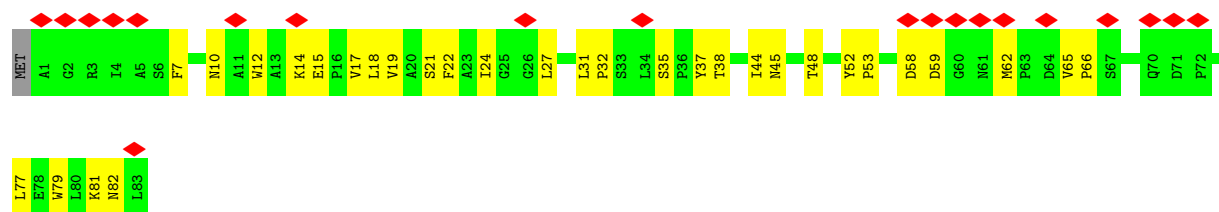
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain 1a: 

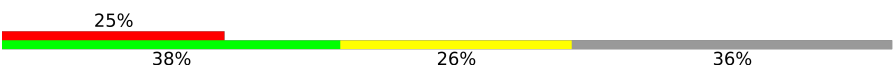


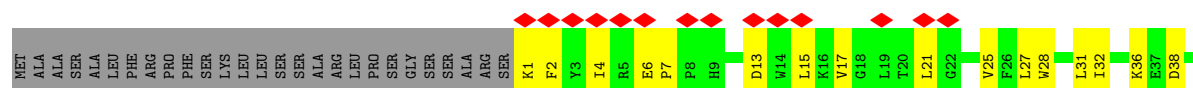
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

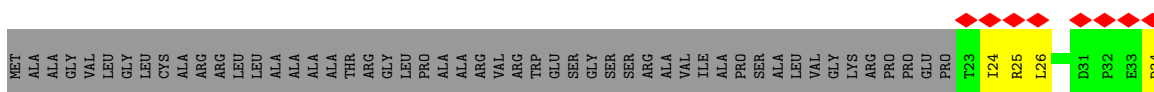
Chain 1b: 

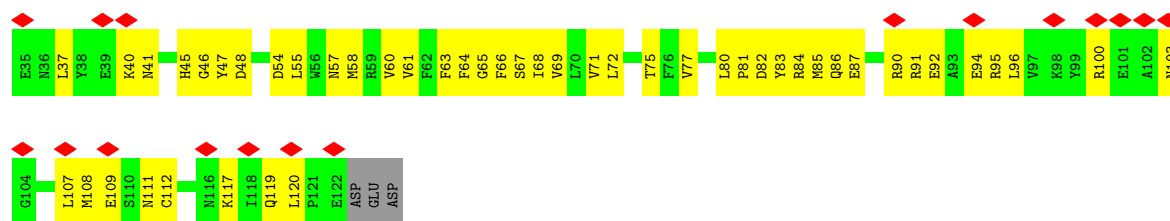


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

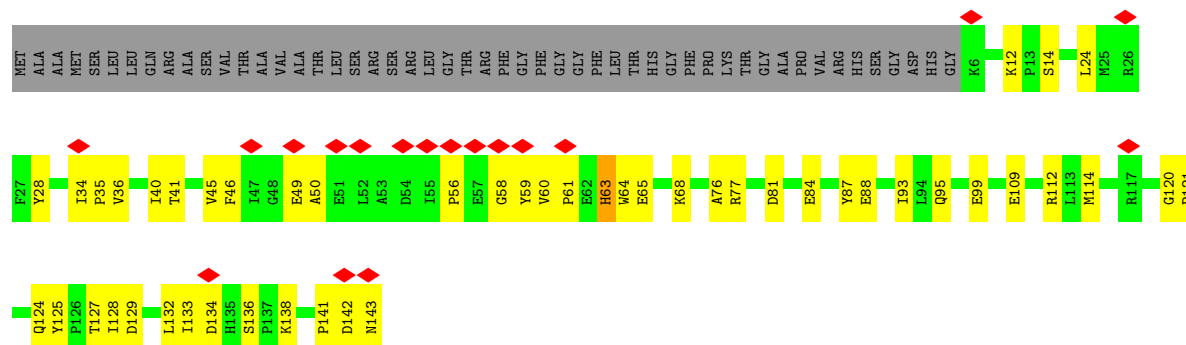
Chain 1c: 



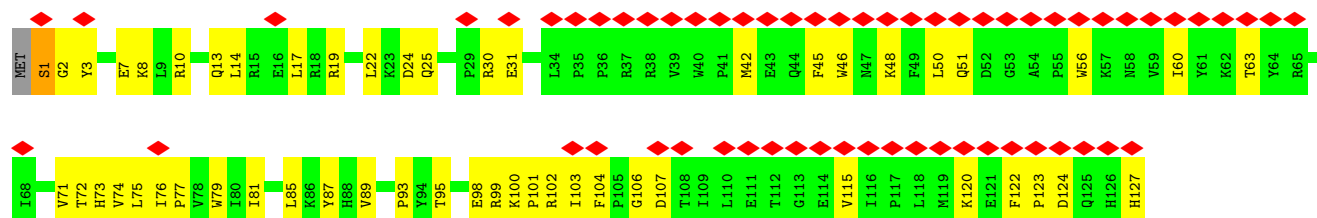




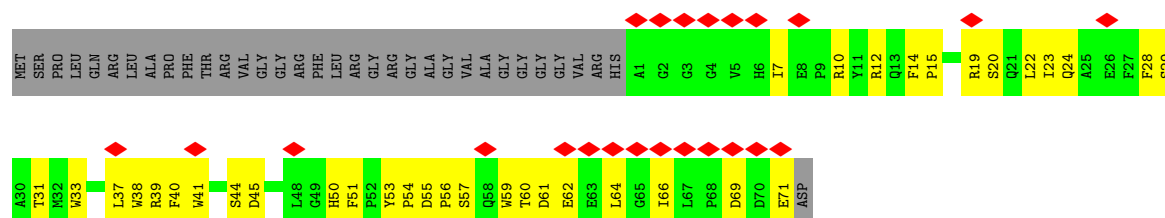
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



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

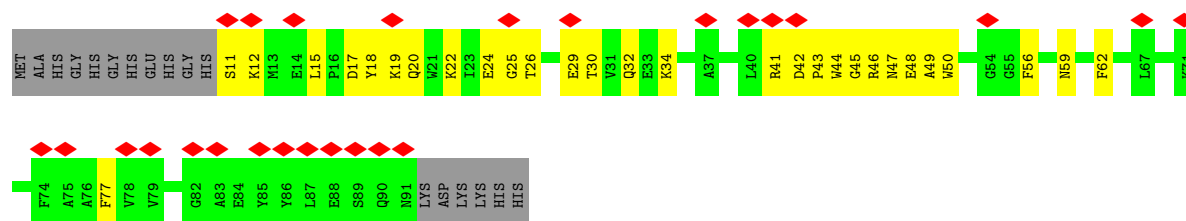


- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

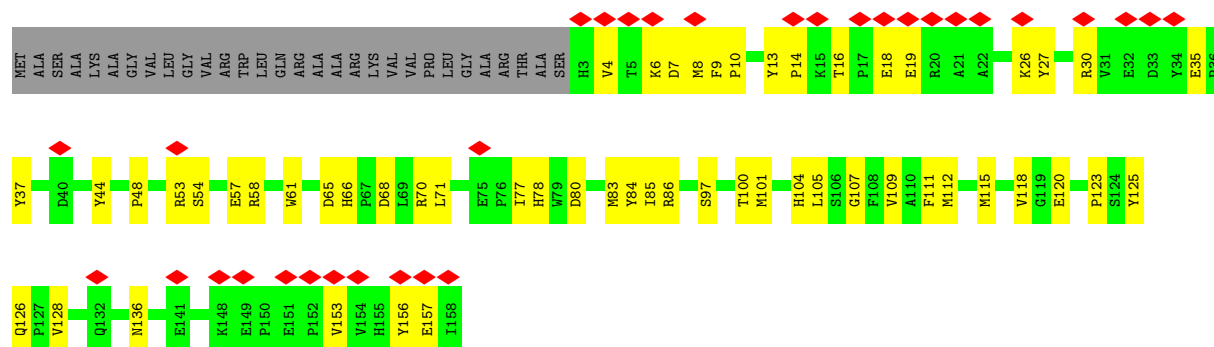


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

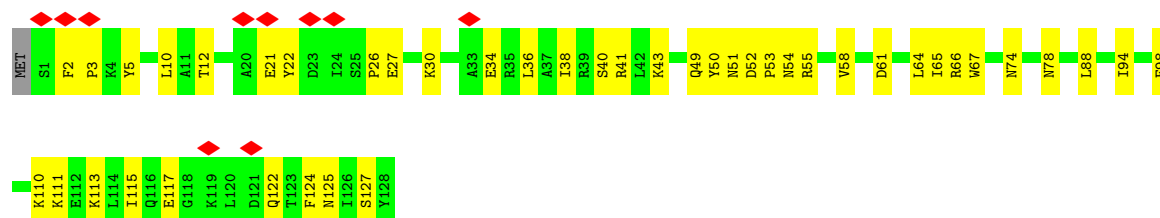




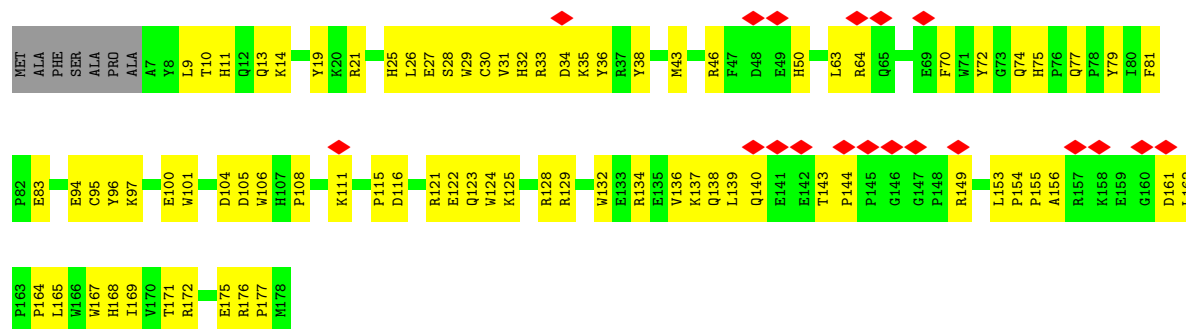
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



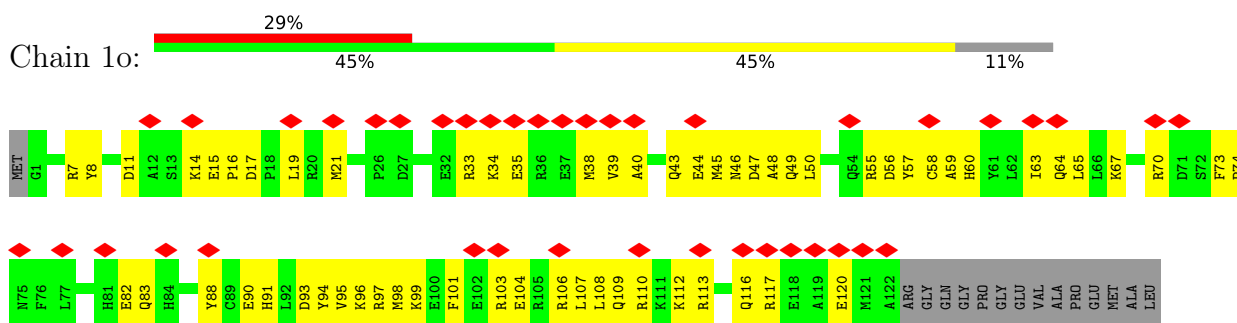
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



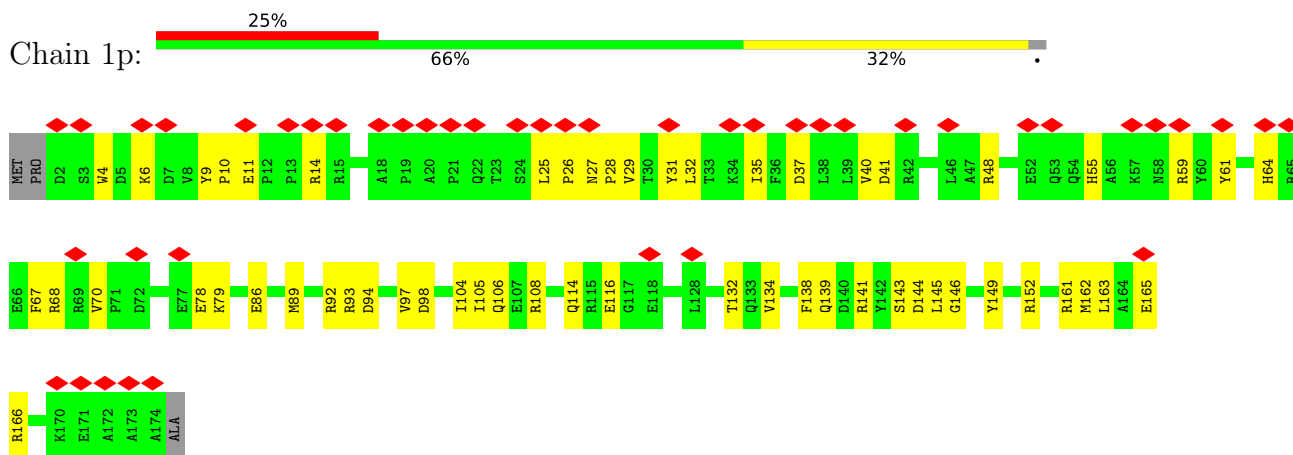
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



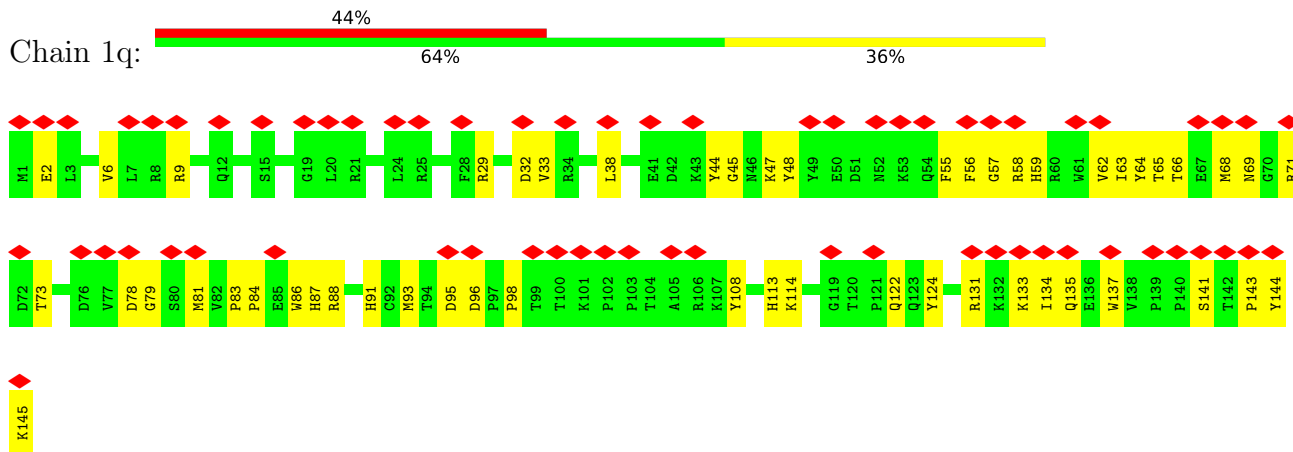
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



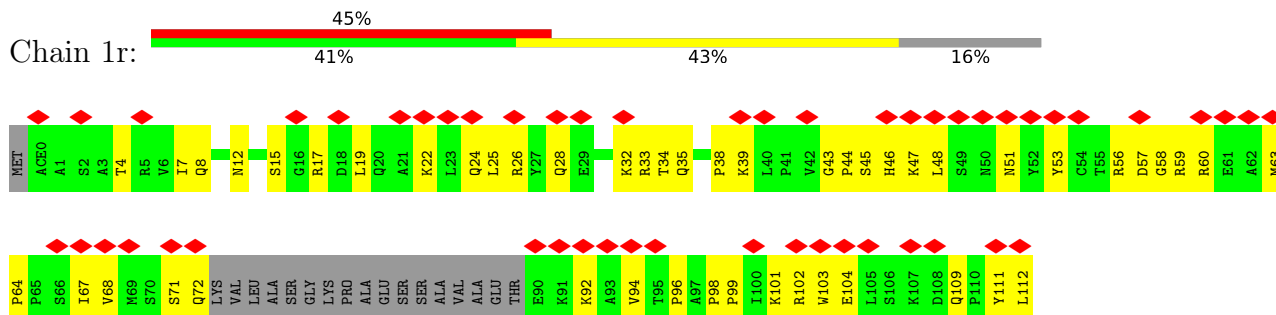
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

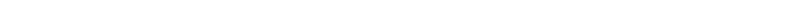


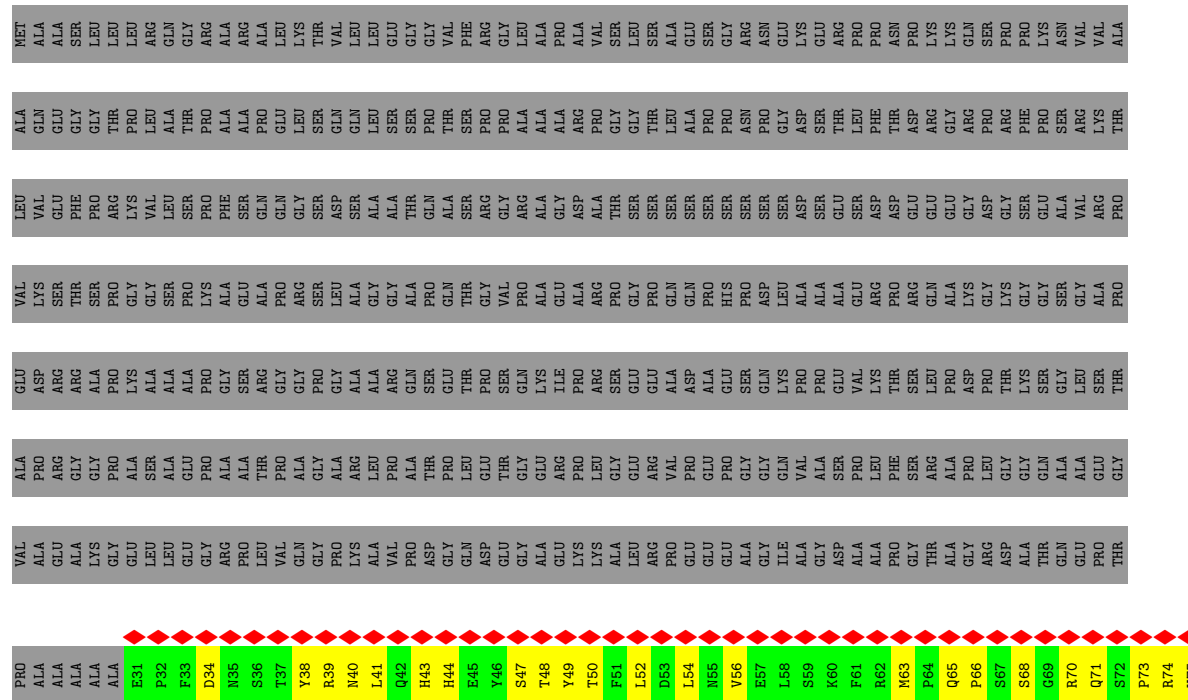
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



- Chain 1s: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	3500	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)	300300	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	0.978	Depositor
Minimum map value	-0.443	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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: MYR, FES, ZN, GTP, FMN, PGT, CDL, PC1, MG, EHZ, K, 3PE, SAC, ACE, SF4, NDP, FME

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	0.14	0/713	0.39	0/975
2	1B	0.30	1/1273 (0.1%)	0.63	2/1722 (0.1%)
3	1C	0.16	0/1791	0.46	1/2439 (0.0%)
4	1D	0.19	1/3457 (0.0%)	0.40	1/4683 (0.0%)
5	1E	0.16	0/1698	0.41	0/2311
6	1F	0.15	0/3401	0.43	0/4595
7	1G	0.14	0/5451	0.39	0/7387
8	1H	0.15	0/2566	0.40	0/3509
9	1I	0.17	0/1443	0.43	0/1952
10	1J	0.13	0/1364	0.39	0/1850
11	1K	0.17	0/751	0.48	0/1018
12	1L	0.14	0/4939	0.40	1/6718 (0.0%)
13	1M	0.13	0/3713	0.32	0/5063
14	1N	0.15	0/2765	0.41	0/3758
15	1O	0.15	0/2650	0.40	1/3588 (0.0%)
16	1P	0.16	0/2828	0.44	0/3834
17	1Q	0.22	0/1070	0.64	1/1446 (0.1%)
18	1R	0.14	0/755	0.40	0/1018
19	1S	0.19	0/711	0.57	0/956
20	1T	0.16	0/701	0.48	0/946
20	1U	0.16	0/706	0.48	0/954
21	1V	0.22	0/946	0.46	0/1281
22	1W	0.22	0/995	0.57	1/1340 (0.1%)
23	1X	0.13	0/1436	0.35	0/1938
24	1Y	0.12	0/1037	0.29	0/1404
25	1Z	0.15	0/1199	0.37	0/1617
26	1a	0.18	0/577	0.35	0/777
27	1b	0.17	0/664	0.44	0/912
28	1c	0.18	0/430	0.41	0/581
29	1d	0.14	0/1024	0.32	0/1383
30	1e	0.16	0/836	0.43	1/1118 (0.1%)
31	1f	0.15	0/499	0.43	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.18	0/858	0.53	0/1165
33	1h	0.14	0/1184	0.39	0/1603
34	1i	0.49	2/1131 (0.2%)	0.65	4/1541 (0.3%)
35	1j	0.13	0/627	0.39	0/858
36	1k	0.13	0/668	0.36	0/903
37	1l	0.14	0/1365	0.38	0/1867
38	1m	0.13	0/1092	0.36	0/1481
39	1n	0.11	0/1549	0.33	0/2098
40	1o	0.13	0/1069	0.38	0/1430
41	1p	0.11	0/1481	0.31	0/1997
42	1q	0.14	0/1253	0.37	1/1704 (0.1%)
43	1r	0.20	0/782	0.50	0/1057
44	1s	0.17	0/394	0.43	0/533
All	All	0.17	4/67842 (0.0%)	0.42	14/91983 (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
8	1H	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	1i	123	PRO	CG-CD	-13.13	1.06	1.50
34	1i	123	PRO	N-CD	7.06	1.57	1.47
4	1D	30	PRO	CA-C	6.05	1.55	1.51
2	1B	80	PRO	CG-CD	-5.60	1.31	1.50

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	123	PRO	N-CD-CG	-13.85	82.42	103.20
34	1i	123	PRO	CA-N-CD	-12.25	94.85	112.00
2	1B	80	PRO	CA-N-CD	-12.09	95.08	112.00
17	1Q	40	PRO	CA-N-CD	-10.53	97.25	112.00
2	1B	80	PRO	N-CD-CG	-8.92	89.82	103.20
22	1W	19	PRO	CA-N-CD	-8.11	100.64	112.00
34	1i	123	PRO	CA-CB-CG	-7.73	89.81	104.50
15	1O	247	PRO	CA-N-CD	-7.12	102.04	112.00

Continued on next page...

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	1L	533	MET	CG-SD-CE	6.67	115.58	100.90
3	1C	116	PRO	CA-N-CD	-5.62	104.13	112.00
4	1D	276	ASP	CB-CA-C	-5.42	109.86	117.23
34	1i	123	PRO	N-CA-CB	-5.22	97.76	103.25
30	1e	46	ILE	N-CA-C	-5.19	108.45	113.53
42	1q	122	GLN	CA-CB-CG	5.07	124.23	114.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1H	196	ALA	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	707	0	757	49	0
2	1B	1242	0	1249	82	0
3	1C	1740	0	1691	112	0
4	1D	3369	0	3305	222	0
5	1E	1658	0	1662	134	0
6	1F	3325	0	3288	223	0
7	1G	5362	0	5388	295	0
8	1H	2504	0	2602	168	0
9	1I	1412	0	1364	107	0
10	1J	1339	0	1337	79	0
11	1K	750	0	798	57	0
12	1L	4818	0	4956	236	0
13	1M	3632	0	3835	145	0
14	1N	2712	0	2872	157	0
15	1O	2590	0	2554	104	0
16	1P	2751	0	2776	134	0
17	1Q	1047	0	1042	63	0
18	1R	741	0	704	36	0
19	1S	700	0	719	57	0
20	1T	689	0	687	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	1U	694	0	691	46	0
21	1V	927	0	972	46	0
22	1W	971	0	975	69	0
23	1X	1398	0	1378	62	0
24	1Y	1016	0	1020	33	0
25	1Z	1168	0	1161	71	0
26	1a	562	0	557	44	0
27	1b	643	0	645	32	0
28	1c	417	0	425	17	0
29	1d	996	0	990	40	0
30	1e	816	0	823	37	0
31	1f	487	0	498	23	0
32	1g	835	0	795	53	0
33	1h	1151	0	1164	41	0
34	1i	1100	0	1106	53	0
35	1j	601	0	546	26	0
36	1k	649	0	626	29	0
37	1l	1310	0	1204	57	0
38	1m	1062	0	1075	50	0
39	1n	1495	0	1434	74	0
40	1o	1045	0	1018	64	0
41	1p	1449	0	1416	59	0
42	1q	1212	0	1174	46	0
43	1r	767	0	791	54	0
44	1s	382	0	351	32	0
45	1A	47	0	69	3	0
45	1L	119	0	161	9	0
45	1N	51	0	82	3	0
45	1Y	51	0	82	2	0
46	1B	8	0	0	2	0
46	1F	8	0	0	3	0
46	1G	16	0	0	1	0
46	1I	16	0	0	2	0
47	1D	54	0	86	7	0
47	1I	44	0	62	9	0
47	1J	35	0	44	4	0
47	1M	44	0	64	6	0
47	1h	46	0	67	2	0
48	1E	4	0	0	2	0
48	1G	4	0	0	0	0
49	1F	31	0	19	3	0
50	1G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
51	1N	77	0	97	4	0
51	1r	61	0	64	6	0
52	1O	32	0	12	3	0
53	1O	1	0	0	0	0
54	1P	48	0	26	3	0
55	1R	1	0	0	0	0
56	1W	37	0	0	0	0
56	1n	37	0	0	2	0
57	1Y	51	0	78	9	0
58	1l	15	0	27	1	0
All	All	67180	0	67461	3070	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 (3070) 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)
21:1V:75:GLN:HE21	21:1V:77:GLU:HG2	1.16	1.06
16:1P:113:ILE:HD12	16:1P:114:PRO:HD3	1.47	0.94
9:1I:146:GLU:HG3	42:1q:124:TYR:HB3	1.51	0.90
18:1R:68:HIS:CD2	18:1R:87:CYS:SG	2.61	0.89
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	1.55	0.89
39:1n:134:ARG:HA	39:1n:137:LYS:HE3	1.57	0.85
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.58	0.85
7:1G:94:MET:HE1	7:1G:119:GLN:HB3	1.59	0.84
35:1j:45:ASP:HB2	35:1j:50:HIS:HB2	1.58	0.84
14:1N:261:MET:HE1	14:1N:340:THR:HA	1.58	0.84
38:1m:122:GLN:HB3	38:1m:125:ASN:HB3	1.60	0.84
5:1E:27:ASN:HA	5:1E:30:ARG:HD2	1.60	0.83
26:1a:64:LYS:HD2	26:1a:68:ASN:HD21	1.43	0.83
7:1G:382:THR:HG22	7:1G:384:PRO:HD3	1.61	0.82
6:1F:118:LEU:HD11	6:1F:225:VAL:HG13	1.60	0.82
14:1N:159:MET:HE1	14:1N:282:MET:HG3	1.60	0.82
4:1D:106:LEU:HD11	4:1D:391:ILE:HD13	1.60	0.81
5:1E:116:ILE:HG23	5:1E:169:ILE:HG21	1.61	0.81
23:1X:49:GLU:HG2	23:1X:134:ARG:HH21	1.46	0.81
43:1r:63:MET:HE3	43:1r:64:PRO:HD2	1.63	0.81
3:1C:204:GLU:HA	17:1Q:50:ASN:HD22	1.46	0.80
12:1L:173:LEU:HD23	13:1M:405:LEU:HD21	1.63	0.80
16:1P:315:ILE:H	16:1P:331:MET:HE1	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:111:LEU:HD11	8:1H:290:TRP:HB3	1.63	0.80
7:1G:350:PRO:HD3	7:1G:458:LEU:HD11	1.63	0.80
43:1r:43:GLY:O	43:1r:46:HIS:ND1	2.15	0.80
5:1E:53:LEU:HD23	44:1s:52:LEU:HG	1.64	0.79
6:1F:102:PRO:HD2	6:1F:302:SER:HB2	1.62	0.79
12:1L:310:LEU:HA	12:1L:313:MET:HG3	1.64	0.79
8:1H:197:PRO:HA	8:1H:279:ARG:HE	1.48	0.79
15:1O:207:LYS:HA	15:1O:211:LEU:HD23	1.63	0.78
5:1E:153:MET:SD	5:1E:153:MET:N	2.58	0.77
4:1D:101:PRO:HB3	4:1D:105:ARG:HH21	1.49	0.77
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.66	0.77
7:1G:400:LEU:O	17:1Q:126:LYS:NZ	2.18	0.76
2:1B:116:MET:HE3	2:1B:156:LEU:HD22	1.67	0.76
6:1F:404:ILE:HG13	7:1G:53:ARG:HD3	1.66	0.76
2:1B:82:GLN:NE2	8:1H:214:GLU:O	2.19	0.76
4:1D:107:ASP:HB3	4:1D:114:ASN:HD21	1.49	0.75
4:1D:116:GLN:NE2	4:1D:276:ASP:OD2	2.20	0.75
12:1L:486:MET:HA	12:1L:489:THR:HG23	1.69	0.74
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.70	0.74
14:1N:235:ASN:HB3	14:1N:311:MET:HE2	1.70	0.74
3:1C:199:LEU:HD12	4:1D:354:GLU:HA	1.69	0.74
12:1L:546:GLN:HG3	13:1M:278:ARG:HH21	1.52	0.74
4:1D:72:MET:HA	4:1D:410:MET:HA	1.68	0.74
6:1F:337:MET:SD	6:1F:341:THR:OG1	2.46	0.74
34:1i:104:PHE:HB3	40:1o:63:ILE:HD11	1.70	0.73
22:1W:17:VAL:HG23	22:1W:77:ARG:HH21	1.54	0.73
15:1O:211:LEU:O	15:1O:215:SER:OG	2.05	0.73
27:1b:10:ASN:OD1	27:1b:14:LYS:NZ	2.19	0.73
4:1D:66:MET:HE2	4:1D:73:VAL:HG21	1.70	0.73
12:1L:381:THR:HB	12:1L:494:THR:HG21	1.71	0.73
8:1H:213:VAL:HG12	8:1H:214:GLU:H	1.53	0.73
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.71	0.73
2:1B:39:TRP:HA	2:1B:42:ARG:HE	1.54	0.73
12:1L:254:VAL:HG13	12:1L:329:ILE:HD12	1.71	0.73
16:1P:2:HIS:HB3	16:1P:5:LEU:HD23	1.71	0.73
20:1U:70:LEU:HD12	20:1U:76:ILE:HD13	1.72	0.72
22:1W:34:GLU:HA	22:1W:37:ARG:HB3	1.71	0.72
7:1G:418:ARG:H	44:1s:74:ARG:HH21	1.36	0.72
5:1E:182:PRO:HB2	5:1E:187:ARG:HH21	1.55	0.72
13:1M:307:TRP:NE1	38:1m:127:SER:OG	2.22	0.72
6:1F:260:GLY:HA3	6:1F:336:VAL:H	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:182:ARG:HA	15:1O:185:LYS:HE2	1.71	0.72
13:1M:295:ALA:HA	13:1M:298:ILE:HD12	1.72	0.71
7:1G:157:THR:OG1	7:1G:161:ARG:NH1	2.23	0.71
15:1O:183:ILE:HD13	15:1O:192:MET:HA	1.72	0.71
21:1V:75:GLN:NE2	21:1V:77:GLU:HG2	2.01	0.71
41:1p:37:ASP:HA	41:1p:41:ASP:HB3	1.72	0.71
3:1C:66:ASP:HB3	21:1V:85:ASN:HD22	1.55	0.71
11:1K:43:MET:HE2	11:1K:43:MET:HA	1.72	0.71
2:1B:148:GLY:HA2	9:1I:118:TYR:HE1	1.56	0.71
16:1P:57:MET:SD	16:1P:60:ARG:NH1	2.62	0.71
35:1j:69:ASP:HA	40:1o:110:ARG:HH12	1.53	0.71
7:1G:365:ASN:ND2	7:1G:490:MET:O	2.24	0.71
16:1P:185:MET:HG3	16:1P:191:VAL:HG13	1.73	0.71
2:1B:32:LYS:HA	2:1B:32:LYS:HE3	1.72	0.70
4:1D:220:PHE:HD2	43:1r:22:LYS:HE2	1.56	0.70
8:1H:120:GLY:HA3	8:1H:132:ALA:HB2	1.73	0.70
19:1S:47:ASN:HB2	19:1S:50:LEU:HB2	1.72	0.70
6:1F:162:ILE:HG21	6:1F:175:VAL:HG12	1.73	0.70
6:1F:391:SER:HB3	43:1r:48:LEU:HD13	1.72	0.70
5:1E:110:LEU:HB3	5:1E:111:ARG:HD3	1.74	0.70
7:1G:71:MET:HE2	7:1G:71:MET:HA	1.71	0.70
19:1S:61:GLN:HE22	19:1S:63:LYS:HE2	1.55	0.70
34:1i:102:ARG:O	40:1o:70:ARG:NH2	2.25	0.70
5:1E:120:ILE:HG22	5:1E:124:LEU:HD23	1.73	0.70
32:1g:107:LEU:HD21	41:1p:134:VAL:HG22	1.73	0.70
14:1N:103:ALA:O	14:1N:107:GLY:N	2.23	0.70
15:1O:72:GLN:HA	15:1O:76:ASN:HA	1.73	0.70
3:1C:138:PHE:HE2	4:1D:388:ARG:HH21	1.39	0.70
6:1F:94:VAL:HB	6:1F:222:VAL:HA	1.73	0.69
7:1G:525:LEU:HD12	7:1G:546:GLN:HE22	1.57	0.69
8:1H:196:ALA:O	8:1H:198:PHE:N	2.25	0.69
13:1M:12:LEU:HD21	13:1M:97:THR:HG23	1.73	0.69
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.74	0.69
39:1n:140:GLN:HA	39:1n:143:THR:HG23	1.74	0.69
13:1M:351:LEU:HD13	13:1M:426:ILE:HG21	1.73	0.69
23:1X:18:LYS:HA	26:1a:54:ILE:HD11	1.73	0.69
10:1J:121:GLY:HA2	11:1K:3:LEU:HG	1.74	0.69
3:1C:150:ARG:NH1	3:1C:154:GLY:O	2.26	0.69
7:1G:349:PHE:HB3	7:1G:509:PRO:HB2	1.75	0.69
34:1i:120:LYS:HG3	40:1o:39:VAL:HG23	1.74	0.69
37:1l:10:PRO:HD3	38:1m:66:ARG:HG2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:116:MET:HG2	2:1B:151:PRO:HG2	1.74	0.69
12:1L:21:MET:HE1	12:1L:26:ILE:HB	1.73	0.69
32:1g:96:LEU:HD11	32:1g:100:ARG:HH21	1.58	0.69
17:1Q:11:ILE:HG23	22:1W:23:ARG:HH12	1.57	0.69
12:1L:108:MET:HB3	12:1L:114:ILE:HD11	1.75	0.68
3:1C:14:ARG:HH22	3:1C:16:ASP:HB2	1.58	0.68
26:1a:12:MET:N	26:1a:12:MET:SD	2.67	0.68
6:1F:68:ARG:HB3	6:1F:254:LYS:HE2	1.75	0.68
32:1g:87:GLU:HA	32:1g:90:ARG:HB3	1.74	0.68
6:1F:378:ARG:O	6:1F:382:GLY:N	2.26	0.68
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.26	0.68
21:1V:76:ILE:H	21:1V:76:ILE:HD12	1.58	0.68
26:1a:34:LYS:NZ	26:1a:61:HIS:O	2.25	0.68
4:1D:84:HIS:HA	4:1D:429:ASP:HB3	1.75	0.68
5:1E:105:THR:HG23	5:1E:107:PRO:HD2	1.76	0.68
6:1F:312:CYS:HA	6:1F:315:VAL:HG12	1.76	0.68
19:1S:41:VAL:O	19:1S:45:LYS:NZ	2.27	0.68
45:1A:201:3PE:H232	27:1b:18:LEU:HD22	1.74	0.68
5:1E:106:THR:HG22	6:1F:349:ARG:HB3	1.76	0.68
2:1B:62:MET:HG3	2:1B:69:MET:HG2	1.74	0.68
7:1G:546:GLN:HG3	7:1G:599:ILE:HD11	1.76	0.68
9:1I:19:ASP:HB3	47:1I:203:PC1:H131	1.76	0.68
15:1O:76:ASN:OD1	15:1O:95:ARG:NE	2.26	0.68
42:1q:55:PHE:HB3	43:1r:25:LEU:HD13	1.74	0.68
9:1I:79:ALA:HB3	9:1I:104:ARG:HE	1.58	0.67
12:1L:575:ILE:O	12:1L:579:ASN:ND2	2.28	0.67
32:1g:63:PHE:O	32:1g:67:SER:OG	2.10	0.67
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.27	0.67
6:1F:197:GLU:OE2	6:1F:204:ARG:NH2	2.27	0.67
15:1O:183:ILE:HA	15:1O:186:LYS:HZ1	1.58	0.67
22:1W:19:PRO:HA	22:1W:77:ARG:HH12	1.58	0.67
39:1n:125:LYS:HE2	39:1n:129:ARG:HE	1.60	0.67
4:1D:151:ILE:O	4:1D:155:THR:OG1	2.11	0.67
43:1r:72:GLN:N	43:1r:72:GLN:OE1	2.27	0.67
22:1W:63:VAL:HA	22:1W:66:MET:HE2	1.75	0.67
23:1X:25:LYS:NZ	23:1X:94:GLN:O	2.23	0.67
27:1b:81:LYS:HE2	27:1b:81:LYS:HA	1.76	0.67
6:1F:365:CYS:HB2	46:1F:502:SF4:S2	2.35	0.67
7:1G:58:GLU:OE1	7:1G:83:SER:OG	2.12	0.67
7:1G:336:ASN:OD1	19:1S:67:ARG:NH1	2.28	0.67
14:1N:215:MET:HG2	14:1N:244:MET:HE1	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:153:LEU:O	10:1J:157:THR:OG1	2.09	0.67
12:1L:593:ILE:O	12:1L:597:ILE:HG22	1.95	0.67
22:1W:35:LEU:HD11	22:1W:86:GLY:HA3	1.76	0.67
2:1B:93:THR:HA	2:1B:132:VAL:HA	1.77	0.67
5:1E:10:ARG:NH1	18:1R:78:GLU:OE1	2.28	0.67
10:1J:112:GLU:OE2	30:1e:73:LYS:NZ	2.27	0.67
12:1L:364:LYS:H	12:1L:364:LYS:HZ3	1.41	0.67
5:1E:109:MET:SD	6:1F:345:LYS:NZ	2.68	0.67
8:1H:195:ARG:HG3	8:1H:196:ALA:H	1.60	0.67
10:1J:167:VAL:HG23	14:1N:42:PRO:HD3	1.77	0.67
13:1M:13:PRO:HB3	45:1N:401:3PE:H2C2	1.77	0.67
16:1P:144:ARG:HH22	16:1P:148:SER:HB3	1.60	0.67
7:1G:221:GLU:OE2	9:1I:81:LYS:NZ	2.23	0.67
12:1L:357:ARG:NH1	39:1n:28:SER:OG	2.28	0.67
29:1d:2:MET:HE1	29:1d:82:MET:HG3	1.76	0.67
32:1g:117:LYS:O	32:1g:119:GLN:NE2	2.25	0.67
3:1C:94:TYR:O	3:1C:95:ASN:ND2	2.27	0.66
5:1E:31:ILE:HG22	5:1E:50:VAL:HG12	1.75	0.66
20:1T:80:ILE:HA	20:1T:83:LYS:HE3	1.77	0.66
22:1W:65:GLU:HA	22:1W:68:MET:HG2	1.76	0.66
3:1C:82:ASP:HB2	3:1C:138:PHE:HE1	1.58	0.66
6:1F:21:ILE:HG12	6:1F:230:VAL:HG13	1.77	0.66
39:1n:136:VAL:HG12	39:1n:140:GLN:HE22	1.61	0.66
40:1o:38:MET:HE2	40:1o:57:TYR:HA	1.77	0.66
7:1G:521:VAL:HG22	7:1G:542:PHE:HB3	1.77	0.66
35:1j:28:PHE:HA	35:1j:31:THR:HG22	1.76	0.66
5:1E:123:LYS:NZ	5:1E:170:GLU:OE1	2.28	0.66
5:1E:163:ASP:HB3	5:1E:186:PRO:HA	1.76	0.66
8:1H:19:PHE:HB3	26:1a:12:MET:HE1	1.76	0.66
12:1L:253:VAL:HG13	12:1L:310:LEU:HD21	1.77	0.66
1:1A:56:PHE:HZ	11:1K:75:LEU:HB3	1.61	0.66
17:1Q:126:LYS:HD2	17:1Q:127:ARG:N	2.10	0.66
5:1E:17:PRO:HD3	5:1E:63:ILE:HD11	1.77	0.66
8:1H:159:SER:H	8:1H:317:GLN:HG2	1.61	0.66
20:1T:70:LEU:HA	20:1T:75:GLU:HB3	1.76	0.66
4:1D:233:ARG:HB2	9:1I:30:LEU:HD21	1.76	0.66
8:1H:196:ALA:HB2	8:1H:274:ARG:HA	1.77	0.66
26:1a:7:PRO:HG3	51:1r:201:CDL:H172	1.77	0.66
4:1D:228:MET:HE1	9:1I:33:GLY:HA2	1.78	0.66
13:1M:134:THR:HB	14:1N:302:LEU:HD12	1.77	0.66
14:1N:162:ILE:HA	14:1N:185:ALA:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1a:57:VAL:HG13	26:1a:59:ARG:HG2	1.76	0.66
2:1B:148:GLY:HA3	2:1B:151:PRO:HG3	1.78	0.66
16:1P:128:LYS:NZ	16:1P:218:ILE:O	2.29	0.66
17:1Q:126:LYS:HE3	17:1Q:128:THR:HB	1.78	0.66
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.29	0.66
7:1G:31:GLU:OE1	7:1G:31:GLU:N	2.27	0.66
13:1M:1:FME:O1	13:1M:3:LYS:NZ	2.28	0.66
14:1N:258:SER:OG	14:1N:336:VAL:N	2.29	0.66
16:1P:82:ARG:HD2	16:1P:86:GLU:HG2	1.76	0.66
6:1F:164:LYS:HA	6:1F:172:ASP:HA	1.78	0.65
3:1C:93:VAL:HG22	3:1C:108:LYS:HG2	1.78	0.65
6:1F:150:GLN:HB3	44:1s:54:LEU:HG	1.78	0.65
7:1G:399:TRP:HE1	44:1s:74:ARG:HH12	1.42	0.65
6:1F:106:LYS:H	6:1F:257:ASN:HD21	1.43	0.65
6:1F:178:VAL:HG21	6:1F:196:ILE:HG23	1.78	0.65
13:1M:269:MET:SD	13:1M:399:ASN:ND2	2.69	0.65
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.29	0.65
5:1E:124:LEU:HD21	5:1E:139:LEU:HD13	1.77	0.65
7:1G:348:VAL:HA	7:1G:510:GLY:HA2	1.78	0.65
12:1L:331:MET:HE1	12:1L:468:ILE:HD12	1.77	0.65
16:1P:201:VAL:HG22	16:1P:235:ARG:HG2	1.77	0.65
22:1W:47:VAL:HG12	22:1W:52:LEU:HD12	1.77	0.65
4:1D:233:ARG:NH1	47:1D:501:PC1:O12	2.28	0.65
12:1L:10:THR:HA	12:1L:13:ILE:HG12	1.78	0.65
13:1M:70:THR:HA	13:1M:103:GLN:HE21	1.61	0.65
14:1N:267:ILE:HD12	14:1N:279:PRO:HB3	1.77	0.65
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.78	0.65
40:1o:21:MET:N	40:1o:21:MET:SD	2.69	0.65
5:1E:111:ARG:NH1	5:1E:150:ASN:O	2.25	0.65
6:1F:21:ILE:HG21	6:1F:230:VAL:HG22	1.79	0.65
11:1K:96:LEU:HB3	14:1N:117:GLU:HB3	1.77	0.65
16:1P:113:ILE:HD12	16:1P:114:PRO:CD	2.26	0.65
2:1B:38:ASN:ND2	2:1B:170:GLU:O	2.30	0.65
8:1H:281:ARG:HB3	8:1H:284:GLN:HG3	1.77	0.65
12:1L:121:LEU:HD22	12:1L:246:LEU:HD23	1.79	0.65
15:1O:23:LYS:HB3	15:1O:25:ILE:HG12	1.78	0.65
2:1B:91:THR:HG21	4:1D:85:ARG:HD3	1.78	0.65
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.15	0.65
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD11	1.78	0.65
57:1Y:201:PGT:H181	57:1Y:201:PGT:H382	1.78	0.65
27:1b:62:MET:HE3	27:1b:62:MET:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:30:ARG:HH12	38:1m:34:GLU:HG2	1.61	0.65
11:1K:70:GLU:HB3	14:1N:60:PHE:HE1	1.62	0.65
4:1D:34:ASN:HB3	15:1O:158:VAL:HG13	1.77	0.65
4:1D:98:GLN:NE2	9:1I:85:ALA:O	2.30	0.65
12:1L:246:LEU:O	12:1L:251:THR:OG1	2.13	0.65
17:1Q:27:GLU:N	17:1Q:27:GLU:OE1	2.28	0.65
20:1U:36:PHE:HA	20:1U:40:LEU:HD13	1.78	0.65
4:1D:158:ALA:O	4:1D:162:GLY:N	2.30	0.64
7:1G:285:ARG:HE	7:1G:558:ASP:HA	1.63	0.64
12:1L:324:LEU:HB3	12:1L:395:ILE:HD11	1.77	0.64
13:1M:43:ASN:HB2	32:1g:80:LEU:HD13	1.79	0.64
35:1j:40:PHE:O	35:1j:44:SER:OG	2.14	0.64
8:1H:193:THR:HG21	8:1H:270:PHE:HE2	1.61	0.64
9:1I:16:SER:OG	9:1I:20:ARG:NH1	2.31	0.64
5:1E:113:SER:HA	5:1E:116:ILE:HD12	1.79	0.64
6:1F:190:THR:HB	6:1F:204:ARG:HB2	1.80	0.64
9:1I:28:THR:HA	47:1I:203:PC1:H221	1.78	0.64
16:1P:203:GLN:NE2	16:1P:232:GLY:O	2.30	0.64
21:1V:39:LYS:HA	21:1V:44:ARG:HD2	1.80	0.64
24:1Y:27:ILE:HG21	45:1Y:202:3PE:H3G1	1.79	0.64
24:1Y:94:CYS:HB2	24:1Y:114:CYS:HA	1.78	0.64
2:1B:118:SER:N	2:1B:148:GLY:O	2.29	0.64
8:1H:110:SER:OG	10:1J:62:GLY:O	2.16	0.64
13:1M:54:LEU:HD13	33:1h:93:ILE:HD12	1.80	0.64
33:1h:120:GLY:O	33:1h:124:GLN:NE2	2.30	0.64
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.63	0.64
4:1D:346:ILE:HD13	7:1G:117:GLN:HA	1.79	0.64
16:1P:13:ARG:NH2	16:1P:61:PRO:O	2.24	0.64
6:1F:106:LYS:HB2	6:1F:255:LEU:HG	1.80	0.64
8:1H:105:MET:HE1	8:1H:233:MET:SD	2.37	0.64
9:1I:138:GLU:N	9:1I:138:GLU:OE2	2.31	0.64
16:1P:56:THR:HA	16:1P:59:LEU:HD23	1.79	0.64
4:1D:66:MET:HE3	4:1D:66:MET:HA	1.80	0.64
5:1E:124:LEU:HB2	5:1E:137:PHE:HD2	1.62	0.64
8:1H:24:GLU:HA	8:1H:271:LEU:HD13	1.79	0.64
12:1L:204:LEU:HD13	38:1m:124:PHE:HD2	1.62	0.64
29:1d:17:GLU:OE1	29:1d:17:GLU:N	2.25	0.64
34:1i:17:LEU:HD11	39:1n:162:LEU:HD12	1.80	0.64
11:1K:59:MET:HA	11:1K:62:ILE:HB	1.80	0.64
15:1O:24:VAL:HG13	15:1O:166:PRO:HA	1.79	0.64
15:1O:95:ARG:NH1	15:1O:281:GLU:O	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:100:ILE:HD11	5:1E:137:PHE:HB3	1.79	0.64
39:1n:167:TRP:O	39:1n:171:THR:OG1	2.15	0.64
8:1H:91:MET:O	8:1H:93:TYR:N	2.31	0.63
3:1C:8:ARG:HG3	3:1C:11:ILE:HG12	1.79	0.63
3:1C:94:TYR:HB2	3:1C:107:VAL:HG22	1.79	0.63
5:1E:150:ASN:HB3	5:1E:163:ASP:HB2	1.80	0.63
7:1G:45:ARG:HH22	7:1G:261:GLU:HG2	1.63	0.63
7:1G:255:HIS:CD2	7:1G:258:ILE:HG12	2.33	0.63
15:1O:211:LEU:HD12	15:1O:220:VAL:HG11	1.80	0.63
42:1q:6:VAL:HG12	51:1r:201:CDL:HA61	1.81	0.63
2:1B:150:PRO:HG3	4:1D:189:MET:HE2	1.80	0.63
7:1G:10:GLU:O	7:1G:75:LYS:NZ	2.31	0.63
18:1R:19:ASP:O	18:1R:25:ARG:NH2	2.28	0.63
34:1i:1:SAC:OAC	34:1i:2:GLY:N	2.31	0.63
2:1B:145:TYR:HB2	9:1I:141:THR:HG23	1.80	0.63
4:1D:292:ASP:OD1	4:1D:292:ASP:N	2.31	0.63
14:1N:63:GLN:NE2	14:1N:105:LYS:O	2.31	0.63
16:1P:20:VAL:HB	16:1P:89:ASN:H	1.61	0.63
16:1P:48:PRO:HB3	16:1P:84:VAL:HG11	1.80	0.63
16:1P:165:ILE:HB	16:1P:227:THR:HG23	1.81	0.63
34:1i:13:GLN:HE22	39:1n:156:ALA:H	1.46	0.63
10:1J:146:LEU:HA	11:1K:58:MET:HE1	1.81	0.63
12:1L:433:GLY:O	36:1k:59:ASN:ND2	2.31	0.63
14:1N:284:MET:HG3	57:1Y:201:PGT:H242	1.79	0.63
42:1q:113:HIS:ND1	42:1q:114:LYS:O	2.32	0.63
6:1F:95:VAL:HG13	6:1F:228:VAL:HG11	1.81	0.63
10:1J:82:VAL:HG13	10:1J:84:VAL:H	1.62	0.63
8:1H:24:GLU:OE2	8:1H:25:ARG:NH1	2.32	0.63
12:1L:481:THR:OG1	40:1o:91:HIS:ND1	2.30	0.63
20:1T:68:GLU:OE1	20:1T:68:GLU:N	2.30	0.63
2:1B:82:GLN:HE21	8:1H:216:ALA:HB2	1.62	0.63
7:1G:703:ILE:O	7:1G:704:CYS:HB3	1.99	0.63
20:1U:8:LEU:HA	20:1U:11:ILE:HD12	1.79	0.63
24:1Y:87:LEU:HD12	24:1Y:90:PHE:HB3	1.80	0.63
5:1E:163:ASP:OD2	5:1E:188:SER:OG	2.17	0.63
12:1L:529:TYR:CE1	12:1L:533:MET:HG3	2.33	0.63
23:1X:19:VAL:HG21	23:1X:24:LEU:HD13	1.80	0.63
25:1Z:121:MET:HE3	25:1Z:137:THR:HG22	1.79	0.63
30:1e:68:ARG:HD2	30:1e:71:THR:HG21	1.80	0.63
28:1c:38:ASP:OD2	29:1d:77:LYS:NZ	2.30	0.62
32:1g:48:ASP:N	32:1g:54:ASP:OD2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:42:MET:HE2	34:1i:42:MET:HA	1.81	0.62
2:1B:60:MET:O	2:1B:64:ALA:N	2.32	0.62
4:1D:49:LEU:HB3	4:1D:66:MET:HB2	1.80	0.62
12:1L:314:MET:HA	12:1L:317:ILE:HD12	1.81	0.62
14:1N:321:LYS:HG2	14:1N:323:MET:H	1.64	0.62
23:1X:8:THR:HA	25:1Z:88:ARG:HH11	1.64	0.62
35:1j:60:THR:HG23	35:1j:62:GLU:H	1.63	0.62
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.81	0.62
12:1L:546:GLN:HB2	13:1M:278:ARG:HE	1.63	0.62
13:1M:26:ASN:OD1	31:1f:13:HIS:NE2	2.32	0.62
41:1p:105:ILE:HG13	41:1p:134:VAL:HG21	1.80	0.62
12:1L:535:ARG:HG2	38:1m:10:LEU:HD22	1.82	0.62
28:1c:41:GLU:OE2	28:1c:45:ARG:NH1	2.32	0.62
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.17	0.62
12:1L:88:MET:HE3	12:1L:326:PHE:HE2	1.61	0.62
2:1B:171:LYS:HG2	2:1B:174:ARG:HE	1.63	0.62
6:1F:109:GLU:HG3	6:1F:112:ARG:HH21	1.64	0.62
6:1F:224:ASN:ND2	49:1F:501:FMN:O2	2.32	0.62
7:1G:272:ASP:OD1	7:1G:683:THR:OG1	2.16	0.62
12:1L:295:GLN:OE1	39:1n:77:GLN:NE2	2.33	0.62
15:1O:97:GLN:HG2	15:1O:135:LEU:HD23	1.82	0.62
22:1W:79:VAL:HA	22:1W:82:LEU:HD23	1.81	0.62
4:1D:87:THR:HG23	4:1D:102:TYR:HD2	1.65	0.62
4:1D:133:ARG:HH21	25:1Z:8:GLN:HG2	1.64	0.62
13:1M:364:LEU:HD22	13:1M:369:LEU:HD11	1.80	0.62
13:1M:430:PHE:HB3	32:1g:46:GLY:HA3	1.81	0.62
15:1O:54:ALA:O	15:1O:104:ARG:NH1	2.32	0.62
25:1Z:86:MET:HG3	25:1Z:128:ARG:HH12	1.64	0.62
43:1r:104:GLU:N	43:1r:104:GLU:OE2	2.33	0.62
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	1.82	0.62
22:1W:70:ASN:HD22	22:1W:82:LEU:HG	1.65	0.62
33:1h:109:GLU:OE1	33:1h:112:ARG:NH2	2.32	0.62
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	1.82	0.62
14:1N:106:LEU:HD21	14:1N:187:MET:HE2	1.81	0.62
25:1Z:98:MET:HE3	30:1e:78:ILE:HD13	1.82	0.62
30:1e:62:PHE:CE1	30:1e:66:LEU:HD21	2.35	0.62
3:1C:61:LEU:HD22	3:1C:124:TYR:HE2	1.65	0.62
13:1M:29:VAL:HG22	32:1g:60:VAL:HG21	1.80	0.62
15:1O:13:ARG:O	15:1O:16:ARG:NH2	2.33	0.62
18:1R:37:GLU:CD	18:1R:37:GLU:H	2.07	0.62
25:1Z:108:GLU:HB2	30:1e:74:ARG:HH12	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:113:VAL:HG13	2:1B:142:VAL:HA	1.82	0.61
14:1N:136:LEU:HG	14:1N:205:LEU:HD21	1.82	0.61
20:1U:22:TYR:HE1	36:1k:43:PRO:HB2	1.63	0.61
22:1W:29:LYS:HG3	22:1W:33:ARG:HH22	1.64	0.61
4:1D:222:ILE:HD13	4:1D:304:MET:HB3	1.80	0.61
20:1T:48:VAL:HG11	22:1W:36:TYR:HB3	1.81	0.61
4:1D:303:GLU:O	4:1D:307:SER:OG	2.14	0.61
6:1F:57:LEU:HG	6:1F:80:SER:HB2	1.81	0.61
8:1H:23:VAL:HG21	26:1a:9:ILE:HD13	1.83	0.61
16:1P:245:ILE:HA	16:1P:248:VAL:HG12	1.83	0.61
4:1D:287:ILE:H	4:1D:287:ILE:HD12	1.65	0.61
6:1F:348:ALA:HA	6:1F:376:MET:HE3	1.82	0.61
7:1G:107:ILE:O	9:1I:104:ARG:NH1	2.33	0.61
12:1L:417:SER:HB3	12:1L:493:VAL:HB	1.80	0.61
16:1P:29:PHE:HB3	16:1P:177:ARG:HH21	1.65	0.61
23:1X:126:LYS:HD3	27:1b:66:PRO:HG3	1.82	0.61
7:1G:27:LEU:HA	7:1G:37:ILE:HD13	1.82	0.61
7:1G:524:LEU:HG	7:1G:527:ALA:HB3	1.81	0.61
8:1H:92:PRO:HG3	8:1H:255:TYR:HB3	1.82	0.61
14:1N:36:ASN:HD21	14:1N:134:GLN:HE22	1.46	0.61
16:1P:30:LEU:HD23	54:1P:501:NDP:H51N	1.81	0.61
17:1Q:28:GLU:OE2	17:1Q:28:GLU:N	2.32	0.61
23:1X:54:ARG:HA	23:1X:54:ARG:CZ	2.30	0.61
4:1D:415:VAL:HA	4:1D:418:ILE:HG12	1.81	0.61
8:1H:215:TYR:HB3	8:1H:219:PRO:HB2	1.83	0.61
13:1M:196:TRP:HH2	13:1M:302:MET:HE1	1.66	0.61
13:1M:237:LYS:HB3	13:1M:316:MET:HE3	1.82	0.61
15:1O:116:LEU:HD23	15:1O:260:ARG:HG3	1.83	0.61
6:1F:31:TRP:O	6:1F:116:HIS:NE2	2.31	0.61
23:1X:3:ILE:HG22	23:1X:5:GLU:H	1.66	0.61
37:1l:7:ASP:O	37:1l:26:LYS:NZ	2.34	0.61
9:1I:5:VAL:HG23	43:1r:112:LEU:HD23	1.83	0.61
14:1N:33:PHE:HE1	14:1N:137:ALA:HB1	1.66	0.61
16:1P:226:LYS:HB3	16:1P:228:PHE:CE1	2.35	0.61
6:1F:394:GLU:HB2	7:1G:129:ARG:HH22	1.65	0.61
11:1K:20:LEU:HD13	12:1L:592:LEU:HB2	1.83	0.61
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.66	0.61
8:1H:96:ILE:HD12	25:1Z:144:THR:HG23	1.83	0.60
9:1I:27:TRP:HB3	9:1I:30:LEU:HB2	1.81	0.60
9:1I:39:SER:OG	9:1I:43:ARG:NH2	2.33	0.60
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:60:SER:HB3	13:1M:457:PRO:HA	1.83	0.60
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.33	0.60
32:1g:68:ILE:HA	32:1g:72:LEU:HB2	1.83	0.60
40:1o:7:ARG:NH2	40:1o:17:ASP:OD2	2.33	0.60
2:1B:49:THR:HG21	2:1B:59:MET:HE1	1.82	0.60
4:1D:326:ASP:O	7:1G:127:ARG:NH2	2.34	0.60
8:1H:102:VAL:HG21	8:1H:154:LEU:HD21	1.82	0.60
8:1H:142:TYR:CD1	8:1H:289:LEU:HD13	2.36	0.60
12:1L:62:ILE:HD12	41:1p:114:GLN:HB2	1.82	0.60
14:1N:236:LYS:HB2	14:1N:311:MET:HE3	1.83	0.60
3:1C:48:LEU:HD22	3:1C:105:ILE:HD12	1.83	0.60
8:1H:68:ILE:HA	8:1H:71:PHE:HB3	1.82	0.60
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.82	0.60
10:1J:5:ILE:HG21	25:1Z:142:TRP:HZ2	1.66	0.60
20:1T:37:MET:N	20:1T:37:MET:SD	2.75	0.60
42:1q:56:PHE:HZ	43:1r:33:ARG:HE	1.50	0.60
4:1D:398:HIS:HB3	4:1D:421:GLN:HG2	1.83	0.60
6:1F:148:ASN:ND2	44:1s:40:ASN:OD1	2.34	0.60
12:1L:100:ILE:HD13	12:1L:246:LEU:HB2	1.83	0.60
12:1L:338:MET:HE1	12:1L:458:LEU:HA	1.82	0.60
21:1V:54:LYS:HD2	21:1V:71:LEU:HB3	1.83	0.60
23:1X:129:LYS:HD3	27:1b:65:VAL:HG23	1.83	0.60
30:1e:46:ILE:HG22	30:1e:50:ARG:HB2	1.83	0.60
43:1r:102:ARG:HH21	43:1r:103:TRP:HB2	1.65	0.60
3:1C:111:THR:HG23	3:1C:115:THR:HB	1.82	0.60
4:1D:133:ARG:NH2	4:1D:202:ASP:OD2	2.34	0.60
7:1G:6:SER:OG	7:1G:7:ASN:N	2.35	0.60
23:1X:9:LEU:HG	25:1Z:88:ARG:HG2	1.83	0.60
4:1D:43:LEU:HD22	11:1K:86:GLY:HA3	1.82	0.60
6:1F:33:LEU:HD22	6:1F:155:GLU:HB3	1.84	0.60
14:1N:213:LEU:HD21	51:1N:402:CDL:H712	1.82	0.60
14:1N:239:VAL:HG11	29:1d:47:ALA:HB1	1.84	0.60
20:1T:46:ASP:OD2	22:1W:64:ARG:NH2	2.34	0.60
32:1g:45:HIS:HB2	32:1g:54:ASP:OD1	2.01	0.60
32:1g:58:MET:HA	32:1g:61:VAL:HG12	1.83	0.60
37:1l:157:GLU:HG2	40:1o:34:LYS:HB3	1.81	0.60
7:1G:194:GLU:HG2	7:1G:195:LEU:HD22	1.82	0.60
7:1G:290:LEU:HD22	42:1q:143:PRO:HB3	1.83	0.60
12:1L:132:VAL:O	12:1L:262:ARG:NH2	2.34	0.60
14:1N:89:MET:HE2	14:1N:98:MET:HG2	1.84	0.60
15:1O:210:PHE:O	15:1O:214:MET:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:96:ASP:OD2	42:1q:96:ASP:N	2.34	0.60
43:1r:57:ASP:OD1	43:1r:57:ASP:N	2.35	0.60
6:1F:293:ASN:HA	6:1F:339:ARG:HG2	1.84	0.60
14:1N:236:LYS:HG3	14:1N:237:MET:HG3	1.84	0.60
17:1Q:126:LYS:HD2	17:1Q:126:LYS:C	2.27	0.60
23:1X:24:LEU:HG	25:1Z:71:LEU:HD11	1.83	0.60
42:1q:47:LYS:HB2	42:1q:63:ILE:HG13	1.83	0.60
8:1H:142:TYR:OH	8:1H:285:LEU:O	2.13	0.60
10:1J:45:LEU:HD23	10:1J:50:SER:HA	1.83	0.60
11:1K:59:MET:HE2	11:1K:63:LEU:HB2	1.83	0.60
12:1L:161:ARG:HH21	12:1L:238:GLU:HG2	1.67	0.60
14:1N:313:MET:HE1	15:1O:103:SER:HA	1.84	0.60
15:1O:247:PRO:HD2	15:1O:248:TRP:H	1.67	0.60
20:1T:70:LEU:HB3	20:1T:76:ILE:HD13	1.83	0.60
23:1X:68:ASP:OD1	23:1X:71:ARG:NH2	2.32	0.60
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.83	0.60
8:1H:113:VAL:HB	8:1H:136:VAL:HG23	1.84	0.60
12:1L:393:ASP:OD1	12:1L:393:ASP:N	2.35	0.60
23:1X:72:GLN:O	23:1X:76:HIS:ND1	2.27	0.60
27:1b:15:GLU:CD	27:1b:18:LEU:HG	2.27	0.60
40:1o:49:GLN:NE2	41:1p:116:GLU:O	2.35	0.60
5:1E:195:PRO:HD2	5:1E:199:LEU:HA	1.83	0.59
7:1G:356:THR:OG1	7:1G:503:LEU:O	2.19	0.59
13:1M:207:MET:HE1	13:1M:240:GLY:HA2	1.82	0.59
14:1N:313:MET:HE3	15:1O:59:ALA:HB2	1.84	0.59
33:1h:49:GLU:OE1	33:1h:50:ALA:N	2.35	0.59
3:1C:29:VAL:HG13	3:1C:63:PHE:HE2	1.66	0.59
3:1C:155:TYR:HD2	22:1W:98:LYS:HA	1.67	0.59
6:1F:307:ILE:HD13	6:1F:311:VAL:HB	1.84	0.59
7:1G:286:ASN:OD1	7:1G:290:LEU:N	2.33	0.59
7:1G:496:ILE:HB	7:1G:499:GLN:HB2	1.83	0.59
9:1I:70:TYR:HE2	18:1R:87:CYS:HA	1.67	0.59
12:1L:306:THR:O	12:1L:310:LEU:HD12	2.02	0.59
15:1O:8:PHE:O	15:1O:13:ARG:NH1	2.31	0.59
7:1G:60:GLU:HG2	7:1G:61:LYS:HG3	1.83	0.59
7:1G:344:CYS:SG	7:1G:345:THR:N	2.75	0.59
7:1G:492:ILE:HD12	7:1G:494:HIS:HD2	1.66	0.59
9:1I:7:MET:SD	9:1I:7:MET:N	2.72	0.59
19:1S:43:LEU:HD23	19:1S:43:LEU:H	1.67	0.59
23:1X:48:GLU:HB2	23:1X:134:ARG:HH22	1.67	0.59
43:1r:32:LYS:O	43:1r:35:GLN:NE2	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:16:ASP:HA	3:1C:19:HIS:HB3	1.82	0.59
7:1G:37:ILE:H	7:1G:37:ILE:HD12	1.65	0.59
7:1G:329:VAL:HG21	7:1G:623:LEU:HB3	1.85	0.59
7:1G:470:VAL:HG22	7:1G:490:MET:HE1	1.84	0.59
8:1H:195:ARG:CG	8:1H:196:ALA:H	2.14	0.59
13:1M:285:LEU:HD22	13:1M:342:MET:HE1	1.83	0.59
19:1S:13:LEU:HD12	19:1S:14:GLY:H	1.67	0.59
23:1X:68:ASP:HA	23:1X:71:ARG:HE	1.68	0.59
2:1B:107:MET:HG2	2:1B:111:ARG:HD3	1.84	0.59
5:1E:149:VAL:HG22	5:1E:190:ARG:HH22	1.67	0.59
6:1F:129:MET:SD	6:1F:221:THR:OG1	2.53	0.59
6:1F:392:LEU:HD12	6:1F:395:ILE:HD11	1.85	0.59
7:1G:45:ARG:NH1	7:1G:261:GLU:OE1	2.35	0.59
7:1G:215:PHE:HB3	9:1I:104:ARG:HD2	1.83	0.59
16:1P:194:ILE:HB	16:1P:288:HIS:NE2	2.17	0.59
25:1Z:6:VAL:HA	43:1r:39:LYS:HB3	1.85	0.59
38:1m:36:LEU:O	38:1m:40:SER:N	2.33	0.59
3:1C:50:ILE:HB	3:1C:107:VAL:HG12	1.83	0.59
4:1D:78:PRO:HB2	4:1D:399:LEU:HD21	1.84	0.59
9:1I:62:ARG:NH2	9:1I:118:TYR:O	2.35	0.59
13:1M:355:MET:HA	13:1M:355:MET:HE2	1.84	0.59
2:1B:64:ALA:HB2	4:1D:171:PHE:HD2	1.66	0.59
7:1G:278:ARG:HH12	7:1G:548:HIS:HB2	1.68	0.59
7:1G:283:MET:HE1	7:1G:293:TYR:HD1	1.66	0.59
12:1L:296:ASN:OD1	12:1L:357:ARG:NH1	2.36	0.59
12:1L:303:ALA:O	12:1L:306:THR:OG1	2.17	0.59
13:1M:231:LEU:HD13	13:1M:235:LEU:HD21	1.83	0.59
16:1P:134:HIS:CE1	16:1P:136:ASN:HB2	2.38	0.59
21:1V:21:GLU:O	21:1V:25:ILE:HG23	2.02	0.59
35:1j:12:ARG:HB3	36:1k:50:TRP:CG	2.37	0.59
5:1E:148:CYS:N	6:1F:105:CYS:SG	2.75	0.59
6:1F:296:ALA:HA	6:1F:308:PRO:HA	1.85	0.59
6:1F:354:TYR:CE2	6:1F:411:ALA:HA	2.38	0.59
12:1L:293:ILE:HG13	12:1L:294:THR:HG23	1.83	0.59
12:1L:570:GLN:O	14:1N:167:TRP:NE1	2.34	0.59
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.84	0.59
24:1Y:123:LEU:HA	24:1Y:126:MET:HG3	1.82	0.59
30:1e:21:SER:HB3	33:1h:133:ILE:HG13	1.85	0.59
1:1A:77:TRP:HZ2	8:1H:100:LEU:HD21	1.68	0.59
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.68	0.59
7:1G:24:THR:HG23	7:1G:28:GLN:HB3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:514:LYS:O	12:1L:514:LYS:HD2	2.03	0.59
14:1N:128:LEU:HD11	14:1N:213:LEU:HG	1.84	0.59
15:1O:210:PHE:HD1	15:1O:211:LEU:HD13	1.67	0.59
21:1V:43:TYR:HE2	21:1V:93:MET:HB2	1.68	0.59
30:1e:29:PRO:HB3	33:1h:138:LYS:HG2	1.85	0.59
34:1i:71:VAL:HA	34:1i:75:LEU:HB2	1.84	0.59
5:1E:100:ILE:HB	5:1E:139:LEU:HA	1.85	0.59
5:1E:124:LEU:HD12	5:1E:126:ILE:H	1.68	0.59
8:1H:13:ILE:HD11	8:1H:229:ALA:HB1	1.85	0.59
8:1H:154:LEU:HA	8:1H:157:ASN:HB3	1.85	0.59
12:1L:533:MET:HA	45:1L:701:3PE:H361	1.85	0.59
19:1S:20:ILE:HD13	19:1S:64:LEU:HD23	1.84	0.59
20:1U:49:GLU:OE2	36:1k:44:TRP:NE1	2.36	0.59
1:1A:88:LEU:HD21	27:1b:32:PRO:HB3	1.83	0.58
4:1D:89:LYS:NZ	4:1D:92:GLU:OE2	2.36	0.58
4:1D:243:GLY:H	4:1D:409:HIS:CE1	2.21	0.58
7:1G:121:MET:HE2	7:1G:121:MET:HA	1.85	0.58
9:1I:53:GLU:HG2	42:1q:58:ARG:HA	1.84	0.58
12:1L:189:PHE:O	12:1L:193:SER:OG	2.20	0.58
13:1M:278:ARG:NH2	37:1l:80:ASP:OD1	2.36	0.58
5:1E:209:PRO:HA	6:1F:40:GLY:HA2	1.84	0.58
9:1I:79:ALA:O	9:1I:104:ARG:NH2	2.32	0.58
20:1T:61:GLU:N	20:1T:61:GLU:OE1	2.33	0.58
37:1l:136:ASN:HA	37:1l:153:VAL:HB	1.85	0.58
4:1D:230:THR:O	4:1D:294:TYR:OH	2.21	0.58
7:1G:194:GLU:OE2	7:1G:194:GLU:N	2.26	0.58
33:1h:142:ASP:O	33:1h:143:ASN:ND2	2.35	0.58
6:1F:204:ARG:HG2	17:1Q:122:PHE:HE2	1.68	0.58
7:1G:681:SER:HB3	7:1G:684:MET:HG2	1.85	0.58
16:1P:192:PRO:O	16:1P:263:TYR:OH	2.14	0.58
23:1X:131:LYS:HD2	27:1b:58:ASP:HB3	1.85	0.58
44:1s:63:MET:O	44:1s:65:GLN:NE2	2.33	0.58
1:1A:104:TYR:HE1	10:1J:166:VAL:HA	1.67	0.58
4:1D:411:LEU:HA	4:1D:414:VAL:HG23	1.86	0.58
6:1F:276:LEU:HD13	6:1F:317:MET:HE1	1.84	0.58
7:1G:524:LEU:N	7:1G:544:ILE:O	2.35	0.58
9:1I:13:ASP:OD1	9:1I:13:ASP:N	2.37	0.58
57:1Y:201:PGT:O4P	57:1Y:201:PGT:O6	2.19	0.58
25:1Z:137:THR:OG1	25:1Z:138:TYR:N	2.37	0.58
3:1C:202:PRO:O	17:1Q:50:ASN:N	2.35	0.58
4:1D:258:VAL:HG12	4:1D:296:ARG:HG2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:164:LEU:HD13	5:1E:169:ILE:HD13	1.84	0.58
6:1F:202:LYS:HE3	6:1F:361:GLN:HB2	1.85	0.58
9:1I:146:GLU:HA	42:1q:124:TYR:HD2	1.68	0.58
12:1L:276:MET:HE2	12:1L:276:MET:HA	1.86	0.58
12:1L:467:ILE:O	12:1L:471:ASN:ND2	2.34	0.58
13:1M:25:ILE:O	13:1M:29:VAL:HG23	2.04	0.58
13:1M:175:ASN:HB3	13:1M:178:ILE:HG22	1.86	0.58
32:1g:68:ILE:HG22	32:1g:72:LEU:HD12	1.84	0.58
39:1n:43:MET:HE3	39:1n:43:MET:O	2.04	0.58
42:1q:78:ASP:H	42:1q:81:MET:HE1	1.69	0.58
4:1D:287:ILE:HD13	9:1I:2:TYR:HD2	1.67	0.58
12:1L:64:SER:O	34:1i:95:THR:OG1	2.22	0.58
12:1L:405:ASN:O	12:1L:407:TRP:N	2.36	0.58
23:1X:141:TYR:HB3	25:1Z:115:ARG:HH11	1.69	0.58
5:1E:126:ILE:HD12	5:1E:127:LYS:H	1.68	0.58
5:1E:145:LEU:N	48:1E:301:FES:S1	2.75	0.58
6:1F:127:ARG:NH1	6:1F:127:ARG:O	2.36	0.58
7:1G:322:LEU:HD11	7:1G:548:HIS:HE2	1.68	0.58
9:1I:70:TYR:CD1	9:1I:76:ARG:HG2	2.39	0.58
12:1L:531:SER:HB2	37:1l:101:MET:HE1	1.86	0.58
22:1W:29:LYS:HE2	22:1W:33:ARG:HH12	1.67	0.58
29:1d:114:GLU:OE1	29:1d:114:GLU:N	2.37	0.58
2:1B:116:MET:HG3	2:1B:156:LEU:HD13	1.86	0.58
3:1C:72:PHE:CE2	3:1C:98:SER:HB3	2.39	0.58
13:1M:312:ALA:O	13:1M:316:MET:HB2	2.04	0.58
15:1O:247:PRO:HD2	15:1O:248:TRP:N	2.18	0.58
19:1S:82:SER:OG	19:1S:84:ASP:OD1	2.22	0.58
8:1H:296:LEU:HA	27:1b:21:SER:HB3	1.85	0.58
20:1U:42:LEU:HD12	20:1U:46:ASP:HB3	1.85	0.58
22:1W:80:ASP:O	22:1W:83:VAL:HG22	2.04	0.58
26:1a:70:ASP:OD1	26:1a:70:ASP:N	2.37	0.58
28:1c:32:ILE:HD12	28:1c:32:ILE:H	1.69	0.58
33:1h:95:GLN:NE2	33:1h:99:GLU:OE2	2.35	0.58
3:1C:85:THR:HB	17:1Q:86:PHE:HA	1.86	0.57
4:1D:72:MET:N	4:1D:72:MET:SD	2.74	0.57
6:1F:57:LEU:O	6:1F:61:LYS:HG2	2.03	0.57
6:1F:150:GLN:HA	6:1F:153:ILE:HG12	1.86	0.57
8:1H:132:ALA:O	8:1H:136:VAL:HG12	2.04	0.57
10:1J:157:THR:HA	11:1K:66:PHE:HZ	1.67	0.57
17:1Q:89:LYS:O	17:1Q:93:VAL:HG23	2.03	0.57
17:1Q:129:ARG:HD3	44:1s:73:PRO:HG3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:22:ASP:OD1	18:1R:24:ARG:N	2.36	0.57
23:1X:59:GLY:O	25:1Z:81:ARG:NH1	2.37	0.57
40:1o:43:GLN:OE1	40:1o:43:GLN:N	2.37	0.57
3:1C:58:ILE:HG13	3:1C:118:GLU:HG3	1.86	0.57
7:1G:285:ARG:NH2	7:1G:557:ALA:O	2.37	0.57
16:1P:201:VAL:HB	16:1P:237:LEU:HD12	1.86	0.57
16:1P:248:VAL:HA	16:1P:334:VAL:HG21	1.86	0.57
2:1B:116:MET:HE2	2:1B:151:PRO:HD2	1.84	0.57
10:1J:137:SER:O	10:1J:139:GLU:N	2.37	0.57
12:1L:6:SER:HA	34:1i:85:LEU:HD12	1.86	0.57
12:1L:49:VAL:HA	12:1L:52:LEU:HD23	1.85	0.57
13:1M:98:MET:HE2	13:1M:132:ILE:HG13	1.86	0.57
13:1M:262:LEU:HD11	13:1M:302:MET:HB2	1.86	0.57
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.04	0.57
15:1O:210:PHE:CD1	15:1O:211:LEU:HD13	2.38	0.57
15:1O:214:MET:HA	15:1O:214:MET:HE3	1.86	0.57
37:1l:125:TYR:OH	40:1o:7:ARG:NH1	2.37	0.57
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.86	0.57
5:1E:91:ASN:ND2	5:1E:93:LYS:O	2.38	0.57
7:1G:644:GLN:OE1	7:1G:644:GLN:N	2.31	0.57
10:1J:157:THR:HA	11:1K:66:PHE:CZ	2.39	0.57
13:1M:237:LYS:H	13:1M:237:LYS:HD2	1.70	0.57
15:1O:65:ASP:HB3	15:1O:67:LYS:HG2	1.86	0.57
19:1S:64:LEU:HB3	19:1S:76:VAL:HG22	1.85	0.57
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.40	0.57
23:1X:142:HIS:ND1	25:1Z:114:THR:OG1	2.37	0.57
4:1D:122:VAL:HG21	4:1D:196:PRO:HG3	1.85	0.57
5:1E:23:PHE:HB3	5:1E:27:ASN:HB2	1.86	0.57
6:1F:63:SER:O	6:1F:251:SER:OG	2.21	0.57
7:1G:198:ASN:OD1	7:1G:268:ARG:NH2	2.38	0.57
8:1H:121:TRP:CH2	10:1J:80:PRO:HG2	2.40	0.57
8:1H:313:SER:O	25:1Z:54:ASN:ND2	2.37	0.57
9:1I:168:ASN:OD1	42:1q:88:ARG:NH1	2.36	0.57
13:1M:8:THR:HA	13:1M:11:LEU:HD12	1.86	0.57
16:1P:271:GLU:HA	16:1P:277:PRO:HB3	1.87	0.57
35:1j:61:ASP:HB2	35:1j:66:ILE:HB	1.86	0.57
4:1D:179:GLU:OE1	43:1r:26:ARG:NH1	2.34	0.57
5:1E:22:ASP:OD1	5:1E:22:ASP:N	2.37	0.57
7:1G:19:MET:SD	7:1G:19:MET:N	2.70	0.57
14:1N:112:HIS:CE1	14:1N:164:ILE:HG21	2.40	0.57
31:1f:38:ARG:HH11	31:1f:54:VAL:HG21	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:40:ALA:HB2	40:1o:60:HIS:HB3	1.86	0.57
44:1s:74:ARG:NH1	44:1s:74:ARG:O	2.37	0.57
5:1E:150:ASN:ND2	5:1E:192:SER:O	2.35	0.57
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.87	0.57
10:1J:119:PHE:HA	11:1K:1:FME:HB2	1.85	0.57
20:1U:51:ILE:O	20:1U:55:GLU:N	2.35	0.57
37:1l:128:VAL:HG21	40:1o:94:TYR:HE1	1.68	0.57
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.86	0.57
6:1F:354:TYR:HE2	6:1F:411:ALA:HA	1.69	0.57
7:1G:230:VAL:HG12	7:1G:322:LEU:HB2	1.86	0.57
7:1G:591:GLY:HA2	16:1P:6:ILE:HD12	1.86	0.57
8:1H:230:ASN:HB3	8:1H:234:MET:HE2	1.86	0.57
16:1P:322:ARG:NH2	16:1P:329:SER:O	2.35	0.57
21:1V:57:MET:HG3	21:1V:70:GLN:HG2	1.85	0.57
25:1Z:143:TYR:OH	26:1a:37:ARG:O	2.22	0.57
36:1k:12:LYS:O	36:1k:12:LYS:HD3	2.05	0.57
39:1n:153:LEU:HD11	39:1n:164:PRO:HB2	1.86	0.57
40:1o:65:LEU:HD11	40:1o:83:GLN:HG2	1.85	0.57
45:1A:201:3PE:H3A1	27:1b:22:PHE:HB3	1.86	0.57
3:1C:112:ASP:O	3:1C:114:LEU:N	2.37	0.57
7:1G:378:LEU:HB2	7:1G:451:VAL:HG22	1.87	0.57
13:1M:294:MET:HA	13:1M:294:MET:HE3	1.85	0.57
19:1S:15:LEU:HA	19:1S:68:TYR:HD1	1.69	0.57
25:1Z:48:TRP:HE1	25:1Z:52:LYS:HD2	1.70	0.57
32:1g:94:GLU:OE1	32:1g:95:ARG:N	2.34	0.57
14:1N:266:ILE:HG21	14:1N:282:MET:HE1	1.86	0.57
15:1O:195:THR:HG23	15:1O:198:TYR:H	1.70	0.57
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.23	0.57
20:1T:12:LYS:NZ	20:1T:74:GLN:OE1	2.38	0.57
40:1o:50:LEU:HD21	40:1o:59:ALA:HB1	1.87	0.57
13:1M:237:LYS:HG3	13:1M:316:MET:HG2	1.87	0.56
30:1e:66:LEU:H	30:1e:66:LEU:HD22	1.70	0.56
43:1r:102:ARG:HE	43:1r:103:TRP:N	2.03	0.56
7:1G:216:THR:O	7:1G:243:ARG:NH2	2.38	0.56
8:1H:310:MET:HE3	8:1H:310:MET:HA	1.86	0.56
12:1L:83:ASP:N	12:1L:86:SER:OG	2.36	0.56
13:1M:198:ALA:HB2	57:1Y:201:PGT:H372	1.86	0.56
15:1O:144:ILE:HD13	15:1O:148:CYS:HB2	1.87	0.56
16:1P:228:PHE:CE2	16:1P:303:LEU:HD21	2.40	0.56
17:1Q:10:LEU:HB3	22:1W:16:SER:HB3	1.87	0.56
3:1C:175:ARG:NH1	3:1C:186:GLU:OE2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:25:LEU:O	6:1F:113:HIS:ND1	2.35	0.56
9:1I:107:THR:HG22	18:1R:14:THR:HB	1.87	0.56
14:1N:270:MET:HB2	14:1N:279:PRO:HG3	1.87	0.56
15:1O:28:ASP:OD2	15:1O:126:ARG:NH1	2.38	0.56
20:1U:86:VAL:O	34:1i:19:ARG:NE	2.39	0.56
25:1Z:101:VAL:HG11	25:1Z:104:TRP:HE3	1.69	0.56
29:1d:107:LYS:HB2	29:1d:112:ILE:HD11	1.86	0.56
34:1i:24:ASP:OD2	39:1n:124:TRP:NE1	2.35	0.56
39:1n:108:PRO:HA	39:1n:111:LYS:HB2	1.86	0.56
2:1B:171:LYS:HB3	2:1B:174:ARG:HB3	1.87	0.56
6:1F:273:SER:HA	6:1F:316:LEU:HB3	1.87	0.56
13:1M:19:LYS:HB3	13:1M:22:MET:HB2	1.87	0.56
15:1O:63:THR:HG23	15:1O:302:ARG:HH22	1.70	0.56
27:1b:14:LYS:HD3	27:1b:14:LYS:N	2.18	0.56
32:1g:40:LYS:HA	32:1g:40:LYS:HE2	1.88	0.56
32:1g:64:PHE:HA	32:1g:68:ILE:HD11	1.87	0.56
32:1g:72:LEU:HD22	47:1h:201:PC1:H3A1	1.88	0.56
32:1g:109:GLU:O	41:1p:141:ARG:NH2	2.37	0.56
34:1i:45:PHE:HA	34:1i:48:LYS:HE2	1.85	0.56
3:1C:150:ARG:NH2	3:1C:156:GLY:H	2.04	0.56
12:1L:384:PRO:HA	12:1L:389:PHE:CD2	2.41	0.56
13:1M:70:THR:HA	13:1M:103:GLN:NE2	2.19	0.56
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.06	0.56
32:1g:83:TYR:O	32:1g:86:GLN:NE2	2.38	0.56
4:1D:22:THR:HG23	4:1D:24:GLU:H	1.71	0.56
4:1D:88:GLU:OE2	4:1D:430:ARG:NE	2.29	0.56
8:1H:130:ILE:O	8:1H:134:ARG:HG2	2.06	0.56
12:1L:60:GLU:OE1	34:1i:99:ARG:NH2	2.39	0.56
20:1U:36:PHE:HB3	20:1U:42:LEU:HD21	1.88	0.56
23:1X:89:ASP:OD1	23:1X:89:ASP:N	2.37	0.56
26:1a:67:GLU:CD	26:1a:67:GLU:H	2.14	0.56
39:1n:175:GLU:O	39:1n:176:ARG:NH1	2.33	0.56
3:1C:125:LYS:NZ	4:1D:252:ASN:OD1	2.39	0.56
4:1D:83:LEU:O	4:1D:83:LEU:HD13	2.06	0.56
5:1E:161:TYR:HD1	5:1E:184:PRO:HA	1.71	0.56
6:1F:189:GLU:HA	6:1F:222:VAL:HG11	1.86	0.56
14:1N:7:THR:HG23	51:1N:402:CDL:H111	1.88	0.56
15:1O:13:ARG:O	15:1O:17:LYS:NZ	2.39	0.56
20:1T:46:ASP:HA	22:1W:64:ARG:HH12	1.71	0.56
22:1W:89:GLU:O	22:1W:93:THR:HG23	2.05	0.56
23:1X:95:LEU:HD13	23:1X:97:ARG:HG2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:66:PHE:O	32:1g:71:VAL:HG23	2.06	0.56
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.06	0.56
43:1r:63:MET:HE3	43:1r:64:PRO:CD	2.35	0.56
1:1A:71:LEU:HD11	10:1J:157:THR:HG21	1.88	0.56
4:1D:193:TYR:HE1	4:1D:201:GLN:H	1.52	0.56
7:1G:180:ASP:OD1	7:1G:180:ASP:N	2.33	0.56
13:1M:5:ILE:HD13	13:1M:108:MET:HG3	1.87	0.56
15:1O:241:LEU:HD13	15:1O:243:CYS:H	1.71	0.56
33:1h:134:ASP:OD1	33:1h:136:SER:OG	2.22	0.56
2:1B:90:GLY:HA2	46:1B:201:SF4:S2	2.46	0.56
4:1D:226:GLU:HG3	25:1Z:23:ARG:HG3	1.88	0.56
5:1E:9:HIS:CD2	5:1E:63:ILE:HD13	2.40	0.56
6:1F:145:GLU:N	6:1F:145:GLU:OE2	2.39	0.56
7:1G:254:MET:HE1	17:1Q:42:ARG:H	1.71	0.56
19:1S:25:ARG:O	19:1S:25:ARG:NE	2.39	0.56
6:1F:134:ALA:HB3	6:1F:175:VAL:HA	1.88	0.56
7:1G:241:SER:OG	7:1G:249:ARG:O	2.18	0.56
10:1J:68:PHE:CE1	11:1K:75:LEU:HD21	2.41	0.56
16:1P:84:VAL:HG23	16:1P:85:VAL:HG13	1.86	0.56
21:1V:35:GLY:HA2	21:1V:44:ARG:HH22	1.69	0.56
24:1Y:85:ASP:OD1	24:1Y:88:ASN:N	2.39	0.56
32:1g:75:THR:HG21	33:1h:36:VAL:HG11	1.87	0.56
37:1l:85:ILE:HG12	37:1l:86:ARG:H	1.70	0.56
7:1G:331:LEU:HG	7:1G:525:LEU:HD13	1.88	0.55
10:1J:163:ILE:HA	10:1J:166:VAL:HG22	1.86	0.55
12:1L:170:GLN:HE21	12:1L:232:TRP:HA	1.70	0.55
12:1L:560:THR:O	12:1L:565:THR:OG1	2.24	0.55
20:1U:21:LEU:HD21	36:1k:47:ASN:HA	1.87	0.55
25:1Z:96:ILE:O	25:1Z:99:LYS:NZ	2.39	0.55
2:1B:54:CYS:SG	4:1D:190:HIS:NE2	2.70	0.55
5:1E:56:ARG:NE	44:1s:48:THR:O	2.40	0.55
6:1F:204:ARG:HG2	17:1Q:122:PHE:CE2	2.41	0.55
47:1I:203:PC1:H11	25:1Z:29:GLY:HA3	1.88	0.55
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.22	0.55
12:1L:367:PRO:HG3	35:1j:22:LEU:HD23	1.89	0.55
16:1P:134:HIS:HE1	16:1P:136:ASN:HB2	1.70	0.55
19:1S:92:ASN:O	19:1S:95:SER:OG	2.23	0.55
23:1X:137:PRO:HG2	23:1X:140:PRO:HG3	1.88	0.55
36:1k:11:SER:OG	36:1k:12:LYS:N	2.33	0.55
1:1A:1:FME:HA	1:1A:1:FME:HE3	1.88	0.55
5:1E:107:PRO:HB2	5:1E:148:CYS:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:186:PRO:HG2	5:1E:191:PHE:O	2.06	0.55
8:1H:5:ASN:HD21	26:1a:23:THR:HG22	1.70	0.55
12:1L:191:THR:O	38:1m:125:ASN:ND2	2.34	0.55
14:1N:28:LEU:HA	14:1N:31:ILE:HB	1.87	0.55
14:1N:108:LEU:HB3	14:1N:161:SER:HB2	1.88	0.55
16:1P:328:THR:HG23	22:1W:51:GLN:HE22	1.71	0.55
23:1X:121:LEU:HD13	25:1Z:62:ILE:HD11	1.88	0.55
34:1i:107:ASP:H	40:1o:67:LYS:HZ2	1.55	0.55
38:1m:34:GLU:HA	39:1n:149:ARG:NH1	2.21	0.55
4:1D:86:GLY:O	4:1D:90:LEU:HD12	2.07	0.55
15:1O:1:LEU:HD11	15:1O:4:GLY:HA3	1.88	0.55
16:1P:201:VAL:HA	16:1P:237:LEU:HA	1.88	0.55
18:1R:52:VAL:HB	18:1R:57:ILE:HG12	1.87	0.55
3:1C:109:THR:OG1	3:1C:110:TYR:N	2.40	0.55
4:1D:228:MET:O	4:1D:232:ASN:ND2	2.38	0.55
6:1F:143:TYR:OH	44:1s:47:SER:O	2.25	0.55
7:1G:380:VAL:HG23	7:1G:409:ILE:HB	1.88	0.55
9:1I:133:GLU:N	9:1I:133:GLU:OE1	2.39	0.55
13:1M:209:LEU:HD21	13:1M:264:LEU:HD13	1.88	0.55
19:1S:13:LEU:HB2	19:1S:68:TYR:HB3	1.88	0.55
22:1W:75:ASP:OD2	22:1W:77:ARG:HG2	2.07	0.55
37:1l:100:THR:O	37:1l:104:HIS:ND1	2.39	0.55
4:1D:311:ILE:H	4:1D:311:ILE:HD12	1.71	0.55
7:1G:534:ARG:HG3	7:1G:537:LEU:HD11	1.88	0.55
12:1L:482:MET:SD	12:1L:482:MET:N	2.80	0.55
16:1P:63:GLY:HA3	16:1P:68:ILE:HD11	1.88	0.55
25:1Z:103:ASP:N	25:1Z:103:ASP:OD1	2.37	0.55
29:1d:17:GLU:H	29:1d:17:GLU:CD	2.15	0.55
29:1d:115:GLU:CD	29:1d:115:GLU:H	2.12	0.55
30:1e:72:MET:O	30:1e:76:SER:N	2.29	0.55
34:1i:10:ARG:HA	34:1i:13:GLN:HE21	1.72	0.55
38:1m:2:PHE:CD2	39:1n:72:TYR:HB2	2.42	0.55
1:1A:72:LEU:HA	10:1J:147:TYR:OH	2.07	0.55
2:1B:63:ALA:HA	2:1B:69:MET:HB2	1.87	0.55
4:1D:405:MET:HE3	4:1D:421:GLN:HE21	1.72	0.55
14:1N:278:MET:HB3	14:1N:279:PRO:HD3	1.89	0.55
17:1Q:33:ARG:NH2	17:1Q:77:ASP:OD1	2.38	0.55
20:1U:37:MET:HB2	20:1U:38:LYS:HE2	1.88	0.55
39:1n:50:HIS:ND1	39:1n:50:HIS:O	2.39	0.55
39:1n:100:GLU:O	39:1n:121:ARG:NH2	2.40	0.55
6:1F:45:THR:HB	6:1F:123:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:528:ASP:OD2	7:1G:545:TYR:OH	2.21	0.55
7:1G:588:THR:HB	22:1W:126:HIS:CE1	2.41	0.55
14:1N:40:MET:HE1	14:1N:134:GLN:CD	2.31	0.55
16:1P:23:VAL:HG12	16:1P:26:ALA:HB2	1.89	0.55
16:1P:174:ARG:NH1	16:1P:316:GLU:OE2	2.34	0.55
21:1V:48:GLU:OE1	21:1V:52:ASN:ND2	2.30	0.55
27:1b:27:LEU:O	27:1b:31:LEU:HD12	2.06	0.55
39:1n:43:MET:HE1	39:1n:46:ARG:HH21	1.71	0.55
39:1n:83:GLU:CD	39:1n:83:GLU:H	2.15	0.55
2:1B:51:GLY:HA2	2:1B:89:ALA:HB3	1.87	0.55
4:1D:261:ARG:NH1	4:1D:268:ASP:OD2	2.39	0.55
4:1D:307:SER:O	4:1D:311:ILE:HD12	2.07	0.55
13:1M:329:LEU:HD23	13:1M:359:TRP:CD2	2.42	0.55
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.70	0.55
23:1X:93:LEU:HB2	23:1X:95:LEU:HD23	1.89	0.55
29:1d:119:VAL:HG21	41:1p:146:GLY:HA2	1.89	0.55
1:1A:97:LEU:HD22	10:1J:162:LEU:HD12	1.88	0.55
7:1G:127:ARG:NH1	43:1r:45:SER:OG	2.40	0.55
7:1G:254:MET:HE1	17:1Q:42:ARG:N	2.22	0.55
8:1H:63:PRO:HG3	8:1H:214:GLU:OE2	2.07	0.55
20:1T:76:ILE:O	20:1T:80:ILE:HG22	2.07	0.55
21:1V:58:VAL:HA	21:1V:67:LEU:HD21	1.89	0.55
1:1A:68:GLU:OE2	10:1J:161:LEU:HB3	2.06	0.54
5:1E:190:ARG:NH1	6:1F:265:PRO:HG2	2.22	0.54
7:1G:383:ASN:HD21	7:1G:386:PHE:HD2	1.54	0.54
11:1K:34:GLU:HA	11:1K:37:MET:HE3	1.89	0.54
11:1K:36:MET:O	11:1K:40:LEU:N	2.28	0.54
12:1L:429:PHE:O	12:1L:436:ARG:NH2	2.40	0.54
15:1O:62:THR:HG21	15:1O:106:LEU:HD21	1.89	0.54
16:1P:146:LEU:HD11	16:1P:289:MET:HE1	1.88	0.54
40:1o:95:VAL:O	40:1o:99:LYS:HG2	2.07	0.54
41:1p:6:LYS:NZ	41:1p:11:GLU:O	2.40	0.54
2:1B:110:PRO:HD2	8:1H:58:LYS:HE3	1.89	0.54
2:1B:127:HIS:CE1	2:1B:134:ARG:HG2	2.42	0.54
2:1B:145:TYR:CZ	9:1I:144:HIS:HB2	2.42	0.54
4:1D:378:LEU:HA	4:1D:389:CYS:HA	1.89	0.54
15:1O:155:VAL:O	15:1O:159:THR:OG1	2.24	0.54
20:1T:22:TYR:OH	20:1T:49:GLU:OE2	2.21	0.54
20:1T:82:ASP:OD1	20:1T:83:LYS:N	2.41	0.54
36:1k:48:GLU:O	36:1k:50:TRP:N	2.40	0.54
39:1n:132:TRP:O	39:1n:136:VAL:HG23	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:109:VAL:HG22	4:1D:149:ASN:HA	1.88	0.54
8:1H:193:THR:HG21	8:1H:270:PHE:CE2	2.42	0.54
9:1I:168:ASN:HD21	42:1q:93:MET:HE1	1.73	0.54
12:1L:294:THR:O	12:1L:295:GLN:NE2	2.40	0.54
13:1M:65:LEU:HD11	13:1M:316:MET:HE1	1.89	0.54
14:1N:324:LYS:NZ	51:1N:402:CDL:OB4	2.34	0.54
16:1P:154:LYS:HD3	16:1P:154:LYS:N	2.21	0.54
18:1R:53:GLY:HA2	18:1R:93:GLN:HE22	1.72	0.54
28:1c:32:ILE:HG22	28:1c:36:LYS:HE3	1.88	0.54
4:1D:220:PHE:HE1	43:1r:17:ARG:HE	1.55	0.54
7:1G:107:ILE:HD12	9:1I:104:ARG:HH11	1.71	0.54
13:1M:329:LEU:HD21	13:1M:359:TRP:HA	1.90	0.54
17:1Q:57:MET:HG3	17:1Q:86:PHE:HE2	1.71	0.54
1:1A:63:LEU:HD11	10:1J:64:MET:HG3	1.88	0.54
4:1D:226:GLU:OE1	4:1D:230:THR:OG1	2.25	0.54
6:1F:137:TYR:HB3	6:1F:192:LEU:HD11	1.89	0.54
7:1G:492:ILE:HD12	7:1G:494:HIS:CD2	2.43	0.54
12:1L:278:LEU:HB3	12:1L:318:GLY:HA3	1.89	0.54
14:1N:161:SER:OG	14:1N:184:ILE:O	2.26	0.54
24:1Y:130:GLU:HB2	24:1Y:132:TRP:NE1	2.22	0.54
32:1g:65:GLY:O	32:1g:69:VAL:HG22	2.07	0.54
37:1l:77:ILE:HD11	38:1m:67:TRP:CG	2.42	0.54
3:1C:80:ALA:H	3:1C:134:ILE:HD11	1.73	0.54
3:1C:128:ASN:HA	3:1C:145:HIS:HE2	1.73	0.54
3:1C:150:ARG:HH21	22:1W:92:GLU:HG3	1.71	0.54
3:1C:167:PRO:HA	17:1Q:82:LEU:HD11	1.90	0.54
5:1E:43:LYS:NZ	5:1E:74:GLN:HE22	2.05	0.54
6:1F:246:GLY:N	6:1F:271:GLU:OE2	2.40	0.54
6:1F:342:ASP:HB3	6:1F:345:LYS:HB3	1.88	0.54
7:1G:362:TYR:OH	19:1S:55:ARG:NH1	2.41	0.54
7:1G:620:ARG:NE	7:1G:633:TYR:OH	2.38	0.54
3:1C:35:LYS:HG2	21:1V:103:VAL:HG23	1.90	0.54
10:1J:129:ASP:OD1	10:1J:130:THR:N	2.41	0.54
12:1L:233:LEU:HD11	12:1L:253:VAL:HG21	1.89	0.54
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.72	0.54
17:1Q:70:MET:HE3	17:1Q:72:TRP:CZ2	2.42	0.54
24:1Y:94:CYS:HB2	24:1Y:114:CYS:CA	2.37	0.54
31:1f:45:LYS:O	41:1p:68:ARG:NH2	2.39	0.54
35:1j:54:PRO:HB2	35:1j:59:TRP:HE1	1.73	0.54
3:1C:53:HIS:NE2	21:1V:104:GLU:OE2	2.34	0.54
3:1C:87:GLN:H	3:1C:87:GLN:CD	2.16	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:254:MET:HA	7:1G:260:GLU:O	2.07	0.54
12:1L:8:THR:HG21	12:1L:82:MET:HG3	1.90	0.54
12:1L:142:ILE:HD13	13:1M:370:PRO:HB2	1.90	0.54
20:1U:88:GLU:N	20:1U:88:GLU:OE1	2.41	0.54
39:1n:134:ARG:HH21	39:1n:161:ASP:HB2	1.72	0.54
1:1A:69:ILE:HG12	8:1H:148:ILE:HD11	1.90	0.54
2:1B:27:GLU:OE1	2:1B:174:ARG:NH1	2.35	0.54
7:1G:171:ASP:OD2	7:1G:189:LYS:NZ	2.33	0.54
7:1G:673:MET:HG2	7:1G:688:VAL:HG11	1.89	0.54
8:1H:149:ILE:HG23	8:1H:181:LEU:HD12	1.89	0.54
12:1L:237:MET:SD	12:1L:303:ALA:HB2	2.48	0.54
18:1R:39:PHE:O	18:1R:43:LEU:HD12	2.07	0.54
24:1Y:91:ILE:HD12	24:1Y:92:GLY:N	2.23	0.54
37:1l:65:ASP:OD1	38:1m:43:LYS:NZ	2.41	0.54
40:1o:93:ASP:N	40:1o:93:ASP:OD1	2.41	0.54
1:1A:92:LEU:HD12	8:1H:302:MET:HG2	1.90	0.54
6:1F:402:HIS:O	7:1G:53:ARG:NE	2.33	0.54
8:1H:92:PRO:HG2	8:1H:256:THR:HG23	1.90	0.54
19:1S:79:ASN:OD1	19:1S:80:ASN:ND2	2.41	0.54
27:1b:59:ASP:OD1	27:1b:59:ASP:N	2.34	0.54
29:1d:34:MET:HA	29:1d:37:LEU:HD12	1.89	0.54
39:1n:122:GLU:OE1	39:1n:123:GLN:NE2	2.41	0.54
40:1o:44:GLU:HA	40:1o:47:ASP:HB3	1.89	0.54
2:1B:68:ASP:CG	2:1B:71:ARG:HB3	2.32	0.53
3:1C:99:LEU:HD11	4:1D:251:LEU:HD11	1.90	0.53
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.08	0.53
8:1H:316:PRO:HG3	25:1Z:57:ARG:HB3	1.89	0.53
13:1M:300:ALA:O	13:1M:308:SER:OG	2.23	0.53
16:1P:111:VAL:C	16:1P:114:PRO:HD2	2.33	0.53
25:1Z:10:MET:SD	25:1Z:11:PRO:HD2	2.48	0.53
26:1a:27:HIS:O	26:1a:31:ASN:ND2	2.29	0.53
33:1h:114:MET:HE3	33:1h:120:GLY:HA3	1.90	0.53
47:1I:203:PC1:H121	25:1Z:35:MET:HE1	1.90	0.53
10:1J:40:GLY:HA2	10:1J:43:ILE:HD12	1.89	0.53
14:1N:36:ASN:ND2	14:1N:134:GLN:HE22	2.05	0.53
19:1S:68:TYR:HE2	19:1S:74:LYS:HG2	1.72	0.53
20:1U:40:LEU:HD12	20:1U:40:LEU:H	1.74	0.53
23:1X:18:LYS:HD2	26:1a:54:ILE:HD11	1.90	0.53
34:1i:72:THR:HG23	34:1i:73:HIS:ND1	2.23	0.53
38:1m:2:PHE:HD2	39:1n:72:TYR:HB2	1.73	0.53
2:1B:155:ALA:HB2	9:1I:137:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:290:ARG:N	4:1D:295:ASP:OD2	2.41	0.53
4:1D:336:ALA:O	4:1D:340:THR:OG1	2.25	0.53
5:1E:105:THR:HA	6:1F:349:ARG:HG3	1.89	0.53
7:1G:181:MET:HA	7:1G:181:MET:HE3	1.89	0.53
12:1L:370:THR:O	12:1L:374:ILE:HG12	2.07	0.53
16:1P:157:ARG:NH1	16:1P:225:GLY:O	2.40	0.53
25:1Z:26:PRO:HD3	43:1r:17:ARG:HH22	1.73	0.53
2:1B:52:LEU:N	2:1B:89:ALA:O	2.30	0.53
4:1D:201:GLN:NE2	9:1I:176:ARG:HA	2.24	0.53
8:1H:114:TYR:HB3	8:1H:118:TRP:CH2	2.43	0.53
8:1H:281:ARG:HD2	8:1H:283:ASP:H	1.73	0.53
11:1K:8:ILE:HB	11:1K:43:MET:HE3	1.90	0.53
16:1P:14:SER:O	17:1Q:65:TRP:NE1	2.32	0.53
17:1Q:97:GLU:OE1	17:1Q:97:GLU:N	2.31	0.53
22:1W:69:LYS:O	22:1W:72:HIS:NE2	2.41	0.53
7:1G:218:ARG:HD2	7:1G:220:TRP:CZ3	2.44	0.53
7:1G:617:ASP:OD1	7:1G:617:ASP:N	2.41	0.53
8:1H:16:ALA:O	8:1H:20:LEU:N	2.41	0.53
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.44	0.53
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.37	0.53
17:1Q:19:ILE:HG22	17:1Q:98:LYS:O	2.09	0.53
19:1S:18:ILE:HG23	19:1S:52:ILE:HA	1.91	0.53
20:1U:37:MET:HE1	20:1U:44:SER:HA	1.91	0.53
40:1o:91:HIS:O	40:1o:95:VAL:HG13	2.08	0.53
4:1D:19:MET:HE2	14:1N:173:THR:HG22	1.91	0.53
4:1D:103:PHE:HA	4:1D:106:LEU:HD12	1.91	0.53
4:1D:218:PHE:O	4:1D:222:ILE:HG13	2.09	0.53
13:1M:420:THR:HB	13:1M:423:ILE:HG12	1.90	0.53
15:1O:116:LEU:HB3	15:1O:260:ARG:HD2	1.90	0.53
23:1X:18:LYS:H	26:1a:69:ILE:HD11	1.72	0.53
23:1X:97:ARG:HA	23:1X:100:ARG:HE	1.74	0.53
31:1f:43:LEU:HD21	41:1p:67:PHE:HD1	1.73	0.53
1:1A:87:MET:HA	10:1J:147:TYR:HB3	1.91	0.53
3:1C:189:GLU:HG3	16:1P:12:GLY:HA3	1.91	0.53
4:1D:101:PRO:HG3	9:1I:121:PHE:HE2	1.73	0.53
4:1D:234:ILE:HB	8:1H:278:PRO:HG2	1.90	0.53
5:1E:27:ASN:O	5:1E:31:ILE:HG13	2.08	0.53
7:1G:619:VAL:O	7:1G:623:LEU:HD23	2.08	0.53
12:1L:343:SER:O	12:1L:346:ILE:HG13	2.09	0.53
16:1P:115:HIS:HB2	16:1P:155:GLU:HB3	1.91	0.53
20:1T:6:LEU:HD12	20:1T:84:LYS:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.42	0.53
2:1B:46:TRP:O	2:1B:83:SER:OG	2.21	0.53
10:1J:117:PHE:HE2	11:1K:9:ILE:HG12	1.73	0.53
15:1O:27:VAL:HB	15:1O:39:ALA:HB2	1.91	0.53
19:1S:57:CYS:HB3	19:1S:60:VAL:HG11	1.91	0.53
30:1e:5:VAL:HG22	30:1e:9:LEU:HD12	1.91	0.53
34:1i:22:LEU:HA	34:1i:25:GLN:HG2	1.90	0.53
43:1r:8:GLN:O	43:1r:12:ASN:ND2	2.42	0.53
2:1B:92:LEU:HB3	2:1B:133:VAL:HG22	1.90	0.53
3:1C:90:PHE:CD2	3:1C:140:VAL:HB	2.44	0.53
3:1C:175:ARG:HE	16:1P:13:ARG:HH21	1.57	0.53
4:1D:101:PRO:HB3	4:1D:105:ARG:NH2	2.21	0.53
5:1E:55:GLN:HB2	5:1E:61:LEU:HD23	1.91	0.53
6:1F:302:SER:OG	6:1F:303:SER:N	2.41	0.53
7:1G:286:ASN:OD1	7:1G:289:GLY:N	2.40	0.53
7:1G:348:VAL:O	7:1G:459:GLN:NE2	2.41	0.53
7:1G:378:LEU:HD21	7:1G:439:PHE:CZ	2.44	0.53
9:1I:31:VAL:HG12	47:1I:203:PC1:H321	1.91	0.53
14:1N:123:SER:OG	14:1N:125:GLN:OE1	2.27	0.53
19:1S:32:VAL:O	19:1S:36:ILE:HG12	2.09	0.53
19:1S:61:GLN:NE2	19:1S:63:LYS:HE2	2.22	0.53
22:1W:70:ASN:OD1	22:1W:70:ASN:N	2.42	0.53
39:1n:169:ILE:O	39:1n:172:ARG:NH1	2.38	0.53
9:1I:113:MET:HE1	9:1I:118:TYR:HE2	1.74	0.53
13:1M:79:ALA:HB2	13:1M:436:LEU:HD11	1.90	0.53
13:1M:135:ARG:HB2	14:1N:302:LEU:HD13	1.91	0.53
16:1P:100:GLU:OE1	16:1P:106:PHE:HB2	2.09	0.53
21:1V:85:ASN:O	21:1V:89:LEU:N	2.29	0.53
27:1b:82:ASN:N	27:1b:82:ASN:OD1	2.42	0.53
39:1n:28:SER:OG	39:1n:75:HIS:ND1	2.42	0.53
5:1E:46:ALA:O	5:1E:50:VAL:HG22	2.08	0.52
6:1F:150:GLN:CB	44:1s:54:LEU:HG	2.39	0.52
6:1F:298:ILE:HG13	6:1F:306:LEU:HD12	1.90	0.52
9:1I:146:GLU:HA	42:1q:124:TYR:CD2	2.44	0.52
13:1M:73:LEU:HD21	13:1M:100:ILE:HD13	1.91	0.52
15:1O:194:ILE:HD11	15:1O:198:TYR:HB3	1.90	0.52
16:1P:169:SER:HB3	16:1P:231:VAL:HG22	1.90	0.52
20:1T:29:LYS:O	20:1T:29:LYS:HD2	2.09	0.52
20:1U:61:GLU:OE1	39:1n:81:PHE:HB2	2.09	0.52
27:1b:12:TRP:HD1	27:1b:19:VAL:HG11	1.74	0.52
36:1k:18:TYR:HB2	36:1k:19:LYS:NZ	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:138:GLN:NE2	39:1n:155:PRO:O	2.40	0.52
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.21	0.52
6:1F:144:ASN:HB3	44:1s:43:HIS:HB2	1.91	0.52
7:1G:348:VAL:H	7:1G:459:GLN:CD	2.17	0.52
11:1K:5:TYR:HA	11:1K:43:MET:HE1	1.91	0.52
12:1L:65:ASN:HD21	12:1L:78:LEU:HD23	1.74	0.52
12:1L:217:LEU:HD12	12:1L:277:THR:HG22	1.90	0.52
14:1N:155:LEU:HD21	14:1N:196:TYR:HE2	1.73	0.52
25:1Z:144:THR:O	26:1a:36:LYS:NZ	2.42	0.52
7:1G:58:GLU:H	7:1G:86:SER:HB3	1.75	0.52
7:1G:231:MET:HB2	7:1G:267:THR:HG22	1.91	0.52
7:1G:444:LYS:NZ	7:1G:476:ASN:O	2.42	0.52
8:1H:12:PRO:HB3	26:1a:18:ILE:HD11	1.90	0.52
21:1V:63:ASP:HB3	21:1V:66:LYS:HB2	1.91	0.52
24:1Y:130:GLU:HB2	24:1Y:132:TRP:HE1	1.74	0.52
37:1l:4:VAL:HG23	37:1l:8:MET:HB2	1.91	0.52
38:1m:2:PHE:HD1	38:1m:3:PRO:CD	2.23	0.52
38:1m:2:PHE:HD1	38:1m:3:PRO:HD2	1.75	0.52
40:1o:14:LYS:HD2	40:1o:112:LYS:HE3	1.91	0.52
3:1C:57:VAL:O	3:1C:61:LEU:HB2	2.10	0.52
3:1C:116:PRO:HB3	3:1C:143:ALA:HB2	1.91	0.52
4:1D:238:ARG:NH1	8:1H:279:ARG:O	2.43	0.52
5:1E:9:HIS:CD2	5:1E:63:ILE:HG21	2.45	0.52
5:1E:45:ALA:HA	6:1F:198:GLY:N	2.24	0.52
5:1E:100:ILE:H	5:1E:100:ILE:HD12	1.74	0.52
19:1S:72:GLN:OE1	19:1S:73:GLU:N	2.42	0.52
22:1W:34:GLU:OE1	22:1W:34:GLU:N	2.36	0.52
25:1Z:93:GLU:O	25:1Z:97:ILE:HG22	2.10	0.52
30:1e:67:LEU:H	30:1e:67:LEU:HD23	1.75	0.52
1:1A:90:MET:HE1	10:1J:151:THR:HA	1.92	0.52
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.39	0.52
7:1G:539:LYS:HD3	7:1G:540:ASP:H	1.73	0.52
12:1L:12:LEU:HA	12:1L:15:LEU:HD12	1.92	0.52
13:1M:39:LEU:HA	13:1M:42:LEU:HD23	1.92	0.52
13:1M:373:ILE:HD11	13:1M:448:THR:HA	1.91	0.52
15:1O:138:MET:HG3	15:1O:143:PHE:HB2	1.91	0.52
15:1O:316:TRP:O	15:1O:320:LYS:HG3	2.09	0.52
41:1p:89:MET:HB3	41:1p:93:ARG:HH21	1.75	0.52
4:1D:134:ALA:O	4:1D:138:ARG:HG2	2.10	0.52
5:1E:203:THR:OG1	5:1E:204:GLU:OE1	2.18	0.52
8:1H:193:THR:HB	8:1H:231:ILE:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:37:MET:HA	11:1K:40:LEU:HD12	1.91	0.52
11:1K:59:MET:HB2	14:1N:27:LEU:HD22	1.91	0.52
13:1M:158:LEU:HD23	14:1N:283:ALA:HB1	1.91	0.52
15:1O:130:SER:O	15:1O:133:VAL:HG12	2.10	0.52
16:1P:19:ILE:H	16:1P:19:ILE:HD12	1.73	0.52
16:1P:130:ILE:HG13	16:1P:164:THR:HB	1.92	0.52
18:1R:9:GLU:OE2	18:1R:33:LYS:NZ	2.43	0.52
22:1W:90:LEU:O	22:1W:94:ILE:HG12	2.09	0.52
35:1j:10:ARG:NH1	35:1j:14:PHE:O	2.42	0.52
35:1j:10:ARG:HG3	35:1j:15:PRO:HA	1.90	0.52
37:1l:77:ILE:HD11	38:1m:67:TRP:CD2	2.45	0.52
4:1D:246:THR:HA	21:1V:11:VAL:HG13	1.92	0.52
4:1D:311:ILE:O	4:1D:315:LEU:HG	2.09	0.52
5:1E:149:VAL:HA	6:1F:259:SER:HB2	1.91	0.52
7:1G:279:LEU:HD21	7:1G:550:GLY:HA3	1.91	0.52
8:1H:70:MET:HA	8:1H:73:ILE:HG22	1.90	0.52
8:1H:110:SER:O	8:1H:113:VAL:HG22	2.10	0.52
12:1L:204:LEU:HD22	38:1m:124:PHE:CE2	2.45	0.52
19:1S:19:ARG:NH1	19:1S:73:GLU:OE1	2.43	0.52
23:1X:19:VAL:CG2	23:1X:24:LEU:HD13	2.39	0.52
24:1Y:84:ASP:OD1	24:1Y:84:ASP:N	2.36	0.52
24:1Y:127:GLY:HA2	24:1Y:132:TRP:CD1	2.45	0.52
37:1l:16:THR:HG23	37:1l:19:GLU:HG3	1.91	0.52
43:1r:59:ARG:HH21	43:1r:60:ARG:HH12	1.58	0.52
4:1D:64:LEU:HD12	4:1D:78:PRO:HB3	1.91	0.52
5:1E:63:ILE:HA	5:1E:66:MET:SD	2.50	0.52
7:1G:320:GLY:O	7:1G:498:SER:OG	2.27	0.52
8:1H:197:PRO:HB2	8:1H:280:PHE:HD2	1.74	0.52
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.45	0.52
9:1I:70:TYR:HD1	9:1I:76:ARG:HG2	1.72	0.52
13:1M:135:ARG:HH22	14:1N:304:MET:HE3	1.75	0.52
23:1X:3:ILE:HG13	25:1Z:105:LYS:NZ	2.25	0.52
25:1Z:68:ARG:HG3	26:1a:43:TYR:CZ	2.45	0.52
32:1g:87:GLU:HG2	32:1g:91:ARG:NH2	2.25	0.52
4:1D:80:ILE:HD13	4:1D:428:VAL:HG22	1.90	0.52
9:1I:43:ARG:HD2	43:1r:24:GLN:HE22	1.74	0.52
10:1J:119:PHE:CD1	11:1K:6:MET:HG3	2.44	0.52
12:1L:464:ALA:HA	12:1L:467:ILE:HB	1.91	0.52
14:1N:189:TRP:CZ3	14:1N:263:LYS:HA	2.45	0.52
15:1O:213:GLU:O	15:1O:217:LYS:NZ	2.40	0.52
33:1h:129:ASP:N	33:1h:129:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:102:ARG:NE	40:1o:48:ALA:O	2.42	0.52
1:1A:3:ILE:O	1:1A:6:THR:OG1	2.28	0.52
1:1A:84:LEU:O	1:1A:88:LEU:N	2.40	0.52
5:1E:110:LEU:HD12	5:1E:111:ARG:HD3	1.92	0.52
6:1F:276:LEU:HD23	6:1F:312:CYS:HB3	1.92	0.52
7:1G:192:MET:N	7:1G:192:MET:SD	2.83	0.52
7:1G:255:HIS:NE2	7:1G:258:ILE:HG12	2.25	0.52
7:1G:450:MET:SD	7:1G:491:ASN:ND2	2.83	0.52
7:1G:460:ARG:HH21	7:1G:657:LEU:HB3	1.75	0.52
7:1G:595:GLU:N	7:1G:595:GLU:OE1	2.42	0.52
10:1J:155:ILE:H	10:1J:155:ILE:HD12	1.75	0.52
12:1L:135:ASN:ND2	12:1L:199:GLN:OE1	2.36	0.52
16:1P:75:GLY:HA2	16:1P:81:ILE:HD11	1.91	0.52
20:1U:63:PRO:HB3	37:1l:61:TRP:CG	2.45	0.52
22:1W:49:LEU:O	22:1W:51:GLN:NE2	2.43	0.52
24:1Y:16:GLU:OE1	24:1Y:18:HIS:NE2	2.42	0.52
24:1Y:61:THR:HG22	24:1Y:103:ARG:HG2	1.92	0.52
24:1Y:69:PHE:HE2	45:1Y:202:3PE:H3F1	1.73	0.52
4:1D:14:PHE:HE2	14:1N:295:ARG:HG3	1.73	0.51
8:1H:12:PRO:HG3	26:1a:19:PRO:HG3	1.91	0.51
8:1H:155:LEU:HD12	8:1H:308:PRO:HG2	1.93	0.51
9:1I:70:TYR:CE2	18:1R:87:CYS:HA	2.45	0.51
13:1M:22:MET:O	13:1M:26:ASN:ND2	2.43	0.51
22:1W:25:MET:O	22:1W:25:MET:HE3	2.11	0.51
29:1d:86:ARG:NH1	29:1d:87:ASP:OD1	2.43	0.51
36:1k:22:LYS:HA	36:1k:46:ARG:HG2	1.91	0.51
42:1q:32:ASP:OD1	42:1q:33:VAL:N	2.43	0.51
44:1s:70:ARG:HB2	44:1s:75:HIS:HB2	1.92	0.51
3:1C:199:LEU:HD21	4:1D:385:ARG:HD3	1.91	0.51
7:1G:364:LEU:HB3	7:1G:577:GLU:HA	1.92	0.51
7:1G:410:GLY:O	7:1G:421:HIS:NE2	2.42	0.51
7:1G:628:PRO:HD2	19:1S:55:ARG:HB3	1.91	0.51
11:1K:31:LEU:O	11:1K:34:GLU:HB2	2.10	0.51
21:1V:82:GLN:HA	21:1V:85:ASN:OD1	2.10	0.51
23:1X:12:LEU:HD21	25:1Z:84:LEU:HD12	1.93	0.51
37:1l:30:ARG:HH12	38:1m:34:GLU:CG	2.23	0.51
41:1p:26:PRO:HB2	41:1p:31:TYR:HE1	1.75	0.51
3:1C:32:ILE:H	3:1C:32:ILE:HD12	1.76	0.51
6:1F:49:LEU:HG	6:1F:127:ARG:HG3	1.92	0.51
7:1G:415:LEU:O	7:1G:417:TYR:N	2.44	0.51
16:1P:133:SER:O	16:1P:167:LYS:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:78:LEU:O	19:1S:81:PHE:HB2	2.10	0.51
20:1T:60:PHE:HE2	20:1T:84:LYS:HD2	1.75	0.51
40:1o:60:HIS:O	40:1o:64:GLN:NE2	2.43	0.51
1:1A:72:LEU:HD23	1:1A:72:LEU:H	1.76	0.51
5:1E:217:LEU:HB3	6:1F:44:LYS:HD2	1.92	0.51
8:1H:172:ILE:HD13	25:1Z:49:SER:HB3	1.92	0.51
8:1H:277:TYR:O	8:1H:279:ARG:NH2	2.43	0.51
10:1J:78:MET:SD	10:1J:79:TYR:N	2.84	0.51
12:1L:76:LEU:HD21	12:1L:196:TRP:HE3	1.74	0.51
12:1L:82:MET:HE2	12:1L:82:MET:N	2.26	0.51
12:1L:526:LEU:HD13	12:1L:530:PRO:HG3	1.92	0.51
23:1X:165:ARG:NH1	29:1d:87:ASP:OD2	2.31	0.51
32:1g:77:VAL:HA	32:1g:80:LEU:HG	1.93	0.51
34:1i:10:ARG:HB2	39:1n:155:PRO:HB3	1.91	0.51
5:1E:108:CYS:HA	5:1E:111:ARG:HH21	1.76	0.51
6:1F:82:MET:HG3	6:1F:129:MET:HB2	1.91	0.51
6:1F:347:ILE:HG21	6:1F:418:LEU:HG	1.93	0.51
7:1G:8:LEU:HD23	7:1G:19:MET:HG2	1.93	0.51
11:1K:94:ASN:HB3	12:1L:583:LEU:HD23	1.93	0.51
12:1L:162:THR:OG1	37:1l:86:ARG:NH2	2.44	0.51
6:1F:320:ASP:HA	6:1F:323:VAL:HG22	1.92	0.51
7:1G:53:ARG:NH1	7:1G:67:ALA:HB2	2.26	0.51
8:1H:272:TRP:HZ2	9:1I:38:LEU:HB2	1.75	0.51
9:1I:76:ARG:NH1	9:1I:128:VAL:O	2.40	0.51
12:1L:4:PHE:CD2	12:1L:61:MET:HG2	2.46	0.51
13:1M:333:ASN:O	13:1M:337:VAL:HG12	2.10	0.51
14:1N:309:ASN:HB3	15:1O:282:ILE:HD12	1.93	0.51
37:1l:58:ARG:HB2	37:1l:70:ARG:HD2	1.93	0.51
39:1n:104:ASP:OD1	39:1n:121:ARG:NH1	2.44	0.51
3:1C:28:TYR:O	3:1C:32:ILE:HD12	2.11	0.51
6:1F:185:ILE:HD11	46:1F:502:SF4:S1	2.51	0.51
8:1H:24:GLU:HG3	8:1H:271:LEU:HD22	1.92	0.51
16:1P:107:GLU:O	16:1P:111:VAL:N	2.43	0.51
20:1U:8:LEU:HD11	20:1U:88:GLU:H	1.76	0.51
27:1b:31:LEU:O	27:1b:35:SER:OG	2.28	0.51
40:1o:73:PHE:O	41:1p:27:ASN:ND2	2.44	0.51
3:1C:42:VAL:HA	3:1C:48:LEU:HA	1.92	0.51
5:1E:44:ALA:O	6:1F:198:GLY:HA3	2.11	0.51
5:1E:136:LEU:C	5:1E:137:PHE:HD1	2.19	0.51
6:1F:186:CYS:O	6:1F:192:LEU:HB2	2.10	0.51
6:1F:367:GLU:N	6:1F:367:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:175:ILE:HB	8:1H:242:PHE:HB3	1.93	0.51
8:1H:202:GLU:HA	8:1H:210:GLY:HA3	1.92	0.51
12:1L:405:ASN:ND2	37:1l:120:GLU:OE1	2.43	0.51
12:1L:597:ILE:HA	12:1L:601:LEU:HB2	1.91	0.51
13:1M:47:GLU:HG2	41:1p:92:ARG:HB3	1.93	0.51
14:1N:78:LEU:HD12	14:1N:82:GLY:HA2	1.93	0.51
15:1O:221:LEU:HD11	15:1O:238:ILE:HG22	1.92	0.51
16:1P:206:TYR:CD1	16:1P:208:VAL:HG12	2.46	0.51
3:1C:16:ASP:OD1	3:1C:19:HIS:ND1	2.43	0.51
3:1C:87:GLN:NE2	21:1V:108:ALA:HB3	2.25	0.51
6:1F:215:VAL:HG12	6:1F:220:THR:HG21	1.93	0.51
9:1I:97:GLU:CD	9:1I:107:THR:HG23	2.36	0.51
14:1N:173:THR:OG1	14:1N:174:GLN:OE1	2.27	0.51
17:1Q:121:ASN:C	17:1Q:122:PHE:HD1	2.19	0.51
37:1l:57:GLU:OE2	38:1m:12:THR:OG1	2.28	0.51
5:1E:39:PRO:HB3	44:1s:66:PRO:HD2	1.92	0.51
7:1G:30:CYS:HB2	7:1G:37:ILE:HD11	1.93	0.51
8:1H:224:PHE:O	8:1H:228:TYR:HB2	2.10	0.51
12:1L:339:LEU:HD22	12:1L:373:LEU:HD22	1.91	0.51
15:1O:174:VAL:HB	15:1O:179:ILE:HD11	1.92	0.51
16:1P:41:MET:SD	16:1P:41:MET:N	2.78	0.51
20:1T:19:LEU:HD11	20:1T:36:PHE:HE1	1.76	0.51
20:1U:22:TYR:CE1	36:1k:43:PRO:HB2	2.44	0.51
32:1g:90:ARG:NE	41:1p:104:ILE:HD11	2.25	0.51
37:1l:156:TYR:O	40:1o:96:LYS:NZ	2.39	0.51
3:1C:79:THR:O	3:1C:93:VAL:N	2.44	0.50
4:1D:149:ASN:ND2	4:1D:370:PRO:HB2	2.25	0.50
6:1F:17:ASP:HA	6:1F:20:ARG:HE	1.76	0.50
7:1G:227:SER:O	7:1G:253:ARG:NH2	2.44	0.50
7:1G:303:VAL:O	7:1G:307:LEU:HD23	2.11	0.50
7:1G:306:MET:HE2	7:1G:306:MET:N	2.26	0.50
7:1G:324:ASP:HB2	7:1G:571:ALA:HB1	1.93	0.50
7:1G:383:ASN:ND2	7:1G:665:GLN:O	2.43	0.50
9:1I:69:ARG:NH1	9:1I:159:ASP:OD1	2.38	0.50
10:1J:59:ILE:O	10:1J:61:LEU:N	2.44	0.50
14:1N:321:LYS:HE2	14:1N:323:MET:HA	1.93	0.50
16:1P:241:LEU:O	16:1P:245:ILE:HG13	2.11	0.50
18:1R:39:PHE:HB3	18:1R:41:ILE:HG22	1.92	0.50
20:1T:71:MET:N	20:1T:71:MET:SD	2.84	0.50
4:1D:239:THR:HG23	4:1D:293:CYS:HB2	1.92	0.50
4:1D:396:PHE:HA	4:1D:428:VAL:HG23	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:316:PRO:HB3	25:1Z:58:ARG:HD2	1.93	0.50
11:1K:70:GLU:HB3	14:1N:60:PHE:CE1	2.45	0.50
12:1L:135:ASN:OD1	12:1L:199:GLN:NE2	2.42	0.50
12:1L:323:HIS:CE1	12:1L:475:MET:HE1	2.46	0.50
12:1L:481:THR:HB	40:1o:94:TYR:CD2	2.46	0.50
14:1N:330:ILE:H	14:1N:330:ILE:HD12	1.75	0.50
17:1Q:124:TRP:CH2	44:1s:66:PRO:HB2	2.46	0.50
18:1R:16:GLN:HE22	18:1R:18:TYR:HD2	1.60	0.50
18:1R:95:HIS:ND1	18:1R:95:HIS:O	2.44	0.50
43:1r:71:SER:OG	43:1r:72:GLN:OE1	2.23	0.50
6:1F:185:ILE:HG12	6:1F:359:CYS:HB3	1.94	0.50
7:1G:12:PHE:HA	7:1G:17:SER:HA	1.92	0.50
11:1K:59:MET:O	11:1K:63:LEU:N	2.32	0.50
12:1L:550:SER:HB2	13:1M:275:ILE:HG23	1.92	0.50
13:1M:266:MET:HG3	13:1M:396:MET:HE3	1.94	0.50
13:1M:447:LEU:HD21	13:1M:454:ILE:HG21	1.93	0.50
15:1O:23:LYS:HA	15:1O:167:HIS:CE1	2.45	0.50
15:1O:173:ASP:HB3	15:1O:222:GLN:NE2	2.27	0.50
20:1U:9:GLU:HA	20:1U:12:LYS:HE3	1.93	0.50
41:1p:25:LEU:HD23	41:1p:25:LEU:H	1.76	0.50
42:1q:44:TYR:HH	42:1q:113:HIS:H	1.57	0.50
43:1r:57:ASP:HB2	43:1r:60:ARG:HG3	1.94	0.50
4:1D:163:ALA:O	4:1D:166:PRO:HD2	2.12	0.50
5:1E:195:PRO:HA	6:1F:264:HIS:HB3	1.93	0.50
10:1J:152:TRP:HZ3	47:1J:201:PC1:H272	1.76	0.50
15:1O:100:LEU:O	15:1O:104:ARG:HG2	2.10	0.50
16:1P:176:ASP:O	16:1P:177:ARG:HG2	2.11	0.50
19:1S:13:LEU:HD12	19:1S:14:GLY:N	2.26	0.50
20:1U:15:VAL:HA	20:1U:54:MET:HE1	1.94	0.50
22:1W:115:PRO:O	22:1W:121:LYS:NZ	2.40	0.50
23:1X:76:HIS:O	23:1X:78:ALA:N	2.42	0.50
25:1Z:97:ILE:HG12	25:1Z:98:MET:HG2	1.93	0.50
4:1D:107:ASP:OD2	4:1D:110:SER:OG	2.29	0.50
5:1E:191:PHE:N	5:1E:194:GLU:OE1	2.39	0.50
9:1I:69:ARG:HD2	42:1q:108:TYR:CG	2.46	0.50
11:1K:80:MET:HE2	11:1K:80:MET:HA	1.94	0.50
14:1N:244:MET:HE2	14:1N:244:MET:HA	1.94	0.50
20:1U:72:CYS:O	20:1U:76:ILE:HG12	2.11	0.50
31:1f:52:GLU:OE1	31:1f:52:GLU:N	2.43	0.50
40:1o:113:ARG:HA	40:1o:116:GLN:NE2	2.26	0.50
4:1D:146:ARG:HG3	4:1D:370:PRO:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:414:VAL:O	4:1D:418:ILE:HG23	2.12	0.50
7:1G:470:VAL:HA	7:1G:473:ILE:HB	1.94	0.50
9:1I:109:TYR:OH	46:1I:202:SF4:S4	2.63	0.50
12:1L:533:MET:HB3	12:1L:534:HIS:CD2	2.47	0.50
12:1L:561:ILE:HG23	12:1L:562:LEU:H	1.77	0.50
23:1X:51:ASP:OD2	23:1X:53:ARG:NE	2.44	0.50
25:1Z:100:ASP:OD1	25:1Z:100:ASP:N	2.40	0.50
26:1a:28:LYS:O	26:1a:33:GLY:N	2.39	0.50
33:1h:61:PRO:HB3	33:1h:65:GLU:HB3	1.93	0.50
6:1F:144:ASN:O	6:1F:147:SER:OG	2.21	0.50
7:1G:231:MET:SD	7:1G:266:LYS:NZ	2.84	0.50
7:1G:284:ILE:HA	7:1G:559:VAL:HG12	1.93	0.50
7:1G:357:ASP:O	19:1S:55:ARG:NH2	2.44	0.50
9:1I:36:MET:HA	9:1I:36:MET:HE3	1.94	0.50
13:1M:131:ILE:HD12	14:1N:302:LEU:HD21	1.94	0.50
14:1N:230:LEU:O	14:1N:233:THR:OG1	2.30	0.50
15:1O:303:LYS:O	15:1O:303:LYS:NZ	2.37	0.50
16:1P:110:PHE:HB2	16:1P:148:SER:HB2	1.94	0.50
18:1R:56:VAL:C	18:1R:57:ILE:HD12	2.36	0.50
23:1X:27:ALA:O	23:1X:29:HIS:N	2.44	0.50
4:1D:151:ILE:HD12	4:1D:177:MET:HE1	1.94	0.50
5:1E:172:ILE:HG23	5:1E:182:PRO:HG2	1.93	0.50
6:1F:146:ALA:O	6:1F:149:LEU:HB3	2.12	0.50
7:1G:59:ILE:HD12	7:1G:77:TRP:CD1	2.47	0.50
7:1G:378:LEU:HD21	7:1G:439:PHE:HZ	1.77	0.50
12:1L:444:ASN:HB2	35:1j:7:ILE:HD13	1.94	0.50
13:1M:76:MET:O	13:1M:80:SER:OG	2.24	0.50
13:1M:194:PHE:CG	57:1Y:201:PGT:H142	2.46	0.50
16:1P:113:ILE:O	16:1P:117:ILE:HG13	2.12	0.50
17:1Q:64:ARG:HG2	17:1Q:64:ARG:HH11	1.76	0.50
25:1Z:6:VAL:O	25:1Z:7:LYS:HD3	2.11	0.50
39:1n:46:ARG:NH1	56:1n:201:EHZ:O1	2.44	0.50
2:1B:145:TYR:N	9:1I:141:THR:O	2.33	0.50
12:1L:529:TYR:O	12:1L:533:MET:HB2	2.11	0.50
18:1R:22:ASP:OD2	18:1R:24:ARG:NH1	2.45	0.50
20:1U:20:LYS:HE3	20:1U:27:PRO:HB3	1.93	0.50
22:1W:52:LEU:HD22	22:1W:104:MET:HE2	1.94	0.50
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.12	0.50
32:1g:45:HIS:CD2	32:1g:55:LEU:HA	2.47	0.50
41:1p:28:PRO:O	41:1p:32:LEU:HD12	2.12	0.50
6:1F:127:ARG:HG2	6:1F:171:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:399:TRP:HE1	44:1s:74:ARG:NH1	2.09	0.49
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.93	0.49
13:1M:201:MET:HG2	57:1Y:201:PGT:H441	1.93	0.49
13:1M:293:HIS:NE2	13:1M:366:ASN:OD1	2.39	0.49
19:1S:81:PHE:CE1	19:1S:85:GLN:HG3	2.47	0.49
29:1d:83:TYR:HD1	29:1d:86:ARG:HE	1.60	0.49
32:1g:25:ARG:HG3	32:1g:26:LEU:HG	1.94	0.49
38:1m:51:ASN:HD22	39:1n:165:LEU:HD22	1.77	0.49
1:1A:84:LEU:HA	1:1A:87:MET:HB3	1.93	0.49
6:1F:234:ILE:O	6:1F:238:GLY:N	2.42	0.49
7:1G:343:LEU:HB3	7:1G:507:TYR:CD2	2.47	0.49
8:1H:150:LEU:O	8:1H:154:LEU:HD12	2.12	0.49
8:1H:199:ASP:HB2	8:1H:279:ARG:HD3	1.92	0.49
12:1L:159:HIS:CD2	13:1M:416:ARG:HA	2.48	0.49
12:1L:474:PRO:HG3	40:1o:65:LEU:HD22	1.94	0.49
15:1O:57:HIS:CD2	15:1O:68:PRO:HB3	2.47	0.49
40:1o:17:ASP:O	40:1o:19:LEU:N	2.45	0.49
41:1p:162:MET:HA	41:1p:165:GLU:HB3	1.94	0.49
2:1B:125:TYR:HE1	9:1I:88:PRO:HB2	1.76	0.49
3:1C:41:GLN:HB3	43:1r:67:ILE:HG22	1.94	0.49
3:1C:162:PHE:CZ	4:1D:88:GLU:HB2	2.47	0.49
7:1G:373:GLU:HG3	7:1G:448:LYS:HG3	1.94	0.49
7:1G:427:LYS:NZ	7:1G:431:ASP:OD2	2.45	0.49
12:1L:232:TRP:HZ3	12:1L:252:MET:HE1	1.77	0.49
16:1P:90:VAL:HG11	16:1P:218:ILE:HG13	1.95	0.49
20:1U:28:GLU:OE2	20:1U:28:GLU:N	2.28	0.49
37:1l:18:GLU:OE1	37:1l:18:GLU:N	2.42	0.49
42:1q:2:GLU:O	42:1q:6:VAL:HG23	2.13	0.49
3:1C:15:ASN:OD1	3:1C:46:ASN:ND2	2.45	0.49
3:1C:49:GLU:HB3	3:1C:108:LYS:HE3	1.94	0.49
6:1F:193:ILE:HD11	6:1F:220:THR:HG21	1.94	0.49
7:1G:26:VAL:HB	7:1G:68:ALA:HB1	1.94	0.49
9:1I:87:CYS:SG	9:1I:91:ALA:N	2.84	0.49
13:1M:14:MET:HE1	13:1M:30:HIS:ND1	2.27	0.49
20:1T:32:VAL:O	20:1T:74:GLN:HG2	2.13	0.49
20:1T:45:LEU:HD23	22:1W:64:ARG:NE	2.27	0.49
21:1V:91:ARG:HG2	21:1V:95:ARG:HH21	1.77	0.49
22:1W:93:THR:HG22	22:1W:98:LYS:HD3	1.94	0.49
32:1g:47:TYR:HB2	32:1g:54:ASP:OD1	2.13	0.49
35:1j:23:ILE:H	35:1j:23:ILE:HD12	1.77	0.49
38:1m:52:ASP:OD1	38:1m:54:ASN:ND2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:94:GLU:HA	39:1n:97:LYS:HG3	1.93	0.49
43:1r:15:SER:O	43:1r:17:ARG:NH1	2.44	0.49
3:1C:47:GLU:OE1	4:1D:363:THR:OG1	2.31	0.49
3:1C:136:ASP:OD2	3:1C:151:ILE:HG22	2.13	0.49
4:1D:183:ARG:HB3	4:1D:204:PRO:HG3	1.92	0.49
7:1G:134:LYS:HB2	18:1R:72:TYR:CG	2.47	0.49
10:1J:65:LEU:HD13	10:1J:68:PHE:CD2	2.47	0.49
12:1L:605:HIS:CD2	12:1L:606:GLU:HG3	2.48	0.49
14:1N:273:ASN:OD1	24:1Y:139:LYS:N	2.45	0.49
17:1Q:66:GLU:HG3	17:1Q:71:GLY:HA2	1.94	0.49
25:1Z:133:ILE:O	25:1Z:137:THR:HG23	2.12	0.49
38:1m:110:LYS:HA	38:1m:113:LYS:HE3	1.94	0.49
42:1q:95:ASP:H	43:1r:34:THR:HG23	1.78	0.49
1:1A:59:ALA:HB1	10:1J:67:VAL:HG22	1.95	0.49
3:1C:130:TYR:HA	4:1D:396:PHE:HE2	1.77	0.49
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.94	0.49
7:1G:8:LEU:HB3	7:1G:19:MET:HB2	1.95	0.49
7:1G:508:LYS:HZ1	7:1G:514:ILE:H	1.60	0.49
7:1G:632:ARG:NH1	19:1S:57:CYS:SG	2.85	0.49
8:1H:26:LYS:HA	8:1H:36:GLY:HA3	1.95	0.49
8:1H:170:GLU:CD	23:1X:97:ARG:HH12	2.21	0.49
12:1L:94:LEU:HA	12:1L:97:THR:HG22	1.95	0.49
13:1M:17:MET:HG2	31:1f:11:TRP:HZ2	1.77	0.49
14:1N:62:THR:HG21	14:1N:114:TRP:CG	2.48	0.49
14:1N:174:GLN:O	14:1N:178:ILE:HD12	2.13	0.49
21:1V:76:ILE:HG22	21:1V:80:ILE:HG23	1.94	0.49
22:1W:43:VAL:O	22:1W:47:VAL:HG22	2.13	0.49
25:1Z:91:LEU:HA	25:1Z:94:GLU:HB3	1.95	0.49
3:1C:118:GLU:HA	3:1C:143:ALA:HB3	1.93	0.49
3:1C:211:GLN:NE2	21:1V:114:PRO:O	2.46	0.49
5:1E:31:ILE:HD12	5:1E:32:GLU:N	2.28	0.49
5:1E:110:LEU:HD11	6:1F:261:HIS:N	2.28	0.49
5:1E:194:GLU:OE1	6:1F:26:TYR:OH	2.30	0.49
6:1F:89:ARG:NH1	6:1F:219:PRO:HD3	2.28	0.49
8:1H:99:ASN:OD1	8:1H:99:ASN:N	2.43	0.49
8:1H:170:GLU:OE2	23:1X:97:ARG:NH1	2.45	0.49
10:1J:160:SER:O	10:1J:164:GLY:N	2.45	0.49
16:1P:182:PHE:HD2	16:1P:245:ILE:HG12	1.78	0.49
22:1W:24:ASP:OD2	22:1W:26:ASN:N	2.42	0.49
24:1Y:65:ILE:HG23	24:1Y:96:GLY:HA3	1.95	0.49
28:1c:15:LEU:H	28:1c:15:LEU:HD12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:6:LYS:HA	37:1l:9:PHE:HD2	1.78	0.49
39:1n:11:HIS:HA	39:1n:14:LYS:HE2	1.93	0.49
4:1D:147:LEU:HB3	4:1D:177:MET:HE3	1.94	0.49
4:1D:231:ASN:N	4:1D:231:ASN:OD1	2.46	0.49
12:1L:530:PRO:HA	12:1L:534:HIS:CD2	2.47	0.49
12:1L:603:ASN:HA	12:1L:605:HIS:CE1	2.48	0.49
17:1Q:81:ASN:O	17:1Q:82:LEU:HD12	2.13	0.49
32:1g:82:ASP:OD2	32:1g:85:MET:HA	2.13	0.49
38:1m:51:ASN:OD1	39:1n:168:HIS:ND1	2.40	0.49
39:1n:27:GLU:HB2	39:1n:36:TYR:HE2	1.78	0.49
4:1D:375:GLY:O	4:1D:392:LYS:N	2.45	0.49
5:1E:97:LYS:H	5:1E:136:LEU:HA	1.78	0.49
8:1H:201:THR:O	8:1H:210:GLY:HA3	2.13	0.49
8:1H:306:SER:O	8:1H:310:MET:HG2	2.13	0.49
9:1I:77:CYS:O	9:1I:105:ARG:NH1	2.45	0.49
13:1M:418:LYS:HD3	39:1n:94:GLU:OE2	2.13	0.49
14:1N:217:MET:HA	14:1N:220:ILE:HD12	1.94	0.49
16:1P:171:ILE:H	16:1P:171:ILE:HD12	1.77	0.49
18:1R:12:THR:HG22	18:1R:35:VAL:HG12	1.95	0.49
34:1i:85:LEU:HA	34:1i:89:VAL:HG22	1.93	0.49
38:1m:38:ILE:HA	38:1m:41:ARG:HH11	1.77	0.49
39:1n:144:PRO:HG2	39:1n:149:ARG:H	1.78	0.49
40:1o:45:MET:SD	40:1o:55:ARG:HG2	2.52	0.49
1:1A:80:GLN:HA	27:1b:45:ASN:HD21	1.76	0.49
2:1B:57:VAL:HA	2:1B:60:MET:HE1	1.94	0.49
3:1C:117:ILE:O	3:1C:143:ALA:N	2.43	0.49
4:1D:318:MET:HE2	4:1D:318:MET:HA	1.94	0.49
5:1E:103:CYS:HB2	5:1E:145:LEU:HG	1.95	0.49
5:1E:108:CYS:HA	5:1E:111:ARG:NH2	2.27	0.49
6:1F:114:ASP:HB3	6:1F:117:LYS:HG3	1.94	0.49
6:1F:256:PHE:CD2	6:1F:270:GLU:HB3	2.48	0.49
7:1G:144:PRO:HA	7:1G:211:LYS:HD2	1.93	0.49
7:1G:159:CYS:HA	7:1G:202:ILE:HD11	1.95	0.49
7:1G:238:ILE:HG22	7:1G:252:PRO:HA	1.95	0.49
7:1G:322:LEU:HA	7:1G:497:ALA:HB3	1.94	0.49
7:1G:343:LEU:HB3	7:1G:507:TYR:CG	2.48	0.49
12:1L:108:MET:HB3	12:1L:114:ILE:CD1	2.43	0.49
16:1P:57:MET:HA	16:1P:60:ARG:HH12	1.78	0.49
28:1c:17:VAL:O	28:1c:21:LEU:HD12	2.13	0.49
37:1l:156:TYR:HB2	40:1o:33:ARG:CZ	2.43	0.49
3:1C:129:TRP:CZ2	4:1D:78:PRO:HD2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:256:SER:OG	4:1D:257:GLY:N	2.44	0.48
7:1G:205:VAL:HG23	7:1G:207:ALA:H	1.78	0.48
12:1L:28:LYS:HB2	12:1L:31:LEU:HG	1.94	0.48
12:1L:227:PHE:N	12:1L:284:THR:OG1	2.41	0.48
45:1L:702:3PE:O14	24:1Y:58:TYR:OH	2.18	0.48
14:1N:147:GLN:HB3	33:1h:125:TYR:CE1	2.48	0.48
15:1O:227:GLU:OE1	15:1O:227:GLU:N	2.43	0.48
16:1P:206:TYR:HD1	16:1P:208:VAL:H	1.61	0.48
18:1R:82:GLY:O	18:1R:91:PHE:N	2.34	0.48
20:1T:20:LYS:HA	20:1T:25:ILE:HG21	1.94	0.48
22:1W:29:LYS:HG3	22:1W:33:ARG:NH2	2.28	0.48
26:1a:55:SER:OG	26:1a:58:ASN:N	2.46	0.48
36:1k:18:TYR:HB2	36:1k:19:LYS:HZ3	1.77	0.48
40:1o:46:ASN:HA	40:1o:55:ARG:HH22	1.77	0.48
4:1D:112:MET:HE1	4:1D:193:TYR:HD2	1.77	0.48
4:1D:226:GLU:HB3	25:1Z:23:ARG:HH11	1.79	0.48
4:1D:425:PHE:HA	4:1D:428:VAL:HG12	1.95	0.48
5:1E:9:HIS:HD2	7:1G:187:ILE:HG22	1.77	0.48
7:1G:418:ARG:H	44:1s:74:ARG:NH2	2.09	0.48
7:1G:515:ARG:O	7:1G:515:ARG:NH1	2.34	0.48
9:1I:7:MET:HG2	9:1I:8:ARG:H	1.78	0.48
13:1M:426:ILE:HG22	39:1n:101:TRP:HH2	1.77	0.48
16:1P:263:TYR:HA	16:1P:266:VAL:HB	1.96	0.48
18:1R:4:THR:HA	18:1R:10:LYS:HA	1.95	0.48
21:1V:54:LYS:NZ	21:1V:70:GLN:O	2.46	0.48
22:1W:28:ALA:O	22:1W:32:VAL:HG13	2.13	0.48
24:1Y:73:SER:O	24:1Y:88:ASN:ND2	2.46	0.48
24:1Y:94:CYS:HB2	24:1Y:114:CYS:O	2.13	0.48
26:1a:21:MET:HE2	26:1a:21:MET:HA	1.95	0.48
38:1m:49:GLN:O	38:1m:55:ARG:HD3	2.13	0.48
1:1A:79:SER:HA	1:1A:87:MET:HE3	1.95	0.48
1:1A:104:TYR:CE1	10:1J:166:VAL:HG12	2.47	0.48
2:1B:148:GLY:HA2	9:1I:118:TYR:CE1	2.43	0.48
2:1B:148:GLY:HA3	2:1B:151:PRO:CG	2.43	0.48
3:1C:180:VAL:HG11	3:1C:182:ARG:NH1	2.27	0.48
7:1G:255:HIS:NE2	7:1G:257:ASP:HB2	2.28	0.48
7:1G:453:LEU:HD11	7:1G:458:LEU:HB2	1.95	0.48
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.49	0.48
10:1J:5:ILE:HG21	25:1Z:142:TRP:CZ2	2.48	0.48
12:1L:62:ILE:HG12	12:1L:81:LYS:HG3	1.96	0.48
13:1M:225:ILE:HG12	13:1M:331:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:346:ARG:NH1	37:1L:68:ASP:OD2	2.47	0.48
14:1N:98:MET:HA	14:1N:98:MET:HE2	1.95	0.48
15:1O:24:VAL:HA	15:1O:122:VAL:HG23	1.95	0.48
19:1S:65:TRP:CE3	19:1S:73:GLU:HG3	2.47	0.48
21:1V:13:LEU:HD23	21:1V:77:GLU:HB2	1.95	0.48
39:1n:10:THR:N	39:1n:13:GLN:OE1	2.44	0.48
39:1n:149:ARG:HD2	39:1n:149:ARG:O	2.13	0.48
3:1C:117:ILE:H	3:1C:142:PHE:HA	1.78	0.48
6:1F:57:LEU:HA	6:1F:60:VAL:HG12	1.94	0.48
8:1H:19:PHE:CB	26:1a:12:MET:HE1	2.43	0.48
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.13	0.48
9:1I:108:ARG:NH1	17:1Q:70:MET:O	2.47	0.48
11:1K:43:MET:O	11:1K:47:ILE:HG13	2.14	0.48
13:1M:449:LEU:HB2	47:1M:501:PC1:H242	1.95	0.48
20:1U:46:ASP:O	20:1U:50:ILE:HG23	2.13	0.48
25:1Z:104:TRP:HH2	30:1e:77:ALA:HB3	1.77	0.48
39:1n:25:HIS:CE1	39:1n:74:GLN:HB2	2.48	0.48
41:1p:59:ARG:NE	41:1p:59:ARG:HA	2.28	0.48
1:1A:18:VAL:O	1:1A:22:PHE:HB2	2.14	0.48
5:1E:150:ASN:HB3	5:1E:163:ASP:CB	2.42	0.48
6:1F:49:LEU:HD11	6:1F:171:TYR:HB2	1.95	0.48
7:1G:648:LEU:HD22	19:1S:44:LYS:HG2	1.94	0.48
8:1H:97:ASN:OD1	8:1H:163:SER:OG	2.27	0.48
8:1H:140:ILE:HG21	10:1J:66:VAL:HG11	1.96	0.48
12:1L:76:LEU:HD11	12:1L:196:TRP:HZ3	1.79	0.48
12:1L:232:TRP:CZ3	12:1L:252:MET:HE1	2.48	0.48
12:1L:420:ALA:O	12:1L:424:THR:HG23	2.12	0.48
15:1O:45:LYS:HE3	15:1O:232:GLU:HA	1.96	0.48
16:1P:117:ILE:HD12	16:1P:118:ALA:N	2.29	0.48
33:1h:41:THR:O	33:1h:45:VAL:HG13	2.14	0.48
34:1i:42:MET:SD	34:1i:46:TRP:NE1	2.86	0.48
37:1L:53:ARG:HH21	38:1m:12:THR:HB	1.77	0.48
40:1o:82:GLU:OE1	40:1o:82:GLU:N	2.35	0.48
2:1B:66:ARG:HG2	4:1D:175:GLU:OE1	2.12	0.48
6:1F:247:ARG:HB3	6:1F:250:ASN:HD22	1.79	0.48
6:1F:309:LYS:HA	6:1F:312:CYS:SG	2.53	0.48
6:1F:351:ILE:HA	6:1F:354:TYR:HB2	1.96	0.48
7:1G:305:GLY:C	7:1G:306:MET:HE2	2.39	0.48
8:1H:26:LYS:NZ	26:1a:4:GLU:O	2.39	0.48
9:1I:174:LEU:HD23	43:1r:38:PRO:HD2	1.94	0.48
12:1L:483:PRO:HG3	35:1j:53:TYR:CE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:396:MET:HE2	13:1M:396:MET:HA	1.96	0.48
14:1N:9:LEU:O	14:1N:12:THR:OG1	2.31	0.48
15:1O:204:ASN:OD1	15:1O:204:ASN:N	2.44	0.48
33:1h:45:VAL:HG23	33:1h:46:PHE:CD1	2.48	0.48
34:1i:122:PHE:O	34:1i:124:ASP:N	2.43	0.48
40:1o:95:VAL:HA	40:1o:98:MET:SD	2.52	0.48
2:1B:48:MET:HG2	2:1B:49:THR:N	2.29	0.48
5:1E:102:VAL:HG13	5:1E:154:VAL:HG22	1.96	0.48
6:1F:66:ARG:H	6:1F:68:ARG:HE	1.62	0.48
8:1H:85:MET:O	8:1H:88:PRO:HD2	2.13	0.48
9:1I:148:LEU:HB3	17:1Q:70:MET:HE1	1.94	0.48
47:1I:203:PC1:H153	25:1Z:35:MET:HE1	1.96	0.48
12:1L:416:THR:O	12:1L:419:THR:OG1	2.23	0.48
28:1c:28:TRP:O	28:1c:32:ILE:HD12	2.13	0.48
32:1g:80:LEU:HD22	32:1g:81:PRO:HD2	1.95	0.48
1:1A:85:LYS:HB3	1:1A:85:LYS:HE3	1.67	0.48
3:1C:150:ARG:HH12	3:1C:155:TYR:HA	1.79	0.48
3:1C:181:LYS:HZ1	16:1P:32:ARG:HH21	1.62	0.48
4:1D:29:LYS:HD2	4:1D:30:PRO:HD2	1.96	0.48
4:1D:410:MET:HE3	8:1H:281:ARG:HD3	1.96	0.48
6:1F:89:ARG:HG2	17:1Q:124:TRP:CD1	2.49	0.48
6:1F:208:PRO:HB2	6:1F:213:VAL:HB	1.95	0.48
7:1G:161:ARG:O	7:1G:165:GLU:N	2.46	0.48
7:1G:319:ALA:N	7:1G:344:CYS:O	2.39	0.48
12:1L:56:HIS:ND1	41:1p:29:VAL:HG11	2.29	0.48
12:1L:401:MET:HE2	12:1L:401:MET:HA	1.96	0.48
12:1L:547:LYS:HG2	37:1l:44:TYR:OH	2.13	0.48
14:1N:66:ALA:CB	14:1N:105:LYS:HG3	2.44	0.48
14:1N:115:VAL:HG12	14:1N:180:ALA:HB1	1.95	0.48
14:1N:159:MET:SD	14:1N:281:LEU:HD12	2.53	0.48
19:1S:19:ARG:HG3	19:1S:53:LEU:HD23	1.95	0.48
19:1S:26:SER:HB3	19:1S:29:SER:HB3	1.96	0.48
27:1b:35:SER:HB2	27:1b:38:THR:HG22	1.96	0.48
4:1D:78:PRO:HG3	4:1D:402:LEU:HD23	1.95	0.48
4:1D:91:ILE:HD11	4:1D:102:TYR:HB2	1.95	0.48
4:1D:149:ASN:O	4:1D:153:ALA:N	2.41	0.48
4:1D:402:LEU:HD22	4:1D:418:ILE:HG22	1.96	0.48
6:1F:276:LEU:HB3	6:1F:312:CYS:HB2	1.95	0.48
8:1H:22:LEU:HB2	8:1H:48:PRO:HD3	1.96	0.48
10:1J:122:LEU:HD12	30:1e:72:MET:HB3	1.95	0.48
10:1J:151:THR:HG23	47:1J:201:PC1:H32	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:1:FME:O1	30:1e:67:LEU:HB2	2.13	0.48
19:1S:63:LYS:HD3	19:1S:75:ASN:ND2	2.29	0.48
20:1U:45:LEU:HD11	39:1n:19:TYR:CZ	2.49	0.48
38:1m:2:PHE:CD1	38:1m:3:PRO:HD2	2.49	0.48
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.39	0.48
7:1G:138:GLU:N	18:1R:74:ASN:HD22	2.12	0.48
7:1G:383:ASN:O	7:1G:387:GLU:HB2	2.14	0.48
7:1G:572:THR:HA	7:1G:582:GLN:HA	1.96	0.48
12:1L:346:ILE:HG22	12:1L:366:MET:SD	2.54	0.48
16:1P:192:PRO:HB2	16:1P:263:TYR:OH	2.14	0.48
36:1k:30:THR:O	36:1k:34:LYS:HG3	2.14	0.48
2:1B:41:ARG:HH11	2:1B:172:ARG:HH11	1.62	0.47
2:1B:101:ARG:NE	2:1B:105:ASP:OD1	2.44	0.47
4:1D:201:GLN:OE1	9:1I:175:TYR:HB3	2.14	0.47
4:1D:298:LEU:HA	4:1D:301:VAL:HG22	1.95	0.47
5:1E:101:GLN:HB2	5:1E:155:GLN:O	2.14	0.47
6:1F:19:ASP:HB3	6:1F:241:TRP:CZ2	2.49	0.47
8:1H:111:LEU:HD13	8:1H:114:TYR:HD2	1.78	0.47
14:1N:207:ILE:HG21	14:1N:262:PRO:HD3	1.96	0.47
19:1S:19:ARG:HB3	19:1S:21:HIS:CE1	2.49	0.47
20:1U:45:LEU:HD21	39:1n:19:TYR:CG	2.49	0.47
43:1r:92:LYS:H	43:1r:92:LYS:HD2	1.79	0.47
7:1G:200:ILE:HD13	7:1G:210:SER:HB3	1.96	0.47
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.96	0.47
12:1L:35:TYR:OH	34:1i:73:HIS:NE2	2.42	0.47
19:1S:49:ASP:OD1	19:1S:50:LEU:HD22	2.14	0.47
20:1T:43:ASP:OD2	20:1T:46:ASP:N	2.37	0.47
20:1T:79:TYR:O	20:1T:83:LYS:HG3	2.13	0.47
20:1U:12:LYS:O	20:1U:16:LEU:HD23	2.14	0.47
23:1X:7:PRO:HD2	25:1Z:84:LEU:HD21	1.96	0.47
34:1i:10:ARG:HH11	34:1i:14:LEU:HD11	1.79	0.47
36:1k:20:GLN:N	36:1k:20:GLN:OE1	2.48	0.47
1:1A:68:GLU:HA	1:1A:71:LEU:HD23	1.94	0.47
3:1C:191:ALA:O	17:1Q:74:SER:OG	2.19	0.47
6:1F:157:TYR:OH	6:1F:174:ASP:HB3	2.14	0.47
7:1G:44:GLU:O	17:1Q:116:LYS:NZ	2.40	0.47
7:1G:233:ALA:HB2	7:1G:496:ILE:C	2.39	0.47
7:1G:310:PHE:CZ	7:1G:520:LYS:HG2	2.49	0.47
7:1G:465:ALA:HB2	7:1G:654:GLN:OE1	2.14	0.47
14:1N:36:ASN:HD21	14:1N:134:GLN:NE2	2.12	0.47
16:1P:315:ILE:HD13	16:1P:319:ARG:HH21	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:35:HIS:HB3	20:1U:38:LYS:HG2	1.97	0.47
28:1c:27:LEU:HD22	29:1d:70:PHE:HD1	1.78	0.47
29:1d:108:THR:OG1	29:1d:111:GLU:OE2	2.32	0.47
4:1D:255:PHE:CZ	4:1D:401:GLY:HA3	2.49	0.47
5:1E:182:PRO:HB2	5:1E:187:ARG:NH2	2.25	0.47
7:1G:41:CYS:HB3	7:1G:52:CYS:HB3	1.95	0.47
7:1G:545:TYR:HB3	7:1G:560:ILE:HG23	1.97	0.47
8:1H:16:ALA:HB2	26:1a:15:CYS:HB3	1.95	0.47
12:1L:136:ASN:OD1	12:1L:139:GLN:N	2.37	0.47
12:1L:270:ASN:OD1	12:1L:273:VAL:N	2.45	0.47
14:1N:20:VAL:HG13	14:1N:29:ILE:HG23	1.95	0.47
14:1N:203:LEU:HD22	14:1N:343:LEU:HD11	1.96	0.47
14:1N:318:GLU:OE2	29:1d:50:ARG:NH1	2.41	0.47
15:1O:25:ILE:HD13	15:1O:167:HIS:HB2	1.97	0.47
15:1O:26:THR:HG22	15:1O:169:VAL:HG12	1.96	0.47
16:1P:300:LEU:HD13	16:1P:305:ILE:HG22	1.95	0.47
17:1Q:133:LYS:HD3	17:1Q:133:LYS:HA	1.66	0.47
21:1V:27:TYR:HB3	21:1V:55:LEU:HD22	1.96	0.47
22:1W:18:LYS:HA	22:1W:18:LYS:HE3	1.95	0.47
23:1X:6:LEU:HB2	25:1Z:84:LEU:HD21	1.97	0.47
23:1X:95:LEU:HD13	23:1X:97:ARG:CG	2.45	0.47
24:1Y:28:GLY:O	24:1Y:62:SER:OG	2.23	0.47
42:1q:48:TYR:HE1	42:1q:86:TRP:CG	2.32	0.47
43:1r:109:GLN:NE2	43:1r:111:TYR:O	2.43	0.47
1:1A:53:MET:N	1:1A:53:MET:HE3	2.29	0.47
1:1A:54:LYS:HE2	1:1A:54:LYS:HB2	1.67	0.47
3:1C:203:TRP:NE1	7:1G:119:GLN:HE22	2.11	0.47
4:1D:65:VAL:HG22	4:1D:77:ASP:HB3	1.96	0.47
4:1D:204:PRO:HG2	4:1D:207:LEU:HB2	1.95	0.47
12:1L:500:LEU:HD11	45:1L:703:3PE:H362	1.96	0.47
12:1L:557:TRP:O	12:1L:561:ILE:HG22	2.15	0.47
14:1N:190:MET:HE1	14:1N:205:LEU:HA	1.96	0.47
14:1N:335:LEU:O	29:1d:33:TYR:OH	2.26	0.47
45:1N:401:3PE:H292	29:1d:54:VAL:HG22	1.95	0.47
16:1P:27:THR:OG1	54:1P:501:NDP:O1X	2.31	0.47
20:1U:8:LEU:H	20:1U:8:LEU:HD12	1.79	0.47
35:1j:38:TRP:HE3	35:1j:39:ARG:HD2	1.79	0.47
42:1q:68:MET:HG2	42:1q:69:ASN:HD22	1.80	0.47
6:1F:24:ASN:CG	6:1F:24:ASN:O	2.57	0.47
6:1F:200:GLN:O	6:1F:202:LYS:N	2.48	0.47
7:1G:388:ALA:HB2	7:1G:493:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:152:SER:HB2	8:1H:304:HIS:HD2	1.80	0.47
9:1I:88:PRO:HD2	46:1I:201:SF4:S3	2.53	0.47
9:1I:175:TYR:CE1	43:1r:38:PRO:HG3	2.49	0.47
13:1M:201:MET:HE1	13:1M:261:PHE:HE1	1.80	0.47
14:1N:120:GLN:HA	14:1N:176:ARG:HE	1.80	0.47
16:1P:262:ALA:HA	16:1P:265:TRP:CD1	2.50	0.47
28:1c:6:GLU:OE2	28:1c:7:PRO:HD2	2.14	0.47
40:1o:106:ARG:HA	40:1o:109:GLN:HE22	1.79	0.47
44:1s:34:ASP:OD2	44:1s:39:ARG:NH2	2.48	0.47
1:1A:54:LYS:HG2	1:1A:113:TRP:HB3	1.96	0.47
1:1A:113:TRP:HH2	8:1H:282:TYR:HE1	1.62	0.47
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	1.97	0.47
3:1C:92:ILE:HD11	3:1C:140:VAL:HG11	1.97	0.47
3:1C:140:VAL:HG13	3:1C:142:PHE:HE2	1.79	0.47
4:1D:152:MET:HG2	4:1D:156:THR:HG21	1.97	0.47
5:1E:183:LYS:HG3	44:1s:44:HIS:HB3	1.95	0.47
6:1F:205:LEU:HB2	17:1Q:118:TYR:CZ	2.50	0.47
6:1F:256:PHE:CE2	6:1F:279:LEU:HD11	2.50	0.47
6:1F:376:MET:HA	6:1F:379:PHE:HB2	1.97	0.47
6:1F:405:CYS:SG	6:1F:407:LEU:HB3	2.55	0.47
7:1G:168:GLY:HA2	7:1G:396:ARG:HH21	1.79	0.47
7:1G:268:ARG:HD2	7:1G:269:PHE:CE2	2.50	0.47
7:1G:288:LYS:HB3	7:1G:288:LYS:HE2	1.70	0.47
7:1G:675:ASP:N	7:1G:675:ASP:OD1	2.48	0.47
8:1H:193:THR:HG22	8:1H:234:MET:HE3	1.96	0.47
8:1H:264:LEU:HD12	8:1H:264:LEU:HA	1.75	0.47
9:1I:44:GLU:HA	26:1a:1:MET:HE1	1.96	0.47
12:1L:40:VAL:HG11	12:1L:97:THR:HG23	1.97	0.47
12:1L:542:LEU:HD23	37:1l:83:MET:HG3	1.96	0.47
13:1M:443:PRO:HB3	47:1M:501:PC1:H2C1	1.95	0.47
15:1O:224:SER:O	15:1O:228:ALA:N	2.46	0.47
20:1T:19:LEU:HD11	20:1T:36:PHE:CE1	2.50	0.47
20:1T:50:ILE:HD12	20:1T:51:ILE:N	2.29	0.47
22:1W:39:TRP:NE1	22:1W:90:LEU:HB2	2.29	0.47
23:1X:11:ASP:OD1	23:1X:11:ASP:N	2.48	0.47
36:1k:17:ASP:OD1	36:1k:18:TYR:N	2.48	0.47
39:1n:9:LEU:O	39:1n:14:LYS:NZ	2.43	0.47
2:1B:53:ALA:HB2	4:1D:83:LEU:HD21	1.97	0.47
7:1G:377:ILE:HD11	7:1G:404:LEU:HD11	1.97	0.47
8:1H:15:LEU:HG	26:1a:15:CYS:SG	2.54	0.47
8:1H:281:ARG:O	8:1H:285:LEU:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:66:TRP:HB2	47:1M:501:PC1:O14	2.14	0.47
12:1L:537:PRO:HG2	45:1L:701:3PE:H362	1.97	0.47
13:1M:61:LEU:HD11	13:1M:244:MET:SD	2.55	0.47
13:1M:257:MET:O	13:1M:260:PRO:HD2	2.15	0.47
14:1N:221:HIS:O	14:1N:319:HIS:NE2	2.47	0.47
15:1O:151:HIS:O	15:1O:155:VAL:HG23	2.15	0.47
17:1Q:28:GLU:H	17:1Q:28:GLU:CD	2.22	0.47
34:1i:46:TRP:O	34:1i:50:LEU:HG	2.14	0.47
40:1o:96:LYS:HE2	40:1o:96:LYS:HB3	1.81	0.47
6:1F:368:GLY:HA3	7:1G:96:PHE:CE1	2.49	0.47
7:1G:46:LEU:HD23	7:1G:161:ARG:HH21	1.80	0.47
7:1G:248:MET:N	7:1G:248:MET:SD	2.88	0.47
9:1I:32:ARG:HH12	47:1I:203:PC1:H31	1.80	0.47
12:1L:420:ALA:HB2	12:1L:494:THR:HG23	1.97	0.47
45:1L:702:3PE:H391	45:1L:702:3PE:H242	1.97	0.47
14:1N:289:ASN:HA	14:1N:292:PHE:CZ	2.50	0.47
16:1P:292:MET:SD	16:1P:294:LEU:HB2	2.55	0.47
19:1S:63:LYS:HG2	19:1S:65:TRP:CD1	2.50	0.47
20:1U:66:ASP:O	20:1U:70:LEU:HD23	2.15	0.47
21:1V:51:THR:O	21:1V:55:LEU:N	2.41	0.47
28:1c:21:LEU:O	28:1c:25:VAL:HG12	2.15	0.47
31:1f:49:ARG:NH2	33:1h:60:VAL:HG22	2.30	0.47
2:1B:125:TYR:CE1	9:1I:88:PRO:HB2	2.50	0.47
3:1C:111:THR:OG1	3:1C:117:ILE:HD11	2.15	0.47
4:1D:213:GLU:OE1	4:1D:216:LYS:NZ	2.48	0.47
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.97	0.47
7:1G:43:HIS:NE2	7:1G:261:GLU:OE2	2.47	0.47
7:1G:126:ASP:OD1	43:1r:56:ARG:NH2	2.47	0.47
7:1G:147:LYS:N	7:1G:209:THR:O	2.35	0.47
7:1G:232:ASP:OD2	7:1G:388:ALA:HA	2.15	0.47
7:1G:276:ARG:HA	42:1q:135:GLN:HB2	1.97	0.47
7:1G:384:PRO:HA	7:1G:388:ALA:H	1.79	0.47
7:1G:689:LYS:O	7:1G:692:THR:OG1	2.31	0.47
10:1J:162:LEU:O	10:1J:165:VAL:HG12	2.15	0.47
13:1M:244:MET:HG3	13:1M:301:ILE:HD12	1.96	0.47
14:1N:202:ILE:O	14:1N:206:LEU:HD12	2.14	0.47
14:1N:260:PHE:CZ	14:1N:264:TRP:HB2	2.50	0.47
15:1O:173:ASP:HB3	15:1O:222:GLN:HE21	1.80	0.47
16:1P:154:LYS:HD3	16:1P:154:LYS:H	1.79	0.47
17:1Q:36:ARG:HG2	17:1Q:38:PHE:HD2	1.80	0.47
25:1Z:86:MET:HE1	25:1Z:125:TYR:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:21:SER:OG	30:1e:36:GLU:HB3	2.14	0.47
38:1m:94:ILE:HD11	38:1m:98:PHE:HD2	1.80	0.47
3:1C:125:LYS:HE2	4:1D:253:TYR:CE1	2.50	0.46
6:1F:36:ALA:HB2	6:1F:116:HIS:CD2	2.50	0.46
7:1G:516:LYS:HD2	7:1G:517:ASN:HB2	1.97	0.46
12:1L:432:LEU:HD13	36:1k:62:PHE:HA	1.97	0.46
13:1M:206:LYS:NZ	13:1M:235:LEU:HD13	2.29	0.46
13:1M:230:VAL:O	13:1M:235:LEU:HG	2.15	0.46
13:1M:424:ASN:ND2	38:1m:55:ARG:HH21	2.14	0.46
16:1P:40:ARG:NH2	22:1W:110:THR:OG1	2.48	0.46
16:1P:78:LYS:HD3	16:1P:78:LYS:C	2.40	0.46
18:1R:32:GLN:HE22	18:1R:34:GLU:HG2	1.80	0.46
20:1T:56:ASP:OD1	20:1T:56:ASP:N	2.48	0.46
22:1W:23:ARG:HB2	22:1W:27:GLU:OE2	2.16	0.46
22:1W:32:VAL:O	22:1W:36:TYR:HB2	2.14	0.46
25:1Z:34:SER:O	25:1Z:38:VAL:HG22	2.16	0.46
29:1d:109:TYR:OH	41:1p:152:ARG:NE	2.48	0.46
32:1g:100:ARG:HG2	32:1g:107:LEU:HA	1.96	0.46
38:1m:21:GLU:H	38:1m:21:GLU:CD	2.22	0.46
4:1D:267:TRP:CE3	4:1D:272:THR:HG21	2.51	0.46
5:1E:206:PRO:HG3	6:1F:29:HIS:CE1	2.50	0.46
6:1F:26:TYR:HB3	6:1F:28:ARG:HG2	1.96	0.46
7:1G:362:TYR:HA	7:1G:492:ILE:HG21	1.97	0.46
8:1H:142:TYR:OH	8:1H:285:LEU:HD12	2.14	0.46
8:1H:306:SER:OG	8:1H:310:MET:SD	2.73	0.46
12:1L:7:LEU:O	12:1L:10:THR:HG22	2.16	0.46
22:1W:17:VAL:HG23	22:1W:77:ARG:NH2	2.28	0.46
29:1d:45:ASP:O	29:1d:49:ARG:HG2	2.15	0.46
37:1l:13:TYR:HD1	37:1l:14:PRO:HD2	1.80	0.46
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.45	0.46
1:1A:66:ASP:OD1	10:1J:59:ILE:HG22	2.15	0.46
4:1D:349:PHE:HE2	7:1G:106:PRO:HA	1.79	0.46
6:1F:132:ARG:HH12	44:1s:66:PRO:HG3	1.80	0.46
14:1N:339:MET:HE1	29:1d:30:ARG:HB3	1.97	0.46
16:1P:226:LYS:HE3	16:1P:226:LYS:HB2	1.76	0.46
24:1Y:86:PRO:HA	24:1Y:125:LYS:HG2	1.97	0.46
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.40	0.46
34:1i:76:ILE:HD12	34:1i:77:PRO:CD	2.45	0.46
34:1i:100:LYS:HZ3	41:1p:116:GLU:HA	1.80	0.46
40:1o:109:GLN:OE1	40:1o:109:GLN:N	2.43	0.46
4:1D:95:THR:O	4:1D:99:ALA:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:224:ASN:HB3	6:1F:227:THR:HG23	1.97	0.46
6:1F:250:ASN:ND2	6:1F:318:ASP:HB2	2.30	0.46
6:1F:395:ILE:HA	6:1F:398:GLN:HG3	1.97	0.46
6:1F:431:GLN:O	6:1F:431:GLN:NE2	2.47	0.46
7:1G:478:ARG:NE	7:1G:478:ARG:O	2.48	0.46
8:1H:19:PHE:HA	8:1H:48:PRO:HB3	1.97	0.46
12:1L:4:PHE:HB2	12:1L:53:MET:HE3	1.96	0.46
12:1L:114:ILE:HD12	12:1L:114:ILE:HA	1.83	0.46
13:1M:258:ALA:HB1	13:1M:262:LEU:HD13	1.97	0.46
14:1N:25:HIS:NE2	30:1e:17:MET:SD	2.89	0.46
16:1P:117:ILE:O	16:1P:121:SER:OG	2.18	0.46
16:1P:280:THR:HG23	16:1P:283:LYS:H	1.80	0.46
19:1S:34:ASP:O	19:1S:38:LYS:HB2	2.16	0.46
21:1V:112:LYS:HG3	21:1V:112:LYS:O	2.16	0.46
22:1W:68:MET:HA	22:1W:71:ALA:HB3	1.98	0.46
24:1Y:139:LYS:HZ3	33:1h:112:ARG:HG3	1.81	0.46
34:1i:93:PRO:HB3	41:1p:4:TRP:CE2	2.50	0.46
35:1j:19:ARG:O	35:1j:23:ILE:HD12	2.15	0.46
37:1l:10:PRO:HB2	38:1m:74:ASN:HD22	1.80	0.46
39:1n:153:LEU:HD21	39:1n:164:PRO:O	2.16	0.46
42:1q:66:THR:O	42:1q:73:THR:N	2.38	0.46
43:1r:4:THR:O	43:1r:8:GLN:HG3	2.15	0.46
1:1A:1:FME:O1	1:1A:2:ASN:N	2.49	0.46
2:1B:68:ASP:OD2	2:1B:71:ARG:N	2.46	0.46
3:1C:155:TYR:HB2	22:1W:102:HIS:CE1	2.50	0.46
5:1E:166:PRO:HB2	5:1E:167:LYS:HE2	1.98	0.46
6:1F:89:ARG:HD2	6:1F:217:GLY:O	2.15	0.46
6:1F:91:LYS:HD2	6:1F:129:MET:O	2.16	0.46
7:1G:623:LEU:HA	7:1G:626:VAL:HG12	1.97	0.46
12:1L:11:THR:HG22	12:1L:46:LEU:HD12	1.98	0.46
13:1M:73:LEU:HA	13:1M:76:MET:SD	2.56	0.46
15:1O:205:ALA:O	15:1O:209:THR:HB	2.15	0.46
15:1O:214:MET:HE3	15:1O:217:LYS:HZ2	1.81	0.46
31:1f:43:LEU:HD21	41:1p:67:PHE:CD1	2.50	0.46
34:1i:79:TRP:HE1	41:1p:40:VAL:HA	1.81	0.46
35:1j:38:TRP:CE3	35:1j:39:ARG:HD2	2.51	0.46
2:1B:47:PRO:HD3	2:1B:74:VAL:HB	1.98	0.46
2:1B:62:MET:HG3	2:1B:69:MET:CG	2.45	0.46
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.50	0.46
4:1D:418:ILE:HG13	4:1D:419:GLY:N	2.30	0.46
5:1E:213:VAL:HA	5:1E:217:LEU:HD22	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:199:ILE:HG22	7:1G:208:LEU:HD23	1.98	0.46
12:1L:339:LEU:HD21	12:1L:376:GLY:HA3	1.98	0.46
12:1L:419:THR:HA	12:1L:422:TYR:CE2	2.51	0.46
13:1M:338:HIS:NE2	32:1g:34:ASP:OD2	2.49	0.46
14:1N:344:SER:O	29:1d:82:MET:HG2	2.16	0.46
16:1P:250:TYR:CZ	16:1P:329:SER:HB2	2.51	0.46
16:1P:315:ILE:O	16:1P:319:ARG:HB2	2.16	0.46
20:1T:63:PRO:HD2	20:1T:66:ASP:OD1	2.16	0.46
30:1e:62:PHE:CD1	30:1e:62:PHE:C	2.94	0.46
34:1i:7:GLU:HA	34:1i:10:ARG:HB3	1.96	0.46
36:1k:48:GLU:OE2	39:1n:33:ARG:NH2	2.47	0.46
2:1B:56:ALA:O	2:1B:59:MET:HB3	2.15	0.46
4:1D:132:PRO:HA	4:1D:135:GLN:HG3	1.98	0.46
4:1D:366:ALA:HB1	4:1D:373:GLU:HG2	1.98	0.46
8:1H:146:LEU:O	8:1H:150:LEU:HG	2.16	0.46
8:1H:193:THR:HG22	8:1H:234:MET:CE	2.46	0.46
8:1H:226:ALA:O	8:1H:230:ASN:ND2	2.48	0.46
12:1L:332:HIS:HA	12:1L:335:PHE:CE1	2.51	0.46
13:1M:114:GLU:OE2	13:1M:174:LEU:HB2	2.15	0.46
14:1N:104:MET:HB2	14:1N:111:PHE:CG	2.51	0.46
14:1N:278:MET:O	14:1N:282:MET:HB2	2.16	0.46
37:1l:128:VAL:HG23	40:1o:97:ARG:HB2	1.98	0.46
41:1p:78:GLU:HG3	41:1p:79:LYS:HG3	1.98	0.46
42:1q:44:TYR:HE2	42:1q:83:PRO:HB3	1.81	0.46
1:1A:77:TRP:CZ2	8:1H:100:LEU:HD21	2.50	0.46
1:1A:102:LEU:O	1:1A:106:TRP:HB2	2.16	0.46
1:1A:113:TRP:HZ2	8:1H:286:MET:HG2	1.81	0.46
4:1D:394:PRO:HB2	4:1D:398:HIS:CE1	2.50	0.46
5:1E:100:ILE:HD12	5:1E:138:THR:H	1.80	0.46
7:1G:365:ASN:N	7:1G:491:ASN:OD1	2.47	0.46
8:1H:77:LEU:HA	8:1H:80:SER:OG	2.16	0.46
10:1J:109:LYS:HA	10:1J:109:LYS:HD2	1.68	0.46
12:1L:231:PRO:C	12:1L:234:PRO:HD2	2.40	0.46
30:1e:79:LYS:HE3	30:1e:79:LYS:HB2	1.79	0.46
32:1g:45:HIS:CD2	32:1g:58:MET:HE3	2.50	0.46
1:1A:72:LEU:O	8:1H:151:LEU:HD21	2.15	0.46
4:1D:301:VAL:O	4:1D:304:MET:HB2	2.16	0.46
6:1F:322:LEU:HB3	6:1F:327:THR:HG23	1.98	0.46
7:1G:415:LEU:C	7:1G:416:THR:HG1	2.24	0.46
8:1H:235:ASN:ND2	8:1H:266:LEU:HB3	2.31	0.46
15:1O:34:GLY:N	52:1O:401:GTP:O3G	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:70:LEU:HD13	20:1U:75:GLU:HB3	1.98	0.46
3:1C:6:ASP:OD1	3:1C:6:ASP:N	2.48	0.46
3:1C:78:LEU:HA	3:1C:93:VAL:O	2.16	0.46
4:1D:170:MET:HE1	4:1D:221:ARG:HB3	1.98	0.46
5:1E:128:VAL:HA	5:1E:139:LEU:HD11	1.98	0.46
6:1F:35:GLY:O	6:1F:38:SER:OG	2.26	0.46
6:1F:116:HIS:O	6:1F:120:GLU:HG3	2.16	0.46
6:1F:224:ASN:O	6:1F:228:VAL:HG12	2.16	0.46
6:1F:362:CYS:N	46:1F:502:SF4:S3	2.78	0.46
7:1G:58:GLU:HA	7:1G:65:VAL:HG12	1.98	0.46
12:1L:100:ILE:O	12:1L:104:SER:N	2.44	0.46
12:1L:363:TYR:HA	12:1L:370:THR:HG21	1.98	0.46
13:1M:2:LEU:HD12	13:1M:6:ILE:HD11	1.98	0.46
16:1P:9:GLY:HA3	16:1P:15:SER:HB3	1.98	0.46
20:1T:51:ILE:HB	20:1T:62:ILE:HD11	1.97	0.46
21:1V:92:LYS:O	21:1V:95:ARG:HD2	2.16	0.46
23:1X:118:ARG:HD2	23:1X:119:PRO:HD2	1.98	0.46
30:1e:58:GLU:OE1	30:1e:58:GLU:N	2.49	0.46
31:1f:42:LEU:HA	31:1f:45:LYS:HB2	1.98	0.46
1:1A:84:LEU:HD23	27:1b:45:ASN:HD22	1.81	0.45
2:1B:171:LYS:HE2	2:1B:171:LYS:HB2	1.71	0.45
3:1C:179:GLU:OE2	16:1P:37:HIS:NE2	2.49	0.45
4:1D:140:LEU:HB2	4:1D:314:CYS:SG	2.56	0.45
6:1F:294:LEU:HD13	6:1F:336:VAL:HG13	1.97	0.45
8:1H:116:ILE:HG12	8:1H:211:PHE:CE1	2.52	0.45
10:1J:168:ILE:O	10:1J:172:THR:HG22	2.17	0.45
23:1X:114:LEU:HB3	23:1X:116:TRP:CE2	2.50	0.45
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.33	0.45
41:1p:145:LEU:HB3	41:1p:149:TYR:HB3	1.98	0.45
42:1q:44:TYR:HB3	42:1q:68:MET:HG3	1.99	0.45
3:1C:21:GLN:HG2	43:1r:96:PRO:O	2.16	0.45
3:1C:55:ASP:OD2	3:1C:56:GLY:N	2.49	0.45
6:1F:101:GLU:HG3	6:1F:102:PRO:HD2	1.97	0.45
9:1I:97:GLU:OE1	9:1I:97:GLU:N	2.49	0.45
10:1J:122:LEU:HD11	30:1e:76:SER:HB2	1.98	0.45
12:1L:511:LEU:HD21	39:1n:38:TYR:CE1	2.52	0.45
14:1N:70:LEU:HD12	14:1N:98:MET:HE1	1.97	0.45
16:1P:236:TYR:HB2	16:1P:241:LEU:HD13	1.99	0.45
23:1X:36:ASP:OD2	23:1X:37:LYS:N	2.49	0.45
24:1Y:120:THR:HA	24:1Y:123:LEU:HD12	1.98	0.45
26:1a:1:MET:HB2	26:1a:3:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:56:PRO:HB2	33:1h:59:TYR:HB3	1.97	0.45
37:1l:123:PRO:O	40:1o:8:TYR:OH	2.28	0.45
40:1o:50:LEU:O	40:1o:55:ARG:NH1	2.40	0.45
4:1D:124:LYS:HD2	4:1D:363:THR:HG21	1.98	0.45
4:1D:232:ASN:HB2	4:1D:235:TRP:HB3	1.98	0.45
4:1D:241:ASP:N	4:1D:292:ASP:OD2	2.38	0.45
4:1D:276:ASP:HB3	4:1D:277:VAL:H	1.59	0.45
6:1F:93:LEU:HD23	6:1F:173:PHE:HZ	1.82	0.45
6:1F:403:THR:OG1	6:1F:405:CYS:O	2.28	0.45
7:1G:41:CYS:SG	7:1G:51:ASN:N	2.89	0.45
8:1H:102:VAL:HB	8:1H:160:TYR:HB3	1.98	0.45
12:1L:511:LEU:HD21	39:1n:38:TYR:CZ	2.51	0.45
16:1P:10:LYS:N	16:1P:10:LYS:HD3	2.31	0.45
16:1P:91:VAL:HG23	16:1P:126:VAL:HG21	1.97	0.45
16:1P:216:ASN:HD22	16:1P:219:LYS:HD3	1.80	0.45
16:1P:268:ARG:O	16:1P:272:VAL:HG23	2.17	0.45
16:1P:315:ILE:HD11	22:1W:53:ASP:HB3	1.98	0.45
25:1Z:6:VAL:C	25:1Z:7:LYS:HD3	2.41	0.45
26:1a:27:HIS:HE1	26:1a:36:LYS:HE2	1.81	0.45
32:1g:112:CYS:HB2	41:1p:141:ARG:HD3	1.99	0.45
37:1l:97:SER:HA	38:1m:5:TYR:CE1	2.51	0.45
42:1q:133:LYS:HG3	42:1q:134:ILE:HG12	1.98	0.45
1:1A:9:THR:HG21	8:1H:6:ILE:HG21	1.98	0.45
1:1A:113:TRP:CH2	8:1H:282:TYR:HE1	2.34	0.45
3:1C:72:PHE:HE1	43:1r:96:PRO:HG3	1.81	0.45
3:1C:176:TYR:HD1	3:1C:177:ASP:H	1.63	0.45
4:1D:315:LEU:HD13	25:1Z:16:TYR:CD2	2.51	0.45
5:1E:190:ARG:HH12	6:1F:265:PRO:HG2	1.81	0.45
5:1E:194:GLU:N	6:1F:26:TYR:OH	2.34	0.45
6:1F:30:ASP:HA	44:1s:39:ARG:HD2	1.98	0.45
7:1G:9:ILE:HD11	7:1G:75:LYS:HB2	1.97	0.45
7:1G:704:CYS:SG	9:1I:104:ARG:HG2	2.56	0.45
8:1H:26:LYS:HZ1	26:1a:4:GLU:C	2.23	0.45
8:1H:187:ILE:HG13	9:1I:27:TRP:CH2	2.52	0.45
9:1I:83:CYS:SG	9:1I:109:TYR:OH	2.74	0.45
12:1L:350:LEU:O	12:1L:353:GLU:HB2	2.16	0.45
13:1M:321:LEU:HD12	13:1M:321:LEU:HA	1.80	0.45
14:1N:109:SER:C	14:1N:112:HIS:HD1	2.22	0.45
16:1P:245:ILE:HD12	16:1P:246:PHE:N	2.32	0.45
17:1Q:91:ASP:OD1	17:1Q:91:ASP:N	2.50	0.45
22:1W:45:ASN:OD1	22:1W:46:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:92:GLU:HB3	22:1W:98:LYS:HD2	1.97	0.45
27:1b:7:PHE:HA	27:1b:10:ASN:HB3	1.98	0.45
31:1f:37:PHE:HA	31:1f:40:LYS:HG3	1.99	0.45
38:1m:26:PRO:O	38:1m:30:LYS:HG3	2.17	0.45
38:1m:27:GLU:HA	38:1m:30:LYS:HE2	1.97	0.45
45:1A:201:3PE:H2D1	8:1H:302:MET:HE1	1.99	0.45
4:1D:326:ASP:OD1	7:1G:127:ARG:NH2	2.50	0.45
5:1E:86:PHE:HZ	6:1F:185:ILE:HG21	1.81	0.45
6:1F:255:LEU:HA	6:1F:269:GLU:HA	1.99	0.45
6:1F:394:GLU:O	6:1F:398:GLN:HG3	2.17	0.45
7:1G:100:ASN:HB3	7:1G:135:ARG:HH21	1.81	0.45
7:1G:121:MET:HB3	7:1G:122:MET:HE2	1.99	0.45
7:1G:337:ARG:HG2	7:1G:609:MET:HB2	1.99	0.45
8:1H:72:ILE:O	8:1H:76:ILE:HG12	2.16	0.45
8:1H:149:ILE:HD11	8:1H:184:MET:HG3	1.98	0.45
8:1H:207:LEU:O	8:1H:209:SER:N	2.49	0.45
12:1L:61:MET:HB2	12:1L:82:MET:HB2	1.98	0.45
13:1M:29:VAL:HG22	32:1g:60:VAL:CG2	2.45	0.45
16:1P:93:ASN:HD22	16:1P:117:ILE:HD11	1.80	0.45
20:1U:36:PHE:HB3	20:1U:42:LEU:CD2	2.47	0.45
23:1X:131:LYS:HD2	23:1X:131:LYS:HA	1.86	0.45
3:1C:94:TYR:C	3:1C:95:ASN:HD22	2.23	0.45
5:1E:10:ARG:H	5:1E:10:ARG:HG2	1.63	0.45
5:1E:127:LYS:HA	5:1E:127:LYS:HD3	1.74	0.45
6:1F:298:ILE:O	6:1F:334:VAL:HA	2.16	0.45
6:1F:327:THR:OG1	6:1F:328:GLY:N	2.50	0.45
7:1G:378:LEU:N	7:1G:450:MET:O	2.47	0.45
8:1H:146:LEU:HD22	8:1H:185:TRP:CZ3	2.52	0.45
12:1L:106:TRP:O	12:1L:109:HIS:ND1	2.38	0.45
14:1N:199:THR:O	14:1N:202:ILE:HG22	2.17	0.45
14:1N:269:GLU:OE1	14:1N:269:GLU:HA	2.16	0.45
17:1Q:67:ASN:HB2	17:1Q:72:TRP:HB2	1.99	0.45
18:1R:95:HIS:O	18:1R:95:HIS:CG	2.69	0.45
20:1T:66:ASP:O	20:1T:70:LEU:HD12	2.16	0.45
20:1U:87:TYR:HA	34:1i:19:ARG:HD3	1.98	0.45
38:1m:111:LYS:O	38:1m:115:ILE:HG13	2.17	0.45
2:1B:41:ARG:HH11	2:1B:172:ARG:NH1	2.14	0.45
4:1D:37:ASP:CG	11:1K:95:LEU:HD11	2.41	0.45
4:1D:100:LEU:HD11	4:1D:115:GLU:HG2	1.99	0.45
4:1D:414:VAL:HA	4:1D:417:ILE:HD12	1.99	0.45
5:1E:180:LYS:NZ	5:1E:181:ILE:H	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:25:LEU:HD11	6:1F:269:GLU:HG2	1.98	0.45
7:1G:189:LYS:HE2	7:1G:189:LYS:HB3	1.64	0.45
7:1G:265:ASP:N	7:1G:265:ASP:OD1	2.47	0.45
7:1G:646:ASN:O	7:1G:650:LYS:HG2	2.16	0.45
8:1H:19:PHE:HA	8:1H:48:PRO:HG3	1.99	0.45
11:1K:19:LEU:HD11	14:1N:65:THR:HG21	1.97	0.45
12:1L:204:LEU:HD22	38:1m:124:PHE:HE2	1.81	0.45
12:1L:319:ILE:O	12:1L:321:GLN:HG2	2.17	0.45
12:1L:435:PRO:HG2	36:1k:56:PHE:CD2	2.51	0.45
12:1L:600:THR:HA	12:1L:605:HIS:CE1	2.51	0.45
13:1M:137:GLY:HA3	13:1M:142:ARG:HD2	1.99	0.45
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.51	0.45
15:1O:270:LEU:O	15:1O:273:THR:OG1	2.27	0.45
16:1P:174:ARG:HB3	16:1P:175:GLU:OE1	2.17	0.45
22:1W:52:LEU:HD11	22:1W:103:ILE:HD12	1.99	0.45
23:1X:165:ARG:NH2	29:1d:86:ARG:HH12	2.14	0.45
24:1Y:132:TRP:CZ3	57:1Y:201:PGT:H141	2.50	0.45
30:1e:64:GLU:O	30:1e:68:ARG:HA	2.16	0.45
38:1m:50:TYR:O	38:1m:55:ARG:NH1	2.48	0.45
41:1p:165:GLU:OE1	41:1p:166:ARG:NH1	2.49	0.45
42:1q:144:TYR:O	42:1q:145:LYS:HG3	2.17	0.45
3:1C:195:ARG:NH1	9:1I:93:THR:HG22	2.32	0.45
6:1F:121:GLY:HA2	6:1F:232:PRO:HG3	1.97	0.45
6:1F:305:PRO:HB3	6:1F:417:GLY:HA3	1.97	0.45
7:1G:112:GLY:HA3	7:1G:219:PRO:HG2	1.99	0.45
12:1L:598:SER:O	12:1L:604:TYR:HB2	2.16	0.45
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.17	0.45
14:1N:264:TRP:HH2	23:1X:169:TRP:HZ3	1.65	0.45
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	1.98	0.45
16:1P:315:ILE:N	16:1P:331:MET:HE1	2.23	0.45
17:1Q:126:LYS:CE	17:1Q:128:THR:HB	2.46	0.45
21:1V:8:THR:HG22	21:1V:77:GLU:HG3	1.99	0.45
21:1V:75:GLN:OE1	21:1V:76:ILE:HD12	2.17	0.45
24:1Y:65:ILE:HD11	24:1Y:100:LEU:HB2	1.98	0.45
25:1Z:111:PHE:CE2	25:1Z:117:VAL:HG21	2.52	0.45
33:1h:93:ILE:HA	33:1h:93:ILE:HD13	1.82	0.45
47:1h:201:PC1:H31	47:1h:201:PC1:H322	1.54	0.45
36:1k:26:THR:O	36:1k:29:GLU:HG2	2.17	0.45
40:1o:56:ASP:OD2	40:1o:58:CYS:N	2.43	0.45
41:1p:55:HIS:O	41:1p:59:ARG:HD2	2.16	0.45
1:1A:73:LEU:HD23	8:1H:151:LEU:HD22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:351:LEU:HA	4:1D:355:GLY:HA2	1.99	0.45
5:1E:25:PRO:O	5:1E:29:LYS:NZ	2.50	0.45
5:1E:46:ALA:O	5:1E:49:PRO:HD2	2.16	0.45
5:1E:183:LYS:NZ	44:1s:41:LEU:HD22	2.32	0.45
5:1E:191:PHE:H	5:1E:194:GLU:CD	2.23	0.45
6:1F:15:LEU:HD22	6:1F:253:THR:OG1	2.17	0.45
6:1F:105:CYS:H	6:1F:257:ASN:CG	2.25	0.45
6:1F:184:TYR:CE1	49:1F:501:FMN:H6	2.52	0.45
7:1G:339:ASP:CG	19:1S:70:PHE:H	2.24	0.45
9:1I:147:LEU:HD23	9:1I:147:LEU:HA	1.77	0.45
10:1J:103:MET:SD	11:1K:6:MET:HE1	2.57	0.45
12:1L:67:HIS:ND1	12:1L:77:SER:OG	2.50	0.45
12:1L:325:ALA:O	12:1L:329:ILE:HG12	2.17	0.45
13:1M:457:PRO:HA	32:1g:84:ARG:HH12	1.82	0.45
19:1S:72:GLN:OE1	19:1S:74:LYS:HD3	2.16	0.45
20:1U:20:LYS:HD3	36:1k:18:TYR:CD2	2.52	0.45
31:1f:42:LEU:HD23	31:1f:42:LEU:H	1.80	0.45
31:1f:49:ARG:HB2	31:1f:52:GLU:HB2	1.99	0.45
32:1g:41:ASN:OD1	32:1g:41:ASN:N	2.43	0.45
32:1g:120:LEU:HD23	41:1p:166:ARG:HG3	1.98	0.45
38:1m:124:PHE:HE1	41:1p:132:THR:HG23	1.81	0.45
40:1o:103:ARG:HG2	40:1o:107:LEU:HD13	1.99	0.45
3:1C:98:SER:N	3:1C:103:SER:O	2.45	0.45
3:1C:206:PHE:CE2	43:1r:59:ARG:HB3	2.52	0.45
47:1D:501:PC1:O32	8:1H:292:SER:OG	2.33	0.45
5:1E:31:ILE:O	5:1E:35:VAL:HG22	2.17	0.45
5:1E:57:GLN:HG3	44:1s:49:TYR:HE2	1.82	0.45
7:1G:354:ALA:HB3	7:1G:361:ASN:HD22	1.82	0.45
7:1G:467:LEU:HA	7:1G:470:VAL:HG12	1.98	0.45
10:1J:167:VAL:O	10:1J:171:ILE:HG23	2.17	0.45
10:1J:171:ILE:HG13	10:1J:172:THR:N	2.32	0.45
12:1L:177:ILE:O	12:1L:180:ILE:HB	2.16	0.45
14:1N:40:MET:HE3	14:1N:40:MET:HB2	1.69	0.45
14:1N:76:ILE:HG22	14:1N:94:ALA:HB2	1.98	0.45
15:1O:129:TYR:HE1	15:1O:160:ALA:HB1	1.81	0.45
22:1W:98:LYS:HB3	22:1W:98:LYS:HE3	1.76	0.45
23:1X:19:VAL:HB	23:1X:23:VAL:CG1	2.47	0.45
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.49	0.45
25:1Z:65:PHE:O	25:1Z:69:ILE:HG12	2.17	0.45
31:1f:49:ARG:NH1	33:1h:58:GLY:O	2.50	0.45
33:1h:64:TRP:NE1	33:1h:77:ARG:HD3	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:101:LYS:HE2	43:1r:101:LYS:HB3	1.75	0.45
2:1B:66:ARG:HA	2:1B:66:ARG:HD3	1.78	0.44
4:1D:145:THR:OG1	4:1D:181:TYR:OH	2.31	0.44
6:1F:51:LYS:HZ3	6:1F:55:TRP:CG	2.35	0.44
6:1F:139:ARG:HD3	6:1F:141:GLU:HB2	1.98	0.44
6:1F:422:PHE:CD1	6:1F:425:GLU:HB2	2.52	0.44
7:1G:18:VAL:HG11	7:1G:32:LYS:HE2	1.99	0.44
7:1G:322:LEU:HD21	7:1G:548:HIS:HE2	1.82	0.44
7:1G:348:VAL:N	7:1G:459:GLN:OE1	2.36	0.44
7:1G:704:CYS:C	9:1I:103:SER:HA	2.42	0.44
8:1H:157:ASN:ND2	8:1H:165:LEU:HA	2.33	0.44
10:1J:122:LEU:HD13	30:1e:75:LEU:HD12	1.98	0.44
11:1K:5:TYR:O	11:1K:9:ILE:HG22	2.17	0.44
12:1L:371:THR:O	12:1L:375:ILE:HG12	2.17	0.44
12:1L:529:TYR:CZ	12:1L:533:MET:HG3	2.51	0.44
16:1P:166:ILE:HG23	16:1P:230:PHE:HE2	1.83	0.44
21:1V:91:ARG:HG2	21:1V:95:ARG:NH2	2.32	0.44
22:1W:27:GLU:H	22:1W:27:GLU:CD	2.19	0.44
32:1g:48:ASP:C	32:1g:48:ASP:OD1	2.60	0.44
34:1i:107:ASP:OD1	34:1i:107:ASP:N	2.50	0.44
39:1n:28:SER:HB2	39:1n:79:TYR:H	1.82	0.44
39:1n:30:CYS:O	39:1n:32:HIS:N	2.49	0.44
4:1D:391:ILE:HB	4:1D:430:ARG:HD2	1.99	0.44
6:1F:298:ILE:HG22	6:1F:301:GLY:H	1.82	0.44
7:1G:339:ASP:OD1	19:1S:70:PHE:N	2.43	0.44
9:1I:153:LYS:HB2	42:1q:124:TYR:HE1	1.83	0.44
12:1L:105:MET:HB2	12:1L:449:LEU:HD13	1.98	0.44
12:1L:377:SER:O	12:1L:381:THR:HG23	2.17	0.44
14:1N:11:MET:HA	14:1N:14:MET:HB2	1.98	0.44
15:1O:198:TYR:O	15:1O:202:ILE:HG12	2.17	0.44
16:1P:216:ASN:HA	16:1P:219:LYS:HG2	1.98	0.44
17:1Q:6:GLN:O	22:1W:18:LYS:NZ	2.50	0.44
24:1Y:100:LEU:O	24:1Y:104:THR:OG1	2.27	0.44
25:1Z:111:PHE:HE2	25:1Z:117:VAL:HG21	1.82	0.44
28:1c:28:TRP:O	28:1c:31:LEU:N	2.49	0.44
28:1c:43:LYS:HZ2	28:1c:49:GLU:HB2	1.82	0.44
31:1f:54:VAL:HG13	31:1f:55:THR:O	2.18	0.44
43:1r:51:ASN:OD1	43:1r:56:ARG:NH1	2.50	0.44
4:1D:180:PHE:O	4:1D:184:VAL:HG22	2.16	0.44
4:1D:377:TYR:HB3	4:1D:390:LYS:HB3	1.99	0.44
7:1G:142:ILE:HG12	7:1G:148:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:379:LEU:H	7:1G:379:LEU:HD12	1.82	0.44
7:1G:508:LYS:HE3	7:1G:513:ALA:HB3	1.98	0.44
8:1H:292:SER:HA	27:1b:17:VAL:HG11	1.99	0.44
12:1L:81:LYS:C	12:1L:82:MET:HE2	2.42	0.44
12:1L:331:MET:N	12:1L:331:MET:SD	2.90	0.44
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.53	0.44
14:1N:214:ALA:O	14:1N:218:LEU:HB2	2.17	0.44
15:1O:20:GLU:OE2	15:1O:23:LYS:NZ	2.46	0.44
17:1Q:55:TRP:O	17:1Q:86:PHE:N	2.38	0.44
22:1W:81:LEU:HA	22:1W:84:ILE:HD12	2.00	0.44
26:1a:31:ASN:OD1	26:1a:60:TYR:OH	2.25	0.44
26:1a:55:SER:HA	26:1a:64:LYS:NZ	2.31	0.44
41:1p:139:GLN:O	41:1p:143:SER:OG	2.26	0.44
44:1s:47:SER:O	44:1s:50:THR:HG23	2.17	0.44
1:1A:18:VAL:HG11	8:1H:76:ILE:HD11	1.99	0.44
1:1A:67:LEU:HD11	11:1K:65:VAL:HA	1.98	0.44
3:1C:131:GLU:HA	3:1C:134:ILE:HG22	1.98	0.44
4:1D:295:ASP:N	4:1D:295:ASP:OD1	2.49	0.44
5:1E:204:GLU:CD	6:1F:17:ASP:HB3	2.43	0.44
8:1H:104:PHE:HB2	10:1J:54:LEU:HD21	2.00	0.44
11:1K:71:ALA:O	11:1K:75:LEU:HD23	2.17	0.44
12:1L:34:ASN:HA	12:1L:105:MET:HE1	2.00	0.44
12:1L:248:HIS:CE1	12:1L:252:MET:HE3	2.53	0.44
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.98	0.44
13:1M:355:MET:HE2	13:1M:358:TRP:HD1	1.82	0.44
14:1N:159:MET:HA	14:1N:159:MET:HE2	2.00	0.44
20:1T:19:LEU:HD23	20:1T:25:ILE:HG12	1.98	0.44
24:1Y:132:TRP:CD1	24:1Y:132:TRP:H	2.34	0.44
28:1c:27:LEU:HD22	29:1d:70:PHE:CD1	2.52	0.44
34:1i:71:VAL:HG22	34:1i:75:LEU:HD12	1.99	0.44
2:1B:52:LEU:HB3	4:1D:83:LEU:HD23	1.99	0.44
4:1D:173:GLU:HA	4:1D:176:LYS:HG3	1.99	0.44
5:1E:99:HIS:ND1	5:1E:138:THR:O	2.50	0.44
6:1F:226:GLU:O	6:1F:230:VAL:HG23	2.17	0.44
7:1G:210:SER:OG	7:1G:213:TYR:HB3	2.17	0.44
7:1G:276:ARG:NH1	7:1G:682:GLN:OE1	2.46	0.44
7:1G:277:GLN:HB3	42:1q:137:TRP:CE2	2.53	0.44
7:1G:569:LYS:NZ	7:1G:596:ASP:OD2	2.40	0.44
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.17	0.44
11:1K:95:LEU:HB3	14:1N:54:GLU:HG3	2.00	0.44
16:1P:50:ARG:NH2	54:1P:501:NDP:O3X	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:338:LYS:HA	16:1P:338:LYS:HD2	1.83	0.44
22:1W:30:ARG:HA	22:1W:30:ARG:HE	1.82	0.44
24:1Y:25:THR:O	24:1Y:29:GLY:N	2.42	0.44
29:1d:25:LYS:NZ	29:1d:27:THR:O	2.50	0.44
37:1l:105:LEU:O	37:1l:109:VAL:HG12	2.18	0.44
42:1q:84:PRO:HD3	42:1q:113:HIS:HD2	1.82	0.44
42:1q:113:HIS:HD1	42:1q:114:LYS:N	2.16	0.44
5:1E:132:THR:HG22	5:1E:134:ASP:H	1.83	0.44
5:1E:146:GLY:N	48:1E:301:FES:S1	2.87	0.44
6:1F:344:VAL:HG12	6:1F:380:VAL:HG22	1.99	0.44
6:1F:372:MET:O	6:1F:376:MET:HG3	2.18	0.44
7:1G:114:CYS:C	7:1G:116:LEU:H	2.26	0.44
7:1G:408:LEU:HB3	7:1G:421:HIS:HB2	2.00	0.44
8:1H:30:TYR:CE1	9:1I:45:PRO:HG3	2.53	0.44
8:1H:253:GLU:HA	26:1a:21:MET:HE1	1.99	0.44
8:1H:264:LEU:HD21	26:1a:9:ILE:HG13	1.99	0.44
12:1L:359:MET:HB2	12:1L:430:ALA:HA	1.99	0.44
13:1M:347:GLY:O	13:1M:348:LEU:HD23	2.18	0.44
14:1N:75:ILE:O	14:1N:79:LEU:N	2.44	0.44
17:1Q:113:PRO:C	17:1Q:114:LYS:HD3	2.43	0.44
20:1T:54:MET:O	20:1T:58:PHE:HB2	2.17	0.44
21:1V:115:ILE:N	21:1V:115:ILE:HD12	2.32	0.44
39:1n:26:LEU:HA	39:1n:29:TRP:HB2	2.00	0.44
43:1r:47:LYS:HE2	43:1r:47:LYS:HB3	1.84	0.44
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.47	0.44
3:1C:129:TRP:HZ3	4:1D:80:ILE:HG12	1.83	0.44
4:1D:178:PHE:CE2	4:1D:189:MET:HG3	2.53	0.44
4:1D:307:SER:O	4:1D:310:ILE:N	2.49	0.44
7:1G:317:ALA:HB3	7:1G:331:LEU:HD11	2.00	0.44
8:1H:200:LEU:HD21	8:1H:280:PHE:O	2.18	0.44
12:1L:231:PRO:HG3	12:1L:529:TYR:HE1	1.82	0.44
14:1N:324:LYS:H	14:1N:324:LYS:HD2	1.81	0.44
15:1O:146:LYS:H	15:1O:146:LYS:HD2	1.83	0.44
15:1O:247:PRO:O	15:1O:251:GLN:HG2	2.18	0.44
16:1P:147:ARG:O	16:1P:151:VAL:HG12	2.17	0.44
19:1S:17:GLU:OE2	19:1S:19:ARG:HD3	2.18	0.44
21:1V:57:MET:SD	21:1V:57:MET:N	2.79	0.44
32:1g:24:ILE:O	32:1g:26:LEU:N	2.48	0.44
33:1h:127:THR:OG1	33:1h:128:ILE:N	2.49	0.44
34:1i:76:ILE:HD12	34:1i:77:PRO:N	2.32	0.44
41:1p:166:ARG:CZ	41:1p:166:ARG:HA	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:57:GLY:H	42:1q:59:HIS:CE1	2.35	0.44
5:1E:47:VAL:HG11	5:1E:83:VAL:HG21	2.00	0.44
7:1G:252:PRO:HG2	17:1Q:44:ASN:ND2	2.33	0.44
7:1G:439:PHE:O	7:1G:442:ILE:HG22	2.18	0.44
9:1I:52:PHE:O	42:1q:62:VAL:HG12	2.17	0.44
9:1I:110:ASP:HA	9:1I:149:TYR:O	2.17	0.44
10:1J:105:TYR:O	10:1J:109:LYS:HG2	2.17	0.44
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.51	0.44
12:1L:206:ASN:O	12:1L:266:LEU:HD11	2.18	0.44
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.18	0.44
13:1M:116:ILE:HG12	13:1M:174:LEU:HD12	1.99	0.44
13:1M:124:ALA:HB1	14:1N:256:PRO:HD3	1.99	0.44
14:1N:176:ARG:NH1	14:1N:225:THR:OG1	2.51	0.44
16:1P:110:PHE:CZ	16:1P:149:LYS:HE2	2.53	0.44
16:1P:135:LEU:HD12	16:1P:229:ALA:HB1	1.98	0.44
17:1Q:93:VAL:O	17:1Q:96:ALA:N	2.47	0.44
18:1R:59:CYS:SG	18:1R:84:CYS:HB2	2.56	0.44
20:1U:7:THR:O	20:1U:11:ILE:HG13	2.18	0.44
22:1W:54:ILE:HB	22:1W:58:GLN:HG3	2.00	0.44
25:1Z:98:MET:SD	25:1Z:101:VAL:HG21	2.57	0.44
25:1Z:121:MET:C	25:1Z:121:MET:SD	3.01	0.44
31:1f:37:PHE:HB3	31:1f:40:LYS:HB2	2.00	0.44
31:1f:43:LEU:HB2	41:1p:70:VAL:HG11	1.99	0.44
32:1g:103:ASN:OD1	32:1g:103:ASN:N	2.51	0.44
2:1B:59:MET:O	2:1B:62:MET:N	2.51	0.44
3:1C:125:LYS:H	3:1C:125:LYS:HG3	1.65	0.44
3:1C:189:GLU:HA	3:1C:189:GLU:OE2	2.18	0.44
4:1D:118:TYR:O	4:1D:122:VAL:HG22	2.18	0.44
4:1D:202:ASP:OD1	4:1D:203:LEU:N	2.51	0.44
5:1E:30:ARG:HA	44:1s:56:VAL:HG22	1.99	0.44
8:1H:301:CYS:O	8:1H:305:ILE:HG22	2.17	0.44
8:1H:316:PRO:HA	25:1Z:58:ARG:NH1	2.32	0.44
10:1J:163:ILE:HG13	14:1N:12:THR:HG21	1.99	0.44
12:1L:511:LEU:HD11	39:1n:38:TYR:CD1	2.53	0.44
13:1M:14:MET:HB2	31:1f:15:LEU:HD23	2.00	0.44
14:1N:71:MET:HE3	14:1N:71:MET:O	2.17	0.44
14:1N:190:MET:HB3	14:1N:204:ASN:HB3	2.00	0.44
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.42	0.44
14:1N:323:MET:O	14:1N:323:MET:HG2	2.18	0.44
15:1O:211:LEU:H	15:1O:211:LEU:HD22	1.83	0.44
16:1P:179:LEU:HD22	16:1P:317:VAL:HG11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:30:ILE:HD12	17:1Q:101:TRP:CD1	2.53	0.44
20:1U:11:ILE:O	20:1U:15:VAL:HG23	2.17	0.44
29:1d:115:GLU:OE1	29:1d:115:GLU:N	2.33	0.44
32:1g:71:VAL:O	32:1g:75:THR:HG23	2.17	0.44
34:1i:101:PRO:HD3	41:1p:14:ARG:HH21	1.83	0.44
34:1i:122:PHE:CD1	40:1o:39:VAL:HG11	2.53	0.44
39:1n:105:ASP:N	39:1n:105:ASP:OD1	2.51	0.44
1:1A:66:ASP:HA	1:1A:69:ILE:HD12	1.99	0.43
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.33	0.43
4:1D:195:ARG:HH21	9:1I:121:PHE:HE1	1.65	0.43
47:1D:501:PC1:H222	9:1I:27:TRP:CE2	2.53	0.43
5:1E:28:TYR:HA	5:1E:31:ILE:HD11	1.99	0.43
6:1F:82:MET:HE2	6:1F:211:ALA:HA	2.00	0.43
6:1F:84:LYS:HG2	6:1F:85:PRO:HD2	1.99	0.43
7:1G:74:MET:N	7:1G:74:MET:SD	2.91	0.43
7:1G:484:THR:HG23	7:1G:487:TRP:H	1.83	0.43
7:1G:537:LEU:HD13	7:1G:541:CYS:HB2	1.99	0.43
10:1J:25:SER:HB3	10:1J:81:GLU:H	1.83	0.43
10:1J:120:ASN:N	11:1K:1:FME:O	2.36	0.43
13:1M:336:ARG:HD2	13:1M:426:ILE:HD12	2.00	0.43
13:1M:346:ARG:NH1	13:1M:346:ARG:HB2	2.33	0.43
16:1P:194:ILE:HG12	16:1P:263:TYR:CE2	2.53	0.43
17:1Q:72:TRP:HA	17:1Q:72:TRP:CE3	2.53	0.43
20:1U:13:ASP:HB3	36:1k:15:LEU:HD11	2.00	0.43
22:1W:18:LYS:O	22:1W:77:ARG:NH2	2.51	0.43
25:1Z:134:LEU:HD11	25:1Z:142:TRP:HZ3	1.82	0.43
30:1e:19:ILE:HD11	33:1h:132:LEU:HD23	2.00	0.43
31:1f:41:SER:O	31:1f:45:LYS:N	2.51	0.43
37:1l:58:ARG:HD3	37:1l:58:ARG:HA	1.84	0.43
40:1o:88:TYR:CD1	40:1o:88:TYR:C	2.96	0.43
42:1q:29:ARG:NH1	42:1q:64:TYR:O	2.41	0.43
42:1q:45:GLY:C	42:1q:65:THR:HB	2.43	0.43
2:1B:158:TYR:OH	42:1q:78:ASP:OD1	2.31	0.43
5:1E:149:VAL:N	6:1F:105:CYS:SG	2.83	0.43
5:1E:150:ASN:HA	5:1E:190:ARG:NH1	2.33	0.43
6:1F:14:SER:O	6:1F:14:SER:OG	2.28	0.43
7:1G:27:LEU:HD21	7:1G:55:CYS:HB2	1.98	0.43
7:1G:372:GLU:HB3	7:1G:402:ASN:ND2	2.33	0.43
9:1I:164:GLU:CD	42:1q:87:HIS:HB3	2.43	0.43
11:1K:2:PRO:HD2	11:1K:5:TYR:HD2	1.82	0.43
12:1L:160:GLY:H	39:1n:95:CYS:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:501:ALA:O	12:1L:505:ASN:ND2	2.48	0.43
45:1L:702:3PE:O13	24:1Y:43:LYS:NZ	2.51	0.43
13:1M:16:TRP:NE1	13:1M:97:THR:OG1	2.51	0.43
17:1Q:64:ARG:HG2	17:1Q:64:ARG:NH1	2.33	0.43
19:1S:28:GLY:C	19:1S:62:PRO:HG3	2.43	0.43
21:1V:79:VAL:O	21:1V:82:GLN:HG2	2.17	0.43
25:1Z:108:GLU:HB2	30:1e:74:ARG:NH1	2.30	0.43
30:1e:6:GLN:H	30:1e:6:GLN:HG2	1.67	0.43
34:1i:31:GLU:OE1	39:1n:115:PRO:HD2	2.18	0.43
34:1i:77:PRO:O	34:1i:81:ILE:HG12	2.18	0.43
38:1m:61:ASP:O	38:1m:65:ILE:HG12	2.18	0.43
40:1o:108:LEU:HA	40:1o:108:LEU:HD23	1.77	0.43
42:1q:68:MET:SD	42:1q:81:MET:HB3	2.58	0.43
43:1r:28:GLN:N	43:1r:28:GLN:OE1	2.51	0.43
2:1B:102:LYS:HG3	2:1B:103:VAL:N	2.33	0.43
3:1C:85:THR:HA	17:1Q:86:PHE:HD1	1.83	0.43
3:1C:113:GLU:OE2	17:1Q:98:LYS:NZ	2.47	0.43
4:1D:22:THR:HG22	4:1D:25:THR:HG23	2.00	0.43
4:1D:290:ARG:HB2	4:1D:292:ASP:OD1	2.18	0.43
5:1E:149:VAL:HG12	6:1F:105:CYS:SG	2.58	0.43
6:1F:292:ASP:C	6:1F:309:LYS:HZ1	2.26	0.43
7:1G:175:THR:HG23	7:1G:182:GLN:HB2	1.99	0.43
7:1G:673:MET:HE1	7:1G:679:ARG:HA	1.99	0.43
8:1H:27:VAL:O	8:1H:31:MET:HG2	2.18	0.43
9:1I:38:LEU:HD21	47:1I:203:PC1:H3C1	2.01	0.43
12:1L:478:PRO:HG2	40:1o:90:GLU:HG3	1.99	0.43
13:1M:225:ILE:HG12	13:1M:331:ASN:CG	2.43	0.43
13:1M:433:GLU:O	13:1M:437:MET:HG2	2.18	0.43
15:1O:139:TYR:HB2	15:1O:144:ILE:HD11	2.00	0.43
18:1R:18:TYR:HE1	18:1R:24:ARG:HB2	1.84	0.43
21:1V:75:GLN:N	21:1V:78:GLU:OE2	2.47	0.43
25:1Z:86:MET:HE2	25:1Z:86:MET:HB2	1.87	0.43
39:1n:128:ARG:HD3	39:1n:167:TRP:CD2	2.53	0.43
4:1D:381:ASP:OD1	4:1D:381:ASP:N	2.49	0.43
5:1E:51:LEU:HD21	5:1E:84:ALA:HB2	2.00	0.43
6:1F:111:ILE:CG2	6:1F:149:LEU:HB2	2.49	0.43
7:1G:148:THR:HB	7:1G:150:MET:HE1	2.00	0.43
10:1J:152:TRP:O	10:1J:156:VAL:HG23	2.17	0.43
12:1L:60:GLU:HB2	12:1L:83:ASP:HA	2.00	0.43
14:1N:40:MET:HE1	14:1N:134:GLN:NE2	2.33	0.43
15:1O:135:LEU:HD11	15:1O:149:VAL:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:69:LYS:HD3	20:1T:70:LEU:HG	1.99	0.43
21:1V:65:LYS:HE2	21:1V:65:LYS:HB3	1.82	0.43
57:1Y:201:PGT:H181	57:1Y:201:PGT:H152	1.65	0.43
25:1Z:36:PHE:O	25:1Z:40:ILE:HG22	2.17	0.43
33:1h:132:LEU:HD23	33:1h:132:LEU:O	2.17	0.43
40:1o:34:LYS:HD3	40:1o:35:GLU:N	2.33	0.43
44:1s:38:TYR:CE1	44:1s:40:ASN:HB3	2.52	0.43
4:1D:347:HIS:CD2	7:1G:121:MET:HE1	2.54	0.43
6:1F:118:LEU:HD13	6:1F:229:ALA:HB2	2.01	0.43
6:1F:292:ASP:C	6:1F:292:ASP:OD1	2.61	0.43
7:1G:195:LEU:HD12	7:1G:198:ASN:ND2	2.34	0.43
7:1G:255:HIS:HE2	7:1G:258:ILE:HG12	1.82	0.43
7:1G:350:PRO:HG2	7:1G:467:LEU:HD13	2.01	0.43
7:1G:512:GLU:HA	7:1G:515:ARG:HB3	2.01	0.43
12:1L:88:MET:C	12:1L:91:PRO:HD2	2.42	0.43
12:1L:316:THR:OG1	12:1L:325:ALA:HB2	2.18	0.43
12:1L:389:PHE:C	12:1L:389:PHE:CD1	2.96	0.43
13:1M:1:FME:O	13:1M:4:ILE:N	2.52	0.43
13:1M:207:MET:HB3	13:1M:298:ILE:HD11	2.00	0.43
13:1M:361:MET:H	13:1M:361:MET:HG2	1.58	0.43
15:1O:164:LEU:HD12	15:1O:247:PRO:HG2	2.00	0.43
15:1O:202:ILE:O	15:1O:206:TYR:HB2	2.18	0.43
16:1P:50:ARG:HB3	16:1P:73:TRP:CD1	2.53	0.43
26:1a:6:LEU:HB3	51:1r:201:CDL:H191	2.00	0.43
32:1g:92:GLU:OE2	41:1p:64:HIS:CE1	2.71	0.43
33:1h:68:LYS:HB3	33:1h:68:LYS:HE2	1.85	0.43
37:1l:35:GLU:OE1	37:1l:35:GLU:N	2.51	0.43
38:1m:50:TYR:O	39:1n:168:HIS:HE1	2.01	0.43
38:1m:53:PRO:HG3	39:1n:128:ARG:NE	2.33	0.43
38:1m:113:LYS:O	38:1m:117:GLU:HG2	2.19	0.43
4:1D:176:LYS:NZ	43:1r:26:ARG:HD2	2.33	0.43
4:1D:373:GLU:H	4:1D:394:PRO:HB3	1.83	0.43
47:1D:501:PC1:H371	8:1H:180:PRO:HB3	2.00	0.43
6:1F:248:GLU:OE1	6:1F:248:GLU:N	2.43	0.43
7:1G:114:CYS:SG	7:1G:117:GLN:N	2.88	0.43
8:1H:152:SER:HB2	8:1H:304:HIS:CD2	2.54	0.43
8:1H:197:PRO:O	8:1H:199:ASP:N	2.49	0.43
12:1L:520:TYR:OH	39:1n:75:HIS:NE2	2.51	0.43
13:1M:38:SER:HB3	13:1M:70:THR:HG21	2.01	0.43
15:1O:179:ILE:O	15:1O:183:ILE:HG23	2.18	0.43
15:1O:207:LYS:HE2	15:1O:207:LYS:HB2	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:50:ARG:HB3	16:1P:73:TRP:NE1	2.34	0.43
19:1S:13:LEU:O	19:1S:69:ALA:N	2.50	0.43
19:1S:72:GLN:CD	19:1S:73:GLU:H	2.27	0.43
20:1T:6:LEU:HD23	20:1T:6:LEU:HA	1.79	0.43
23:1X:9:LEU:HD23	23:1X:9:LEU:HA	1.89	0.43
32:1g:87:GLU:OE1	32:1g:87:GLU:N	2.47	0.43
37:1l:70:ARG:HE	37:1l:86:ARG:NE	2.17	0.43
41:1p:32:LEU:HA	41:1p:35:ILE:HG22	2.01	0.43
2:1B:122:GLY:N	9:1I:114:THR:OG1	2.52	0.43
3:1C:88:ASN:HB2	21:1V:110:GLN:OE1	2.19	0.43
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.53	0.43
5:1E:146:GLY:HA3	6:1F:142:PHE:CZ	2.53	0.43
6:1F:21:ILE:HD11	6:1F:234:ILE:HG23	2.00	0.43
7:1G:59:ILE:HD13	7:1G:59:ILE:HA	1.89	0.43
8:1H:305:ILE:O	8:1H:308:PRO:HD2	2.19	0.43
12:1L:183:VAL:HG13	13:1M:393:ILE:HD11	2.00	0.43
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.53	0.43
12:1L:533:MET:O	45:1L:701:3PE:H361	2.19	0.43
12:1L:544:MET:O	12:1L:548:SER:OG	2.28	0.43
14:1N:11:MET:O	14:1N:15:SER:N	2.42	0.43
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.01	0.43
15:1O:94:TYR:CD1	15:1O:148:CYS:HB3	2.54	0.43
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	2.01	0.43
17:1Q:123:SER:OG	17:1Q:124:TRP:N	2.49	0.43
57:1Y:201:PGT:H472	57:1Y:201:PGT:H232	1.99	0.43
32:1g:91:ARG:O	32:1g:94:GLU:OE1	2.37	0.43
37:1l:6:LYS:HA	37:1l:6:LYS:HD2	1.69	0.43
40:1o:7:ARG:HA	40:1o:15:GLU:HG3	1.99	0.43
42:1q:6:VAL:HG22	42:1q:9:ARG:HH21	1.83	0.43
6:1F:46:LYS:O	6:1F:50:LEU:HG	2.19	0.43
6:1F:55:TRP:O	6:1F:55:TRP:HD1	2.00	0.43
6:1F:105:CYS:H	6:1F:257:ASN:ND2	2.16	0.43
7:1G:455:SER:O	7:1G:459:GLN:HG2	2.18	0.43
9:1I:112:ASP:C	9:1I:112:ASP:OD1	2.62	0.43
13:1M:182:TRP:HE1	41:1p:79:LYS:HA	1.83	0.43
13:1M:229:MET:O	13:1M:233:ALA:N	2.48	0.43
13:1M:262:LEU:O	13:1M:266:MET:HB2	2.18	0.43
14:1N:122:ILE:HD11	14:1N:127:GLY:HA2	2.00	0.43
15:1O:137:ALA:HA	15:1O:140:ARG:NH1	2.33	0.43
17:1Q:63:GLU:HG2	17:1Q:65:TRP:HE3	1.83	0.43
19:1S:19:ARG:HB3	19:1S:21:HIS:HE1	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:67:LEU:HD12	21:1V:67:LEU:HA	1.87	0.43
22:1W:19:PRO:HA	22:1W:77:ARG:NH1	2.27	0.43
29:1d:100:ASP:C	29:1d:100:ASP:OD1	2.62	0.43
34:1i:101:PRO:O	34:1i:103:ILE:HG23	2.19	0.43
37:1l:8:MET:N	37:1l:8:MET:HE2	2.34	0.43
37:1l:30:ARG:HH22	38:1m:34:GLU:C	2.27	0.43
2:1B:34:ASP:OD2	2:1B:35:ASP:N	2.52	0.43
4:1D:156:THR:HG22	4:1D:167:PHE:CE2	2.54	0.43
4:1D:165:THR:HA	8:1H:32:GLN:HG2	2.01	0.43
4:1D:261:ARG:HH12	4:1D:368:GLU:CD	2.26	0.43
4:1D:298:LEU:HB3	9:1I:5:VAL:HG22	1.99	0.43
5:1E:15:ASN:OD1	5:1E:63:ILE:HG23	2.18	0.43
5:1E:122:LYS:HE2	5:1E:122:LYS:HB3	1.87	0.43
7:1G:234:VAL:HG11	7:1G:390:LEU:HD12	2.01	0.43
7:1G:332:LYS:HA	7:1G:343:LEU:HD11	2.00	0.43
7:1G:616:LEU:HD11	7:1G:620:ARG:HH22	1.83	0.43
9:1I:64:GLU:O	9:1I:134:GLY:N	2.52	0.43
12:1L:226:GLN:HG3	12:1L:314:MET:HE1	2.01	0.43
12:1L:488:MET:HE3	12:1L:488:MET:H	1.84	0.43
12:1L:572:LYS:HA	12:1L:572:LYS:HD3	1.70	0.43
13:1M:71:TRP:O	13:1M:74:PRO:HD2	2.19	0.43
13:1M:424:ASN:CG	38:1m:55:ARG:HH21	2.27	0.43
47:1M:501:PC1:H351	33:1h:40:ILE:HG21	2.01	0.43
15:1O:45:LYS:HD3	15:1O:235:VAL:HG21	1.99	0.43
16:1P:304:GLY:O	16:1P:306:GLN:NE2	2.47	0.43
20:1U:46:ASP:O	20:1U:49:GLU:HG3	2.19	0.43
21:1V:75:GLN:CD	21:1V:76:ILE:N	2.77	0.43
22:1W:58:GLN:O	22:1W:62:LYS:HB2	2.19	0.43
29:1d:53:VAL:HG23	29:1d:54:VAL:HG23	2.01	0.43
30:1e:62:PHE:HE1	30:1e:66:LEU:HD21	1.82	0.43
35:1j:41:TRP:HB2	36:1k:77:PHE:HZ	1.84	0.43
1:1A:83:ASN:ND2	47:1J:201:PC1:H122	2.33	0.43
1:1A:83:ASN:HD22	47:1J:201:PC1:H122	1.83	0.43
7:1G:114:CYS:SG	7:1G:116:LEU:HB3	2.58	0.43
8:1H:162:LEU:HA	8:1H:165:LEU:HD23	2.01	0.43
8:1H:272:TRP:CZ2	9:1I:34:LEU:HB3	2.53	0.43
8:1H:272:TRP:CD2	9:1I:34:LEU:HD12	2.54	0.43
10:1J:127:ILE:HD13	11:1K:2:PRO:HG3	2.00	0.43
10:1J:132:ASP:HB3	26:1a:46:ASN:ND2	2.34	0.43
12:1L:236:ALA:HB1	12:1L:248:HIS:CD2	2.54	0.43
13:1M:432:ARG:HG3	32:1g:47:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:179:MET:SD	14:1N:215:MET:HE1	2.59	0.43
14:1N:202:ILE:HG23	14:1N:346:LEU:HD13	2.00	0.43
15:1O:105:LEU:HA	15:1O:128:ILE:HD11	2.01	0.43
19:1S:70:PHE:HD2	19:1S:72:GLN:HB2	1.83	0.43
21:1V:46:TYR:O	21:1V:50:ILE:HG13	2.19	0.43
23:1X:101:LYS:H	23:1X:101:LYS:HD2	1.82	0.43
30:1e:6:GLN:OE1	30:1e:13:LEU:HB2	2.19	0.43
38:1m:22:TYR:HD1	39:1n:64:ARG:HD2	1.84	0.43
38:1m:74:ASN:OD1	38:1m:78:ASN:ND2	2.52	0.43
43:1r:39:LYS:HD3	43:1r:39:LYS:HA	1.69	0.43
5:1E:81:TYR:O	5:1E:85:THR:HG22	2.20	0.42
7:1G:342:SER:OG	7:1G:514:ILE:HD13	2.18	0.42
8:1H:222:MET:HE3	8:1H:222:MET:HB3	1.78	0.42
9:1I:74:GLU:OE1	18:1R:88:GLY:HA3	2.19	0.42
12:1L:96:VAL:O	12:1L:100:ILE:HG22	2.19	0.42
12:1L:178:GLY:O	12:1L:219:ALA:HA	2.19	0.42
14:1N:119:THR:O	14:1N:176:ARG:HD2	2.19	0.42
15:1O:83:TYR:CE1	15:1O:194:ILE:HB	2.54	0.42
16:1P:181:TYR:O	16:1P:184:SER:OG	2.24	0.42
17:1Q:32:THR:O	17:1Q:62:ARG:NH2	2.52	0.42
19:1S:14:GLY:O	19:1S:15:LEU:HD23	2.18	0.42
20:1T:37:MET:HE1	20:1T:47:GLN:HG3	2.01	0.42
22:1W:30:ARG:HA	22:1W:30:ARG:NE	2.34	0.42
23:1X:19:VAL:HB	23:1X:23:VAL:HG11	2.01	0.42
23:1X:76:HIS:CG	23:1X:114:LEU:HD21	2.54	0.42
27:1b:77:LEU:HA	27:1b:79:TRP:NE1	2.33	0.42
29:1d:95:LYS:HE3	29:1d:95:LYS:HB3	1.83	0.42
32:1g:90:ARG:NH1	41:1p:9:TYR:OH	2.52	0.42
33:1h:24:LEU:O	33:1h:28:TYR:N	2.45	0.42
37:1l:77:ILE:HD12	37:1l:78:HIS:O	2.19	0.42
39:1n:21:ARG:HD2	39:1n:70:PHE:CZ	2.53	0.42
40:1o:11:ASP:OD1	40:1o:11:ASP:N	2.51	0.42
40:1o:110:ARG:HH11	40:1o:110:ARG:HG3	1.84	0.42
41:1p:10:PRO:HD2	41:1p:108:ARG:CD	2.49	0.42
41:1p:10:PRO:HD2	41:1p:108:ARG:HD2	2.01	0.42
4:1D:329:LYS:HE2	43:1r:53:TYR:CZ	2.53	0.42
5:1E:194:GLU:HB2	5:1E:199:LEU:HD13	2.01	0.42
6:1F:124:VAL:HG11	6:1F:232:PRO:HB3	2.00	0.42
6:1F:135:TYR:HE1	6:1F:176:PHE:HD2	1.64	0.42
7:1G:260:GLU:HB2	7:1G:261:GLU:H	1.71	0.42
7:1G:341:ASP:OD2	19:1S:16:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:533:THR:HG23	7:1G:535:GLN:H	1.84	0.42
8:1H:91:MET:HE3	8:1H:91:MET:HB2	1.81	0.42
8:1H:216:ALA:HA	8:1H:220:PHE:HB2	2.01	0.42
8:1H:231:ILE:N	8:1H:231:ILE:HD13	2.34	0.42
9:1I:54:LYS:HB3	9:1I:54:LYS:HE3	1.79	0.42
10:1J:35:VAL:O	10:1J:39:VAL:HG13	2.20	0.42
12:1L:101:MET:HG3	12:1L:118:PHE:HE2	1.84	0.42
13:1M:30:HIS:O	13:1M:34:ILE:HG12	2.19	0.42
14:1N:296:LEU:HD23	14:1N:296:LEU:HA	1.94	0.42
16:1P:58:HIS:O	16:1P:61:PRO:HD2	2.19	0.42
20:1T:53:ALA:HA	20:1T:57:GLU:OE1	2.20	0.42
22:1W:61:ASP:C	22:1W:61:ASP:OD1	2.63	0.42
32:1g:111:ASN:HA	41:1p:161:ARG:NH2	2.33	0.42
33:1h:12:LYS:HB2	33:1h:12:LYS:HE3	1.88	0.42
41:1p:162:MET:SD	41:1p:162:MET:N	2.72	0.42
3:1C:72:PHE:CZ	3:1C:98:SER:HB3	2.54	0.42
3:1C:147:ASP:OD2	3:1C:149:ARG:NH1	2.39	0.42
4:1D:101:PRO:CB	4:1D:105:ARG:HH21	2.27	0.42
4:1D:104:ASP:OD1	4:1D:111:MET:HB3	2.19	0.42
4:1D:221:ARG:O	4:1D:225:LEU:HD12	2.20	0.42
4:1D:354:GLU:O	4:1D:384:SER:HB2	2.18	0.42
47:1D:501:PC1:H231	47:1D:501:PC1:H282	2.01	0.42
5:1E:126:ILE:HG12	5:1E:130:GLU:HB3	2.01	0.42
5:1E:202:LEU:HD22	6:1F:28:ARG:HG2	2.02	0.42
6:1F:256:PHE:HB3	6:1F:258:ILE:HD11	2.01	0.42
7:1G:156:CYS:N	46:1G:802:SF4:S1	2.93	0.42
7:1G:302:ARG:O	7:1G:306:MET:HG2	2.20	0.42
7:1G:399:TRP:NE1	44:1s:74:ARG:HH12	2.15	0.42
8:1H:236:ALA:HB1	8:1H:259:PHE:HZ	1.83	0.42
8:1H:260:VAL:HG23	26:1a:16:LEU:HB2	2.02	0.42
10:1J:74:MET:SD	10:1J:74:MET:N	2.86	0.42
10:1J:146:LEU:CA	11:1K:58:MET:HE1	2.47	0.42
12:1L:37:LYS:HE2	12:1L:37:LYS:HB3	1.94	0.42
12:1L:283:ILE:HD13	37:1l:112:MET:HG2	2.00	0.42
13:1M:94:LEU:HD23	45:1N:401:3PE:H351	2.01	0.42
13:1M:207:MET:HG3	13:1M:298:ILE:CG1	2.49	0.42
14:1N:85:THR:HG21	33:1h:128:ILE:HG12	2.01	0.42
15:1O:32:CYS:HA	52:1O:401:GTP:O2G	2.20	0.42
15:1O:46:LEU:HD11	15:1O:238:ILE:HD11	2.01	0.42
16:1P:29:PHE:HB3	16:1P:177:ARG:NH2	2.32	0.42
16:1P:93:ASN:O	16:1P:94:LEU:HD13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:294:LEU:HD21	16:1P:297:LEU:HD12	2.01	0.42
20:1U:21:LEU:CD2	36:1k:47:ASN:HA	2.49	0.42
25:1Z:38:VAL:O	25:1Z:42:THR:HG23	2.18	0.42
26:1a:2:TRP:HH2	51:1r:201:CDL:H751	1.84	0.42
29:1d:25:LYS:HZ2	29:1d:28:ASP:HA	1.84	0.42
31:1f:40:LYS:HA	31:1f:45:LYS:HZ3	1.85	0.42
32:1g:37:LEU:HD23	32:1g:46:GLY:HA2	2.01	0.42
35:1j:71:GLU:N	35:1j:71:GLU:OE1	2.53	0.42
40:1o:74:PRO:HD3	41:1p:27:ASN:HA	2.01	0.42
42:1q:38:LEU:HD23	42:1q:38:LEU:HA	1.81	0.42
3:1C:83:VAL:HG12	3:1C:85:THR:HG22	2.00	0.42
4:1D:212:TYR:CZ	4:1D:216:LYS:HD3	2.54	0.42
6:1F:353:PHE:O	6:1F:357:GLU:HG2	2.19	0.42
7:1G:175:THR:CG2	7:1G:182:GLN:HB2	2.49	0.42
7:1G:220:TRP:CE2	9:1I:85:ALA:HB2	2.54	0.42
7:1G:535:GLN:OE1	7:1G:535:GLN:N	2.52	0.42
9:1I:121:PHE:HA	9:1I:124:GLU:OE1	2.19	0.42
10:1J:111:GLU:HB3	10:1J:121:GLY:H	1.83	0.42
11:1K:30:LEU:HD13	11:1K:75:LEU:HD22	2.01	0.42
12:1L:10:THR:O	12:1L:14:ILE:HG12	2.19	0.42
12:1L:486:MET:HG3	58:1l:201:MYR:H31	2.01	0.42
14:1N:130:LEU:O	14:1N:134:GLN:HB2	2.19	0.42
20:1T:25:ILE:HD11	20:1T:40:LEU:HD21	2.02	0.42
28:1c:27:LEU:HD23	28:1c:27:LEU:HA	1.84	0.42
29:1d:5:ARG:CZ	29:1d:85:LEU:HD11	2.49	0.42
30:1e:74:ARG:O	30:1e:78:ILE:HG12	2.19	0.42
3:1C:48:LEU:HD22	3:1C:105:ILE:CD1	2.49	0.42
4:1D:49:LEU:HD22	4:1D:50:ASN:H	1.84	0.42
4:1D:329:LYS:NZ	7:1G:125:SER:O	2.52	0.42
5:1E:151:ALA:N	5:1E:163:ASP:HA	2.35	0.42
5:1E:165:THR:O	5:1E:168:ASP:N	2.51	0.42
6:1F:96:ASN:ND2	6:1F:192:LEU:HD13	2.35	0.42
6:1F:305:PRO:HA	6:1F:414:PRO:HA	2.00	0.42
9:1I:160:LYS:HD2	9:1I:161:TRP:NE1	2.35	0.42
12:1L:305:SER:O	12:1L:309:GLN:HG2	2.20	0.42
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	2.01	0.42
14:1N:291:TYR:HE1	14:1N:295:ARG:HH21	1.68	0.42
15:1O:104:ARG:HH21	15:1O:126:ARG:HG2	1.84	0.42
15:1O:285:GLY:O	15:1O:289:SER:OG	2.25	0.42
18:1R:22:ASP:OD1	18:1R:24:ARG:HD3	2.20	0.42
18:1R:55:ARG:HE	18:1R:55:ARG:HB3	1.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:60:PHE:CE2	20:1T:84:LYS:HD2	2.53	0.42
21:1V:68:GLU:O	21:1V:72:GLN:N	2.53	0.42
23:1X:42:PHE:HB2	23:1X:58:GLU:HB3	2.01	0.42
29:1d:2:MET:N	29:1d:2:MET:SD	2.92	0.42
37:1l:6:LYS:HA	37:1l:9:PHE:CD2	2.54	0.42
37:1l:13:TYR:HD1	37:1l:14:PRO:CD	2.33	0.42
4:1D:80:ILE:HG22	4:1D:425:PHE:CE2	2.55	0.42
4:1D:240:VAL:HG12	4:1D:294:TYR:CG	2.54	0.42
5:1E:89:MET:HG3	6:1F:181:ALA:O	2.19	0.42
6:1F:161:LEU:HD13	6:1F:167:CYS:HB3	2.02	0.42
7:1G:252:PRO:HB3	7:1G:263:ILE:HG12	2.00	0.42
7:1G:322:LEU:HD11	7:1G:548:HIS:NE2	2.35	0.42
7:1G:460:ARG:NE	7:1G:659:ASP:OD1	2.52	0.42
8:1H:116:ILE:HG12	8:1H:211:PHE:CD1	2.54	0.42
11:1K:64:LEU:HD23	11:1K:64:LEU:HA	1.87	0.42
12:1L:19:ILE:HD11	12:1L:122:VAL:HB	2.01	0.42
12:1L:76:LEU:HD11	12:1L:196:TRP:CZ3	2.55	0.42
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.36	0.42
12:1L:371:THR:HG23	35:1j:29:SER:HB2	2.01	0.42
13:1M:80:SER:HB3	13:1M:226:ALA:HB2	2.01	0.42
13:1M:249:ILE:O	13:1M:249:ILE:HG13	2.20	0.42
14:1N:341:PRO:HB2	29:1d:79:GLN:NE2	2.35	0.42
18:1R:15:GLY:HA3	42:1q:131:ARG:HH12	1.84	0.42
19:1S:75:ASN:OD1	19:1S:75:ASN:C	2.62	0.42
19:1S:79:ASN:O	19:1S:81:PHE:HD2	2.02	0.42
21:1V:22:ARG:O	21:1V:26:LEU:HG	2.19	0.42
26:1a:64:LYS:HB2	26:1a:64:LYS:HE2	1.65	0.42
29:1d:76:LEU:O	29:1d:79:GLN:HB3	2.20	0.42
35:1j:55:ASP:OD2	35:1j:57:SER:OG	2.37	0.42
36:1k:42:ASP:OD2	36:1k:45:GLY:N	2.52	0.42
37:1l:37:TYR:CG	37:1l:44:TYR:HD2	2.38	0.42
2:1B:109:GLU:HG2	2:1B:110:PRO:HA	2.01	0.42
3:1C:17:VAL:HA	3:1C:20:LYS:NZ	2.33	0.42
6:1F:275:PRO:HA	6:1F:315:VAL:O	2.20	0.42
7:1G:53:ARG:HH12	7:1G:67:ALA:HB2	1.85	0.42
8:1H:113:VAL:HA	8:1H:116:ILE:HG13	2.01	0.42
8:1H:174:MET:HE3	8:1H:174:MET:HB2	1.76	0.42
12:1L:44:PHE:CE1	12:1L:95:PHE:HB2	2.54	0.42
12:1L:103:PHE:CE2	12:1L:242:PRO:HG3	2.55	0.42
12:1L:142:ILE:HA	13:1M:370:PRO:HG2	2.01	0.42
12:1L:155:ILE:HD11	12:1L:248:HIS:NE2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:581:LYS:NZ	24:1Y:44:PRO:HD2	2.35	0.42
14:1N:6:TYR:CZ	14:1N:10:ILE:HD11	2.55	0.42
14:1N:131:LEU:HA	14:1N:131:LEU:HD12	1.80	0.42
26:1a:18:ILE:HG13	26:1a:19:PRO:HD3	2.01	0.42
29:1d:106:LYS:HD3	29:1d:106:LYS:HA	1.93	0.42
31:1f:37:PHE:O	33:1h:88:GLU:HB3	2.19	0.42
31:1f:49:ARG:HH22	33:1h:60:VAL:H	1.67	0.42
34:1i:104:PHE:HD2	40:1o:67:LYS:HD3	1.83	0.42
39:1n:63:LEU:HD23	39:1n:63:LEU:HA	1.84	0.42
40:1o:110:ARG:HG3	40:1o:110:ARG:NH1	2.34	0.42
42:1q:71:ARG:O	42:1q:73:THR:HG23	2.18	0.42
2:1B:52:LEU:HD12	2:1B:91:THR:O	2.20	0.42
2:1B:150:PRO:HD3	4:1D:190:HIS:CD2	2.55	0.42
4:1D:371:LYS:HE2	4:1D:371:LYS:HB3	1.62	0.42
6:1F:362:CYS:HB2	7:1G:53:ARG:HG3	2.01	0.42
9:1I:78:ILE:HD12	18:1R:86:TYR:HA	2.01	0.42
10:1J:55:MET:O	10:1J:59:ILE:HG13	2.20	0.42
12:1L:137:LEU:H	12:1L:196:TRP:HB3	1.85	0.42
13:1M:441:ILE:HD12	13:1M:441:ILE:HA	1.94	0.42
15:1O:198:TYR:CZ	15:1O:202:ILE:HD11	2.55	0.42
20:1U:25:ILE:HD12	20:1U:25:ILE:N	2.35	0.42
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.53	0.42
26:1a:26:ILE:HG12	26:1a:30:THR:HG23	2.02	0.42
34:1i:103:ILE:HG13	40:1o:47:ASP:OD1	2.19	0.42
34:1i:106:GLY:O	34:1i:115:VAL:HG23	2.19	0.42
36:1k:22:LYS:HB2	36:1k:24:GLU:OE1	2.20	0.42
37:1l:115:MET:HA	37:1l:118:VAL:HG22	2.01	0.42
40:1o:98:MET:HA	40:1o:101:PHE:HB3	2.01	0.42
43:1r:19:LEU:H	43:1r:19:LEU:HD12	1.85	0.42
3:1C:136:ASP:OD2	3:1C:150:ARG:HA	2.20	0.42
5:1E:194:GLU:HG2	5:1E:195:PRO:O	2.20	0.42
5:1E:194:GLU:HB3	6:1F:26:TYR:CE2	2.54	0.42
6:1F:35:GLY:O	6:1F:39:ARG:HG3	2.20	0.42
6:1F:204:ARG:HH12	6:1F:214:GLY:HA2	1.83	0.42
6:1F:398:GLN:OE1	7:1G:92:GLY:HA2	2.19	0.42
7:1G:80:LEU:HD22	7:1G:83:SER:HB2	2.01	0.42
7:1G:201:ASP:OD1	7:1G:268:ARG:NH1	2.53	0.42
7:1G:562:PRO:HB2	7:1G:593:ALA:HB2	2.01	0.42
7:1G:620:ARG:HA	7:1G:623:LEU:HD21	2.02	0.42
8:1H:43:TYR:CZ	51:1r:201:CDL:H141	2.55	0.42
8:1H:96:ILE:HD13	8:1H:96:ILE:HA	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:235:ASN:HD22	8:1H:266:LEU:HB3	1.83	0.42
8:1H:305:ILE:O	8:1H:309:ILE:HD12	2.20	0.42
10:1J:151:THR:HB	10:1J:152:TRP:H	1.68	0.42
12:1L:89:PHE:CE2	12:1L:128:MET:HE3	2.55	0.42
12:1L:200:GLN:NE2	41:1p:106:GLN:OE1	2.37	0.42
12:1L:489:THR:HA	12:1L:492:ILE:HD12	2.02	0.42
13:1M:4:ILE:C	13:1M:7:PRO:HD2	2.45	0.42
14:1N:258:SER:HB2	14:1N:333:SER:C	2.45	0.42
15:1O:50:HIS:HE2	15:1O:125:GLU:CD	2.27	0.42
15:1O:210:PHE:CD1	15:1O:210:PHE:C	2.98	0.42
15:1O:266:LYS:O	15:1O:269:VAL:HG22	2.20	0.42
16:1P:24:PHE:HB2	16:1P:93:ASN:HA	2.01	0.42
16:1P:219:LYS:NZ	16:1P:220:ASP:OD1	2.51	0.42
17:1Q:72:TRP:HA	17:1Q:72:TRP:HE3	1.85	0.42
18:1R:52:VAL:HG11	18:1R:91:PHE:CD2	2.55	0.42
23:1X:9:LEU:O	23:1X:13:LYS:NZ	2.52	0.42
25:1Z:129:THR:HG22	25:1Z:132:GLU:HG2	2.01	0.42
33:1h:81:ASP:OD1	33:1h:81:ASP:N	2.53	0.42
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.55	0.42
41:1p:59:ARG:HB3	41:1p:61:TYR:HE1	1.85	0.42
43:1r:98:PRO:HA	43:1r:99:PRO:HD2	1.98	0.42
43:1r:109:GLN:HE22	43:1r:112:LEU:HA	1.84	0.42
2:1B:54:CYS:O	4:1D:189:MET:HE1	2.20	0.42
4:1D:200:HIS:CE1	4:1D:201:GLN:HG2	2.55	0.42
4:1D:242:ILE:HA	4:1D:409:HIS:NE2	2.34	0.42
4:1D:255:PHE:HB3	4:1D:259:MET:HB3	2.02	0.42
4:1D:379:VAL:HG22	4:1D:388:ARG:O	2.20	0.42
5:1E:110:LEU:HD21	6:1F:336:VAL:O	2.20	0.42
5:1E:186:PRO:HG2	5:1E:192:SER:HA	2.01	0.42
6:1F:74:PRO:HB2	6:1F:77:LEU:HD13	2.01	0.42
6:1F:117:LYS:HA	6:1F:120:GLU:HG3	2.02	0.42
7:1G:693:GLU:O	7:1G:696:GLN:NE2	2.50	0.42
9:1I:49:ASN:O	9:1I:49:ASN:OD1	2.37	0.42
10:1J:7:PHE:HE2	11:1K:3:LEU:HD13	1.85	0.42
11:1K:40:LEU:HD22	14:1N:71:MET:HB3	2.01	0.42
11:1K:73:LEU:HD11	14:1N:60:PHE:CD1	2.55	0.42
12:1L:577:VAL:HG21	14:1N:167:TRP:HB3	2.01	0.42
14:1N:258:SER:HB3	14:1N:336:VAL:HG12	2.02	0.42
20:1U:83:LYS:HA	20:1U:83:LYS:HD3	1.82	0.42
23:1X:31:TYR:HB2	23:1X:69:PHE:CE2	2.55	0.42
25:1Z:48:TRP:CD1	25:1Z:48:TRP:C	2.98	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1a:48:MET:HB3	26:1a:48:MET:HE3	1.74	0.42
32:1g:91:ARG:HG2	32:1g:95:ARG:NH2	2.34	0.42
35:1j:51:PHE:HB3	40:1o:91:HIS:CD2	2.54	0.42
42:1q:32:ASP:OD1	42:1q:32:ASP:C	2.63	0.42
43:1r:47:LYS:O	43:1r:51:ASN:ND2	2.44	0.42
3:1C:88:ASN:ND2	3:1C:112:ASP:OD2	2.53	0.41
5:1E:140:ILE:HG23	5:1E:142:VAL:HG13	2.02	0.41
6:1F:96:ASN:CG	6:1F:192:LEU:HD13	2.45	0.41
7:1G:315:VAL:HG23	7:1G:521:VAL:HG12	2.01	0.41
8:1H:247:HIS:HD2	8:1H:255:TYR:HD2	1.68	0.41
10:1J:123:GLY:O	10:1J:126:VAL:HG22	2.20	0.41
12:1L:72:GLN:HB3	12:1L:73:THR:H	1.57	0.41
12:1L:455:LYS:HB3	12:1L:455:LYS:HE3	1.78	0.41
16:1P:144:ARG:NH1	16:1P:144:ARG:O	2.52	0.41
16:1P:180:ASN:HA	16:1P:321:HIS:NE2	2.35	0.41
20:1T:51:ILE:O	20:1T:55:GLU:HG2	2.20	0.41
27:1b:31:LEU:N	27:1b:32:PRO:HD2	2.35	0.41
30:1e:31:ARG:HH21	30:1e:68:ARG:NH2	2.18	0.41
38:1m:52:ASP:OD1	39:1n:132:TRP:NE1	2.53	0.41
2:1B:42:ARG:HB2	2:1B:164:GLN:HG3	2.03	0.41
2:1B:101:ARG:HA	2:1B:101:ARG:HD2	1.59	0.41
2:1B:148:GLY:CA	9:1I:118:TYR:HE1	2.30	0.41
5:1E:6:LEU:O	5:1E:92:ARG:NH1	2.49	0.41
6:1F:31:TRP:HH2	6:1F:151:VAL:HG21	1.84	0.41
6:1F:114:ASP:OD1	6:1F:114:ASP:N	2.53	0.41
6:1F:322:LEU:H	6:1F:322:LEU:HD12	1.85	0.41
7:1G:45:ARG:NH2	7:1G:261:GLU:HG2	2.33	0.41
7:1G:59:ILE:HD12	7:1G:77:TRP:HD1	1.83	0.41
7:1G:317:ALA:HB2	7:1G:523:PHE:HB2	2.02	0.41
8:1H:153:VAL:HG11	8:1H:241:LEU:HD22	2.00	0.41
11:1K:12:PHE:CG	14:1N:72:MET:HE3	2.55	0.41
13:1M:341:THR:HG21	38:1m:64:LEU:HD21	2.01	0.41
14:1N:113:PHE:O	14:1N:116:PRO:HD2	2.20	0.41
14:1N:159:MET:CE	14:1N:282:MET:HG3	2.40	0.41
16:1P:146:LEU:O	16:1P:150:ALA:N	2.53	0.41
16:1P:210:VAL:O	16:1P:214:ILE:HG12	2.19	0.41
33:1h:84:GLU:O	33:1h:88:GLU:HG2	2.20	0.41
39:1n:139:LEU:O	39:1n:143:THR:HG23	2.21	0.41
40:1o:16:PRO:HB3	40:1o:104:GLU:OE1	2.19	0.41
41:1p:163:LEU:HD23	41:1p:163:LEU:HA	1.81	0.41
2:1B:141:PRO:HB3	16:1P:57:MET:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:82:ASP:HB2	3:1C:138:PHE:CE1	2.47	0.41
47:1D:501:PC1:H331	9:1I:27:TRP:CZ2	2.56	0.41
5:1E:145:LEU:HB2	5:1E:160:TYR:OH	2.21	0.41
5:1E:190:ARG:HH21	5:1E:193:CYS:HA	1.85	0.41
6:1F:258:ILE:HA	6:1F:334:VAL:HG13	2.02	0.41
6:1F:393:TRP:O	6:1F:397:LYS:HG2	2.20	0.41
7:1G:106:PRO:HD2	18:1R:86:TYR:OH	2.20	0.41
7:1G:384:PRO:HD2	7:1G:415:LEU:HD22	2.02	0.41
7:1G:618:GLN:O	7:1G:621:SER:OG	2.36	0.41
9:1I:144:HIS:O	9:1I:144:HIS:ND1	2.54	0.41
13:1M:32:LEU:O	13:1M:35:SER:OG	2.31	0.41
13:1M:249:ILE:HG23	13:1M:250:LEU:HD13	2.02	0.41
13:1M:316:MET:HE2	13:1M:316:MET:HB3	1.92	0.41
13:1M:325:MET:HE3	13:1M:440:HIS:HB2	2.02	0.41
13:1M:352:LEU:HD11	13:1M:426:ILE:HD11	2.02	0.41
14:1N:30:TRP:CE2	14:1N:71:MET:HG2	2.55	0.41
14:1N:66:ALA:HB3	14:1N:105:LYS:HG3	2.02	0.41
15:1O:126:ARG:HG3	15:1O:130:SER:HB3	2.03	0.41
15:1O:295:LYS:O	15:1O:299:LEU:HG	2.21	0.41
16:1P:198:LYS:HD3	16:1P:198:LYS:HA	1.88	0.41
22:1W:68:MET:HE3	22:1W:68:MET:HB3	1.94	0.41
40:1o:117:ARG:NH1	40:1o:120:GLU:OE2	2.53	0.41
1:1A:113:TRP:CD1	1:1A:113:TRP:N	2.88	0.41
3:1C:11:ILE:HD12	43:1r:58:GLY:N	2.36	0.41
3:1C:23:SER:O	3:1C:26:GLY:N	2.54	0.41
4:1D:132:PRO:O	4:1D:136:TRP:HD1	2.03	0.41
6:1F:16:LYS:HA	6:1F:16:LYS:HD3	1.81	0.41
6:1F:49:LEU:HG	6:1F:127:ARG:HE	1.85	0.41
6:1F:385:ARG:HG3	6:1F:386:PRO:HD2	2.02	0.41
7:1G:252:PRO:HG2	17:1Q:44:ASN:HD22	1.86	0.41
7:1G:622:ARG:HA	7:1G:625:GLU:HG2	2.02	0.41
7:1G:667:THR:OG1	7:1G:669:LYS:NZ	2.48	0.41
9:1I:4:PHE:CD2	9:1I:7:MET:HE1	2.56	0.41
9:1I:6:ASN:C	9:1I:6:ASN:HD22	2.28	0.41
10:1J:68:PHE:HD1	11:1K:27:MET:HE1	1.85	0.41
12:1L:51:LEU:HD23	12:1L:51:LEU:HA	1.88	0.41
12:1L:216:LEU:HD12	12:1L:216:LEU:HA	1.93	0.41
12:1L:313:MET:HE1	12:1L:329:ILE:HD13	2.02	0.41
12:1L:488:MET:SD	12:1L:492:ILE:HD11	2.59	0.41
14:1N:46:LYS:HA	14:1N:46:LYS:HD3	1.82	0.41
14:1N:86:ILE:HG23	14:1N:86:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:329:MET:O	14:1N:333:SER:OG	2.31	0.41
15:1O:133:VAL:HG13	15:1O:134:PHE:CD2	2.55	0.41
16:1P:186:ARG:O	16:1P:186:ARG:NE	2.38	0.41
16:1P:328:THR:HG23	22:1W:51:GLN:NE2	2.36	0.41
17:1Q:34:LYS:HE3	17:1Q:34:LYS:HB3	1.75	0.41
17:1Q:38:PHE:HE2	17:1Q:58:GLU:HB3	1.85	0.41
17:1Q:125:ASN:HA	44:1s:68:SER:OG	2.20	0.41
19:1S:40:TYR:OH	19:1S:52:ILE:HB	2.20	0.41
22:1W:112:ALA:O	22:1W:114:ARG:HD2	2.20	0.41
23:1X:47:TRP:O	23:1X:50:LYS:HG2	2.20	0.41
31:1f:30:SER:O	31:1f:33:LYS:HB2	2.20	0.41
37:1l:66:HIS:N	37:1l:71:LEU:O	2.51	0.41
41:1p:94:ASP:HA	41:1p:97:VAL:HG12	2.02	0.41
41:1p:98:ASP:HB3	41:1p:138:PHE:HE1	1.85	0.41
44:1s:71:GLN:HB2	44:1s:75:HIS:CE1	2.55	0.41
1:1A:85:LYS:O	1:1A:89:THR:HG22	2.20	0.41
2:1B:61:HIS:CE1	4:1D:174:ARG:HG2	2.55	0.41
4:1D:98:GLN:O	4:1D:101:PRO:HD2	2.21	0.41
5:1E:130:GLU:O	5:1E:139:LEU:HD23	2.21	0.41
6:1F:96:ASN:HB2	6:1F:222:VAL:HG13	2.01	0.41
6:1F:376:MET:HE2	6:1F:376:MET:C	2.46	0.41
7:1G:115:ASP:O	7:1G:119:GLN:HB2	2.20	0.41
7:1G:147:LYS:HG2	7:1G:149:ILE:HD12	2.01	0.41
8:1H:299:ALA:HB1	27:1b:24:ILE:HB	2.02	0.41
9:1I:78:ILE:HG22	9:1I:78:ILE:O	2.21	0.41
12:1L:435:PRO:HB3	12:1L:437:PHE:CE2	2.56	0.41
12:1L:597:ILE:HG13	12:1L:602:PHE:CD2	2.56	0.41
13:1M:50:LEU:N	13:1M:58:SER:O	2.53	0.41
14:1N:25:HIS:HE2	30:1e:17:MET:HG2	1.85	0.41
16:1P:135:LEU:HA	16:1P:167:LYS:HE3	2.02	0.41
16:1P:157:ARG:HA	16:1P:157:ARG:HD3	1.94	0.41
16:1P:283:LYS:O	16:1P:287:VAL:HG23	2.21	0.41
17:1Q:95:PHE:O	17:1Q:98:LYS:HG2	2.21	0.41
20:1T:75:GLU:OE1	20:1T:75:GLU:N	2.53	0.41
20:1U:15:VAL:HG21	20:1U:77:VAL:HB	2.01	0.41
25:1Z:81:ARG:O	25:1Z:85:GLN:HB2	2.21	0.41
33:1h:14:SER:HB3	39:1n:106:TRP:CD1	2.55	0.41
34:1i:127:HIS:HA	40:1o:88:TYR:CE2	2.56	0.41
39:1n:25:HIS:CD2	39:1n:70:PHE:HE1	2.39	0.41
44:1s:52:LEU:O	44:1s:56:VAL:HG23	2.21	0.41
2:1B:76:PHE:O	2:1B:76:PHE:CG	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:171:PHE:CE1	4:1D:174:ARG:HD3	2.55	0.41
4:1D:270:ARG:HE	4:1D:270:ARG:HB2	1.70	0.41
4:1D:347:HIS:NE2	7:1G:126:ASP:HA	2.36	0.41
4:1D:417:ILE:O	4:1D:420:THR:HG22	2.20	0.41
47:1D:501:PC1:H271	8:1H:187:ILE:HD12	2.03	0.41
5:1E:9:HIS:NE2	5:1E:63:ILE:HD13	2.35	0.41
5:1E:78:MET:O	5:1E:82:GLU:HG3	2.20	0.41
6:1F:131:ALA:HB3	6:1F:173:PHE:HE1	1.85	0.41
6:1F:263:ASN:N	6:1F:286:GLY:O	2.50	0.41
6:1F:306:LEU:HD21	6:1F:343:ILE:HD11	2.03	0.41
7:1G:144:PRO:HB3	7:1G:698:VAL:HB	2.02	0.41
7:1G:160:ILE:HD13	7:1G:172:LEU:HB3	2.03	0.41
11:1K:48:ILE:HD13	11:1K:56:ALA:HB1	2.01	0.41
12:1L:37:LYS:HD3	12:1L:98:TRP:HE1	1.85	0.41
12:1L:335:PHE:HE2	12:1L:380:LEU:HG	1.85	0.41
12:1L:400:ASN:O	37:1l:126:GLN:NE2	2.53	0.41
13:1M:357:THR:O	13:1M:361:MET:HG2	2.20	0.41
13:1M:365:THR:HG21	13:1M:441:ILE:HD11	2.02	0.41
13:1M:407:SER:O	13:1M:410:MET:HE3	2.20	0.41
14:1N:200:MET:HA	14:1N:203:LEU:HB3	2.03	0.41
15:1O:31:ILE:HG23	52:1O:401:GTP:O1A	2.20	0.41
15:1O:32:CYS:O	15:1O:182:ARG:HD3	2.19	0.41
15:1O:156:LYS:HD3	15:1O:160:ALA:HB3	2.02	0.41
16:1P:203:GLN:HB2	16:1P:235:ARG:HD2	2.03	0.41
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.20	0.41
20:1U:44:SER:OG	56:1n:201:EHZ:O6	2.35	0.41
29:1d:120:ARG:HD3	41:1p:144:ASP:OD2	2.20	0.41
30:1e:23:GLU:HA	30:1e:23:GLU:OE2	2.21	0.41
34:1i:48:LYS:O	34:1i:51:GLN:NE2	2.54	0.41
35:1j:61:ASP:HA	35:1j:64:LEU:HB2	2.01	0.41
38:1m:88:LEU:HD23	38:1m:88:LEU:HA	1.85	0.41
41:1p:6:LYS:HB2	41:1p:6:LYS:HE2	1.77	0.41
2:1B:42:ARG:CD	2:1B:168:LYS:HG3	2.51	0.41
2:1B:50:PHE:CE2	2:1B:103:VAL:HG11	2.56	0.41
2:1B:118:SER:N	46:1B:201:SF4:S1	2.94	0.41
2:1B:130:TYR:CD1	2:1B:131:SER:HB2	2.55	0.41
4:1D:147:LEU:HD12	4:1D:147:LEU:HA	1.89	0.41
4:1D:322:GLU:CD	4:1D:322:GLU:H	2.29	0.41
5:1E:46:ALA:HB3	5:1E:73:LEU:HD21	2.03	0.41
6:1F:126:GLY:O	6:1F:130:GLY:N	2.54	0.41
7:1G:383:ASN:ND2	7:1G:386:PHE:HD2	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:676:SER:HA	7:1G:679:ARG:HB2	2.03	0.41
8:1H:72:ILE:O	8:1H:75:PRO:HD2	2.21	0.41
8:1H:90:PRO:HG2	8:1H:240:ILE:HG12	2.02	0.41
9:1I:175:TYR:CD1	43:1r:38:PRO:HG3	2.55	0.41
10:1J:159:TRP:HE1	14:1N:12:THR:HG22	1.86	0.41
13:1M:369:LEU:HD12	13:1M:369:LEU:H	1.86	0.41
14:1N:12:THR:O	14:1N:16:GLY:N	2.42	0.41
24:1Y:49:LEU:HD23	24:1Y:49:LEU:H	1.85	0.41
26:1a:1:MET:HB2	26:1a:3:PHE:CE2	2.56	0.41
37:1l:85:ILE:HG12	37:1l:86:ARG:N	2.34	0.41
40:1o:74:PRO:HG3	41:1p:28:PRO:HD3	2.02	0.41
4:1D:319:PRO:HA	4:1D:320:PRO:HD3	1.97	0.41
5:1E:103:CYS:SG	5:1E:144:CYS:HA	2.61	0.41
6:1F:163:GLY:N	6:1F:173:PHE:O	2.48	0.41
6:1F:378:ARG:NE	6:1F:383:ASP:O	2.54	0.41
6:1F:385:ARG:HG2	6:1F:387:ALA:H	1.86	0.41
8:1H:318:SER:O	25:1Z:61:GLN:NE2	2.50	0.41
10:1J:52:LEU:HD12	11:1K:41:PHE:CZ	2.56	0.41
10:1J:152:TRP:CG	30:1e:13:LEU:HG	2.56	0.41
12:1L:298:ILE:HG22	12:1L:354:GLN:O	2.21	0.41
12:1L:401:MET:SD	40:1o:94:TYR:OH	2.77	0.41
13:1M:134:THR:O	13:1M:142:ARG:NH2	2.45	0.41
15:1O:30:ASN:OD1	15:1O:173:ASP:HA	2.21	0.41
15:1O:100:LEU:HD12	15:1O:100:LEU:HA	1.87	0.41
15:1O:134:PHE:CD2	15:1O:134:PHE:N	2.89	0.41
16:1P:33:TYR:O	16:1P:37:HIS:ND1	2.34	0.41
18:1R:77:LYS:HD2	18:1R:77:LYS:HA	1.73	0.41
18:1R:84:CYS:SG	18:1R:87:CYS:N	2.68	0.41
25:1Z:48:TRP:NE1	25:1Z:52:LYS:HD2	2.35	0.41
25:1Z:72:MET:HE2	27:1b:52:TYR:HB2	2.03	0.41
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.21	0.41
36:1k:17:ASP:CG	36:1k:18:TYR:H	2.29	0.41
2:1B:59:MET:O	2:1B:62:MET:HG2	2.21	0.41
3:1C:23:SER:HB2	43:1r:68:VAL:HG11	2.02	0.41
3:1C:152:LEU:HD23	3:1C:152:LEU:HA	1.85	0.41
3:1C:172:VAL:CG2	3:1C:185:ALA:HB1	2.50	0.41
4:1D:112:MET:HB3	4:1D:194:ILE:HD12	2.02	0.41
4:1D:182:GLU:HG3	9:1I:58:SER:HB3	2.03	0.41
4:1D:258:VAL:HG13	4:1D:299:CYS:SG	2.60	0.41
4:1D:281:VAL:HG11	4:1D:310:ILE:HG23	2.02	0.41
4:1D:347:HIS:CG	7:1G:121:MET:HE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:172:ILE:HG13	5:1E:187:ARG:NH1	2.36	0.41
6:1F:123:LEU:HB2	6:1F:162:ILE:HD11	2.02	0.41
6:1F:132:ARG:O	6:1F:173:PHE:HA	2.21	0.41
6:1F:259:SER:OG	6:1F:260:GLY:N	2.54	0.41
6:1F:277:LYS:HA	6:1F:291:TRP:CZ3	2.56	0.41
6:1F:391:SER:O	6:1F:395:ILE:HG13	2.21	0.41
7:1G:16:GLN:H	7:1G:16:GLN:CD	2.29	0.41
7:1G:36:GLN:NE2	17:1Q:49:VAL:HG23	2.36	0.41
7:1G:44:GLU:H	7:1G:44:GLU:CD	2.27	0.41
7:1G:107:ILE:CD1	9:1I:104:ARG:HD3	2.51	0.41
7:1G:408:LEU:HD22	7:1G:415:LEU:HD11	2.02	0.41
8:1H:30:TYR:CD2	26:1a:5:ILE:HD11	2.56	0.41
8:1H:54:LYS:HE2	8:1H:54:LYS:HB2	1.60	0.41
8:1H:72:ILE:HD13	8:1H:72:ILE:HA	1.92	0.41
10:1J:125:TRP:CD1	10:1J:125:TRP:H	2.38	0.41
11:1K:55:LEU:HG	30:1e:25:PRO:HD3	2.02	0.41
12:1L:65:ASN:ND2	12:1L:78:LEU:HD23	2.36	0.41
12:1L:66:TRP:CE3	47:1M:501:PC1:H11	2.55	0.41
12:1L:106:TRP:CH2	12:1L:345:SER:HA	2.56	0.41
12:1L:154:LEU:HD23	12:1L:154:LEU:HA	1.78	0.41
12:1L:239:GLY:O	12:1L:299:LYS:NZ	2.54	0.41
12:1L:362:LEU:HA	12:1L:365:ALA:HB3	2.03	0.41
14:1N:7:THR:HG21	51:1N:402:CDL:H322	2.03	0.41
15:1O:279:LEU:HB2	15:1O:282:ILE:HG22	2.02	0.41
16:1P:2:HIS:CG	16:1P:3:HIS:N	2.89	0.41
16:1P:46:ILE:HD13	18:1R:26:VAL:HG11	2.03	0.41
16:1P:201:VAL:CG2	16:1P:235:ARG:HG2	2.47	0.41
19:1S:16:ARG:HH11	19:1S:69:ALA:HB2	1.85	0.41
19:1S:32:VAL:HA	19:1S:35:PHE:HB3	2.01	0.41
19:1S:84:ASP:OD1	19:1S:85:GLN:N	2.54	0.41
20:1T:51:ILE:H	20:1T:51:ILE:HG13	1.70	0.41
20:1U:17:TYR:O	20:1U:21:LEU:HB2	2.20	0.41
20:1U:26:ASP:HB2	20:1U:28:GLU:OE2	2.21	0.41
22:1W:27:GLU:HA	22:1W:30:ARG:HB3	2.01	0.41
23:1X:100:ARG:HA	23:1X:100:ARG:HD3	1.65	0.41
24:1Y:109:ILE:HD12	24:1Y:109:ILE:HA	1.91	0.41
29:1d:10:PRO:HG2	30:1e:7:LYS:HB2	2.03	0.41
29:1d:82:MET:HE2	29:1d:82:MET:HB2	1.90	0.41
33:1h:60:VAL:HA	33:1h:61:PRO:HD3	1.89	0.41
34:1i:10:ARG:NH1	34:1i:14:LEU:HD11	2.35	0.41
35:1j:20:SER:O	35:1j:24:GLN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:7:ASP:C	37:1l:8:MET:HE2	2.46	0.41
37:1l:27:TYR:CZ	37:1l:48:PRO:HD3	2.56	0.41
37:1l:107:GLY:O	37:1l:111:PHE:HB3	2.20	0.41
39:1n:29:TRP:CE2	39:1n:75:HIS:HD2	2.39	0.41
39:1n:43:MET:CE	39:1n:46:ARG:HH21	2.33	0.41
44:1s:50:THR:C	44:1s:54:LEU:HD23	2.45	0.41
1:1A:74:PRO:HB3	10:1J:143:ILE:HD13	2.03	0.41
4:1D:153:ALA:O	4:1D:157:HIS:HB2	2.21	0.41
4:1D:255:PHE:HZ	4:1D:401:GLY:HA3	1.85	0.41
5:1E:196:ALA:HB3	6:1F:264:HIS:CE1	2.56	0.41
6:1F:110:ILE:H	6:1F:110:ILE:HG13	1.63	0.41
6:1F:135:TYR:HE2	6:1F:216:PHE:HE2	1.69	0.41
6:1F:139:ARG:HG2	6:1F:140:GLY:N	2.36	0.41
6:1F:213:VAL:HG13	6:1F:217:GLY:HA2	2.02	0.41
7:1G:156:CYS:C	7:1G:158:ARG:H	2.29	0.41
7:1G:516:LYS:HE3	7:1G:516:LYS:HB3	1.84	0.41
7:1G:684:MET:O	7:1G:688:VAL:HG22	2.21	0.41
8:1H:100:LEU:HD22	8:1H:160:TYR:HD2	1.86	0.41
8:1H:227:GLU:OE1	8:1H:230:ASN:ND2	2.51	0.41
9:1I:116:CYS:SG	9:1I:117:ILE:N	2.94	0.41
10:1J:7:PHE:CE2	11:1K:3:LEU:HD13	2.56	0.41
12:1L:47:SER:C	12:1L:50:PRO:HD2	2.45	0.41
12:1L:111:ASP:OD1	39:1n:96:TYR:OH	2.26	0.41
12:1L:169:LEU:HD13	45:1L:701:3PE:H232	2.03	0.41
14:1N:75:ILE:HA	14:1N:78:LEU:HB3	2.03	0.41
14:1N:116:PRO:O	14:1N:119:THR:OG1	2.38	0.41
14:1N:172:GLN:OE1	14:1N:177:LYS:HG2	2.21	0.41
14:1N:228:LEU:HD23	15:1O:276:PRO:HB2	2.02	0.41
14:1N:245:MET:HE3	14:1N:245:MET:HB3	1.86	0.41
17:1Q:90:GLU:H	17:1Q:90:GLU:CD	2.29	0.41
19:1S:63:LYS:HE2	19:1S:63:LYS:HB2	1.84	0.41
21:1V:79:VAL:HA	21:1V:82:GLN:NE2	2.37	0.41
23:1X:77:CYS:HB2	23:1X:109:CYS:HB3	2.02	0.41
27:1b:44:ILE:HD13	27:1b:44:ILE:HA	1.83	0.41
28:1c:1:LYS:HZ3	28:1c:4:ILE:HA	1.85	0.41
42:1q:78:ASP:OD1	42:1q:79:GLY:N	2.54	0.41
4:1D:19:MET:CE	14:1N:173:THR:HG22	2.51	0.40
4:1D:201:GLN:HE22	9:1I:176:ARG:HA	1.86	0.40
4:1D:284:ASP:O	4:1D:306:GLN:HG3	2.20	0.40
4:1D:347:HIS:NE2	7:1G:125:SER:O	2.49	0.40
5:1E:103:CYS:SG	5:1E:105:THR:HG22	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:106:THR:OG1	5:1E:107:PRO:HD3	2.20	0.40
5:1E:195:PRO:HB3	6:1F:264:HIS:CD2	2.56	0.40
6:1F:79:TRP:HH2	6:1F:228:VAL:HA	1.85	0.40
6:1F:156:ALA:HB1	6:1F:162:ILE:HB	2.03	0.40
7:1G:194:GLU:OE1	7:1G:385:ARG:HD2	2.20	0.40
7:1G:365:ASN:HB3	7:1G:488:LYS:HD3	2.03	0.40
7:1G:514:ILE:HG13	7:1G:519:PRO:HD3	2.04	0.40
7:1G:544:ILE:HG23	7:1G:559:VAL:HG23	2.02	0.40
7:1G:582:GLN:HB3	7:1G:633:TYR:CE1	2.56	0.40
8:1H:85:MET:HE1	8:1H:109:SER:N	2.35	0.40
47:1I:203:PC1:H261	47:1I:203:PC1:H232	1.93	0.40
10:1J:65:LEU:HA	10:1J:68:PHE:HD2	1.85	0.40
12:1L:103:PHE:CE1	12:1L:341:MET:HB2	2.56	0.40
12:1L:123:LEU:HB2	12:1L:150:MET:HE2	2.03	0.40
12:1L:373:LEU:HG	12:1L:431:PHE:CE1	2.56	0.40
45:1L:702:3PE:H221	45:1L:702:3PE:H2	1.55	0.40
13:1M:67:VAL:HG22	47:1M:501:PC1:H2E2	2.03	0.40
14:1N:147:GLN:CD	14:1N:147:GLN:H	2.29	0.40
15:1O:65:ASP:HB2	28:1c:2:PHE:CE1	2.55	0.40
15:1O:156:LYS:HE3	15:1O:156:LYS:HB2	1.88	0.40
21:1V:8:THR:HG21	21:1V:13:LEU:HB3	2.04	0.40
22:1W:39:TRP:O	22:1W:42:GLU:HG3	2.21	0.40
27:1b:10:ASN:O	27:1b:14:LYS:NZ	2.51	0.40
32:1g:111:ASN:HA	41:1p:161:ARG:HH22	1.86	0.40
34:1i:60:ILE:HA	34:1i:63:THR:HG22	2.02	0.40
40:1o:107:LEU:HA	40:1o:110:ARG:HB3	2.02	0.40
3:1C:58:ILE:HB	3:1C:59:PRO:HD3	2.03	0.40
3:1C:149:ARG:NH2	4:1D:77:ASP:OD1	2.55	0.40
4:1D:96:TYR:CE1	4:1D:386:PRO:HG3	2.57	0.40
4:1D:146:ARG:HH12	4:1D:368:GLU:HG3	1.86	0.40
4:1D:156:THR:HG22	4:1D:167:PHE:HE2	1.86	0.40
6:1F:146:ALA:O	6:1F:150:GLN:HG2	2.21	0.40
7:1G:67:ALA:O	7:1G:71:MET:HB2	2.21	0.40
7:1G:490:MET:SD	7:1G:491:ASN:N	2.94	0.40
7:1G:611:LEU:HD13	7:1G:613:TYR:OH	2.21	0.40
9:1I:56:PRO:HB2	43:1r:33:ARG:NH2	2.36	0.40
12:1L:324:LEU:HD13	12:1L:476:THR:HG21	2.03	0.40
13:1M:218:LYS:O	13:1M:222:GLU:HG2	2.21	0.40
13:1M:348:LEU:HD12	13:1M:415:GLN:HE22	1.86	0.40
13:1M:425:ASN:ND2	38:1m:58:VAL:HG13	2.36	0.40
14:1N:251:MET:HB3	14:1N:293:TYR:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:134:PHE:CD2	15:1O:202:ILE:HD12	2.56	0.40
19:1S:17:GLU:C	19:1S:17:GLU:OE1	2.64	0.40
22:1W:27:GLU:OE1	22:1W:27:GLU:N	2.36	0.40
22:1W:40:TYR:CD1	22:1W:40:TYR:N	2.89	0.40
22:1W:102:HIS:HA	22:1W:105:ARG:HH12	1.87	0.40
23:1X:47:TRP:CE3	33:1h:141:PRO:HA	2.56	0.40
23:1X:49:GLU:HG2	23:1X:134:ARG:NH2	2.24	0.40
25:1Z:58:ARG:HE	25:1Z:58:ARG:HB3	1.62	0.40
33:1h:87:TYR:OH	41:1p:86:GLU:OE1	2.32	0.40
34:1i:56:TRP:CD1	34:1i:56:TRP:C	2.98	0.40
34:1i:98:GLU:HA	41:1p:114:GLN:HE21	1.85	0.40
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.53	0.40
2:1B:60:MET:HA	2:1B:63:ALA:HB3	2.03	0.40
3:1C:23:SER:C	3:1C:26:GLY:H	2.28	0.40
3:1C:52:ILE:HG21	3:1C:60:VAL:HG11	2.02	0.40
3:1C:136:ASP:CG	3:1C:150:ARG:HA	2.47	0.40
3:1C:178:ASP:H	16:1P:36:ASN:ND2	2.19	0.40
3:1C:209:TYR:CD2	4:1D:360:PRO:HD2	2.56	0.40
4:1D:197:GLY:O	4:1D:325:VAL:HG13	2.22	0.40
4:1D:281:VAL:HG23	4:1D:313:GLN:HB2	2.04	0.40
5:1E:53:LEU:O	5:1E:57:GLN:NE2	2.54	0.40
6:1F:188:GLU:HA	49:1F:501:FMN:O2'	2.20	0.40
6:1F:230:VAL:O	6:1F:234:ILE:HG12	2.21	0.40
8:1H:139:THR:HG23	8:1H:192:GLU:HG2	2.03	0.40
8:1H:195:ARG:HE	8:1H:195:ARG:HA	1.87	0.40
10:1J:82:VAL:HG13	10:1J:84:VAL:N	2.34	0.40
10:1J:115:ILE:O	10:1J:117:PHE:N	2.54	0.40
11:1K:12:PHE:CE2	14:1N:72:MET:HG2	2.57	0.40
12:1L:264:TYR:N	12:1L:265:PRO:HD2	2.37	0.40
13:1M:116:ILE:HG22	23:1X:168:PHE:HE1	1.85	0.40
14:1N:162:ILE:HD13	14:1N:282:MET:HG2	2.01	0.40
16:1P:4:ALA:C	16:1P:5:LEU:HD22	2.46	0.40
20:1T:52:MET:SD	20:1T:55:GLU:HG3	2.62	0.40
20:1U:24:LYS:HD2	36:1k:41:ARG:HH21	1.85	0.40
21:1V:1:ALA:HA	21:1V:65:LYS:H	1.85	0.40
22:1W:77:ARG:O	22:1W:81:LEU:HD23	2.22	0.40
27:1b:15:GLU:OE2	27:1b:18:LEU:HG	2.20	0.40
29:1d:91:PHE:O	29:1d:94:VAL:HG22	2.21	0.40
36:1k:25:GLY:N	36:1k:29:GLU:OE2	2.55	0.40
36:1k:32:GLN:NE2	36:1k:42:ASP:HB3	2.37	0.40
37:1l:70:ARG:HH21	37:1l:86:ARG:CZ	2.33	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:60:HIS:O	40:1o:63:ILE:HG22	2.21	0.40
42:1q:86:TRP:CZ3	42:1q:98:PRO:HD2	2.56	0.40
42:1q:91:HIS:HB2	42:1q:93:MET:HG3	2.03	0.40
43:1r:7:ILE:HD11	51:1r:201:CDL:H522	2.03	0.40
3:1C:207:PRO:HB3	3:1C:210:ARG:HH12	1.87	0.40
4:1D:87:THR:HG23	4:1D:102:TYR:CD2	2.50	0.40
4:1D:112:MET:HG3	4:1D:181:TYR:CZ	2.57	0.40
4:1D:128:ILE:HD13	4:1D:128:ILE:HA	1.85	0.40
4:1D:150:HIS:HA	4:1D:153:ALA:HB3	2.03	0.40
4:1D:401:GLY:O	4:1D:405:MET:HE2	2.21	0.40
5:1E:24:THR:HG22	5:1E:27:ASN:OD1	2.21	0.40
7:1G:131:LEU:HD12	7:1G:132:GLU:HG2	2.03	0.40
7:1G:285:ARG:HD2	7:1G:289:GLY:O	2.21	0.40
7:1G:350:PRO:HG3	7:1G:463:GLY:C	2.47	0.40
7:1G:545:TYR:O	7:1G:560:ILE:HA	2.22	0.40
10:1J:71:THR:HG21	11:1K:75:LEU:HD12	2.03	0.40
12:1L:15:LEU:O	12:1L:18:PRO:HD2	2.22	0.40
12:1L:132:VAL:HG23	12:1L:133:THR:HG23	2.03	0.40
12:1L:293:ILE:H	12:1L:293:ILE:HG12	1.68	0.40
12:1L:396:ILE:HA	12:1L:399:VAL:HG12	2.01	0.40
13:1M:65:LEU:HD21	13:1M:316:MET:HE3	2.04	0.40
13:1M:183:SER:O	41:1p:152:ARG:NH1	2.52	0.40
14:1N:120:GLN:CD	14:1N:176:ARG:HH21	2.29	0.40
14:1N:338:PRO:HA	23:1X:169:TRP:HZ2	1.86	0.40
24:1Y:68:ILE:HD11	24:1Y:96:GLY:HA2	2.03	0.40
30:1e:93:PRO:HA	30:1e:94:PRO:HD3	1.90	0.40
39:1n:153:LEU:HD12	39:1n:154:PRO:HD2	2.03	0.40
2:1B:42:ARG:HD2	2:1B:168:LYS:HG3	2.03	0.40
2:1B:60:MET:HE2	2:1B:60:MET:HB2	1.97	0.40
3:1C:69:ASN:ND2	43:1r:94:VAL:O	2.50	0.40
4:1D:119:SER:O	4:1D:123:GLU:HG3	2.21	0.40
4:1D:318:MET:SD	4:1D:319:PRO:HD2	2.61	0.40
4:1D:374:PHE:HA	4:1D:394:PRO:HD3	2.02	0.40
5:1E:29:LYS:H	5:1E:29:LYS:HG2	1.68	0.40
6:1F:101:GLU:HB3	6:1F:104:THR:HG21	2.03	0.40
6:1F:349:ARG:HA	6:1F:349:ARG:HD2	1.83	0.40
6:1F:378:ARG:HH12	7:1G:131:LEU:HD13	1.86	0.40
7:1G:149:ILE:HD13	7:1G:152:ARG:NH2	2.36	0.40
8:1H:163:SER:O	8:1H:166:ILE:HG22	2.21	0.40
10:1J:72:THR:O	10:1J:76:THR:HB	2.21	0.40
11:1K:1:FME:HE2	11:1K:5:TYR:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:158:TRP:O	12:1L:160:GLY:N	2.55	0.40
12:1L:357:ARG:O	12:1L:436:ARG:NE	2.51	0.40
12:1L:538:THR:H	12:1L:538:THR:HG23	1.68	0.40
13:1M:107:ILE:O	13:1M:111:THR:HG22	2.21	0.40
13:1M:201:MET:O	13:1M:205:VAL:HG23	2.21	0.40
14:1N:218:LEU:HD21	14:1N:240:ILE:HD12	2.03	0.40
15:1O:7:ALA:O	15:1O:10:LEU:HG	2.22	0.40
25:1Z:69:ILE:HG21	27:1b:53:PRO:HD2	2.03	0.40
25:1Z:129:THR:HG23	25:1Z:131:GLU:H	1.86	0.40
32:1g:100:ARG:NH2	32:1g:108:MET:HA	2.37	0.40
34:1i:3:TYR:HB2	34:1i:8:LYS:HE2	2.04	0.40
34:1i:30:ARG:NH2	39:1n:116:ASP:OD1	2.55	0.40
35:1j:56:PRO:HA	35:1j:59:TRP:CD2	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	
3	1C	13/264 (5%)	13 (100%)	0	0	100	100
4	1D	199/476 (42%)	193 (97%)	6 (3%)	0	100	100
5	1E	112/249 (45%)	102 (91%)	10 (9%)	0	100	100
6	1F	131/464 (28%)	117 (89%)	14 (11%)	0	100	100
7	1G	46/727 (6%)	43 (94%)	3 (6%)	0	100	100
8	1H	145/318 (46%)	131 (90%)	11 (8%)	3 (2%)	5	31
9	1I	22/239 (9%)	18 (82%)	4 (18%)	0	100	100
12	1L	135/606 (22%)	124 (92%)	11 (8%)	0	100	100
13	1M	49/459 (11%)	48 (98%)	1 (2%)	0	100	100
14	1N	323/347 (93%)	306 (95%)	17 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	1O	32/357 (9%)	30 (94%)	2 (6%)	0	100	100
16	1P	213/377 (56%)	195 (92%)	17 (8%)	1 (0%)	24	59
17	1Q	127/175 (73%)	109 (86%)	18 (14%)	0	100	100
18	1R	94/123 (76%)	86 (92%)	8 (8%)	0	100	100
19	1S	45/99 (46%)	39 (87%)	6 (13%)	0	100	100
20	1U	57/156 (36%)	52 (91%)	5 (9%)	0	100	100
21	1V	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
22	1W	113/128 (88%)	105 (93%)	7 (6%)	1 (1%)	14	47
23	1X	117/172 (68%)	111 (95%)	6 (5%)	0	100	100
24	1Y	137/141 (97%)	129 (94%)	8 (6%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	74 (91%)	7 (9%)	0	100	100
28	1c	47/76 (62%)	46 (98%)	1 (2%)	0	100	100
29	1d	117/123 (95%)	111 (95%)	6 (5%)	0	100	100
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	1f	55/135 (41%)	47 (86%)	7 (13%)	1 (2%)	6	34
32	1g	98/154 (64%)	89 (91%)	9 (9%)	0	100	100
33	1h	136/189 (72%)	122 (90%)	13 (10%)	1 (1%)	18	53
34	1i	124/128 (97%)	112 (90%)	12 (10%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	75 (95%)	3 (4%)	1 (1%)	9	40
37	1l	154/186 (83%)	143 (93%)	11 (7%)	0	100	100
38	1m	126/129 (98%)	117 (93%)	9 (7%)	0	100	100
39	1n	170/179 (95%)	166 (98%)	3 (2%)	1 (1%)	21	55
40	1o	120/137 (88%)	111 (92%)	9 (8%)	0	100	100
41	1p	171/176 (97%)	167 (98%)	4 (2%)	0	100	100
42	1q	143/145 (99%)	127 (89%)	15 (10%)	1 (1%)	18	53
43	1r	90/114 (79%)	81 (90%)	9 (10%)	0	100	100
44	1s	43/471 (9%)	37 (86%)	6 (14%)	0	100	100
All	All	4350/8942 (49%)	4033 (93%)	307 (7%)	10 (0%)	44	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	1H	197	PRO
36	1k	49	ALA
8	1H	213	VAL
16	1P	174	ARG
33	1h	63	HIS
42	1q	141	SER
39	1n	31	VAL
31	1f	36	ALA
22	1W	96	VAL
8	1H	196	ALA

5.3.2 Protein sidechains ⓘ

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	$\# Z > 2$
34	SAC	1i	1	-	7,8,9	0.55	0	7,9,11	1.17	1 (14%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	1.06	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	0.96	1 (12%)
8	FME	1H	1	8	8,9,10	0.52	0	8,9,11	1.04	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	0.98	1 (12%)
10	FME	1J	1	10	8,9,10	0.57	0	8,9,11	0.94	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	FME	1M	1	13	8,9,10	0.58	0	8,9,11	0.81	1 (12%)
11	FME	1K	1	11	8,9,10	0.54	0	8,9,11	1.00	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
34	SAC	1i	1	-	-	3/7/8/10	-
1	FME	1A	1	1	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
14	FME	1N	1	14	-	1/7/9/11	-
10	FME	1J	1	10	-	2/7/9/11	-
13	FME	1M	1	13	-	0/7/9/11	-
11	FME	1K	1	11	-	2/7/9/11	-

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	-3.00	117.04	124.77
8	1H	1	FME	O-C-CA	-2.71	117.79	124.77
1	1A	1	FME	O-C-CA	-2.65	117.97	124.77
10	1J	1	FME	O-C-CA	-2.58	118.14	124.77
11	1K	1	FME	O-C-CA	-2.53	118.25	124.77
12	1L	1	FME	O-C-CA	-2.50	118.34	124.77
14	1N	1	FME	O-C-CA	-2.41	118.56	124.77
13	1M	1	FME	O-C-CA	-2.20	119.11	124.77

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	1J	1	FME	O-C-CA-CB
11	1K	1	FME	O-C-CA-CB
14	1N	1	FME	O1-CN-N-CA
34	1i	1	SAC	O-C-CA-CB
10	1J	1	FME	N-CA-CB-CG

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

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	1i	1	SAC	1	0
1	1A	1	FME	2	0
13	1M	1	FME	2	0
11	1K	1	FME	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
54	NDP	1P	501	-	51,52,52	0.53	0	71,80,80	0.84	2 (2%)
47	PC1	1h	201	-	45,45,53	0.28	0	51,53,61	0.38	0
45	3PE	1L	702	-	30,30,50	0.34	0	33,35,55	0.63	1 (3%)
47	PC1	1D	501	-	53,53,53	0.26	0	59,61,61	0.30	0
51	CDL	1r	201	-	60,60,99	0.33	0	66,72,111	0.41	0
57	PGT	1Y	201	-	50,50,50	0.49	0	53,56,56	0.45	0
45	3PE	1L	701	-	45,45,50	0.32	0	48,50,55	0.47	0
56	EHZ	1W	201	-	31,36,37	0.22	0	36,44,47	1.17	1 (2%)
49	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.64	1 (2%)
47	PC1	1I	203	-	43,43,53	0.29	0	49,51,61	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	SF4	1G	801	7	0,12,12	-	-	-		
45	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.40	0
46	SF4	1G	802	7	0,12,12	-	-	-		
46	SF4	1I	201	9	0,12,12	-	-	-		
47	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.32	0
56	EHZ	1n	201	-	31,36,37	0.19	0	36,44,47	1.31	1 (2%)
46	SF4	1F	502	6	0,12,12	-	-	-		
58	MYR	1l	201	-	13,14,15	0.30	0	12,13,15	0.30	0
46	SF4	1I	202	9	0,12,12	-	-	-		
45	3PE	1L	703	-	41,41,50	0.31	0	44,46,55	1.26	4 (9%)
48	FES	1G	803	7	0,4,4	-	-	-		
51	CDL	1N	402	-	76,76,99	0.32	0	82,88,111	0.37	0
47	PC1	1M	501	-	43,43,53	0.30	0	49,51,61	0.37	0
46	SF4	1B	201	2	0,12,12	-	-	-		
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.55	1 (2%)
52	GTP	1O	401	53	33,34,34	0.59	0	50,54,54	0.65	0
45	3PE	1Y	202	-	50,50,50	0.27	0	53,55,55	0.35	0
48	FES	1E	301	5	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
54	NDP	1P	501	-	-	7/34/77/77	0/5/5/5
47	PC1	1h	201	-	-	4/49/49/57	-
45	3PE	1L	702	-	-	8/34/34/54	-
47	PC1	1D	501	-	-	8/57/57/57	-
51	CDL	1r	201	-	-	13/71/71/110	-
57	PGT	1Y	201	-	-	23/55/55/55	-
45	3PE	1L	701	-	-	7/49/49/54	-
56	EHZ	1W	201	-	-	7/42/44/45	-
49	FMN	1F	501	-	-	2/18/18/18	0/3/3/3
47	PC1	1I	203	-	-	6/47/47/57	-
45	3PE	1N	401	-	-	10/54/54/54	-
46	SF4	1G	801	7	-	-	0/6/5/5
46	SF4	1G	802	7	-	-	0/6/5/5
46	SF4	1I	201	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	PC1	1J	201	-	-	4/38/38/57	-
56	EHZ	1n	201	-	-	10/42/44/45	-
58	MYR	1l	201	-	-	0/12/12/13	-
46	SF4	1F	502	6	-	-	0/6/5/5
46	SF4	1I	202	9	-	-	0/6/5/5
45	3PE	1L	703	-	-	4/45/45/54	-
48	FES	1G	803	7	-	-	0/1/1/1
51	CDL	1N	402	-	-	10/87/87/110	-
47	PC1	1M	501	-	-	6/47/47/57	-
46	SF4	1B	201	2	-	-	0/6/5/5
45	3PE	1A	201	-	-	8/50/50/54	-
52	GTP	1O	401	53	-	3/22/38/38	0/3/3/3
45	3PE	1Y	202	-	-	7/54/54/54	-
48	FES	1E	301	5	-	-	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1n	201	EHZ	C10-S1-C9	7.40	123.70	101.84
56	1W	201	EHZ	C10-S1-C9	6.50	121.07	101.84
45	1L	703	3PE	O21-C21-C22	6.04	124.54	111.48
54	1P	501	NDP	P2B-O2B-C2B	-4.22	112.17	123.43
54	1P	501	NDP	O4D-C1D-C2D	-2.93	100.35	106.62
45	1L	703	3PE	O21-C21-O22	-2.77	117.23	123.70
45	1L	703	3PE	C2-O21-C21	2.64	124.11	117.80
45	1L	703	3PE	O21-C2-C1	2.57	117.57	108.34
45	1L	702	3PE	O21-C21-C22	2.33	116.53	111.48
45	1A	201	3PE	O21-C2-C1	2.12	115.93	108.34
49	1F	501	FMN	C4-N3-C2	-2.10	121.91	125.64

There are no chirality outliers.

All (147) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1A	201	3PE	C1-O11-P-O13
45	1A	201	3PE	C1-O11-P-O14
45	1L	701	3PE	C1-O11-P-O12
45	1L	701	3PE	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
45	1L	702	3PE	C1-O11-P-O13
45	1L	702	3PE	C1-O11-P-O14
45	1L	702	3PE	O32-C31-O31-C3
45	1L	702	3PE	C32-C31-O31-C3
45	1L	702	3PE	O22-C21-O21-C2
45	1L	702	3PE	C22-C21-O21-C2
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2
45	1N	401	3PE	C1-O11-P-O14
45	1Y	202	3PE	C1-O11-P-O14
45	1Y	202	3PE	C2-C1-O11-P
47	1I	203	PC1	C11-O13-P-O12
47	1I	203	PC1	C11-O13-P-O11
47	1I	203	PC1	O21-C2-C3-O31
47	1J	201	PC1	C1-O11-P-O13
47	1M	501	PC1	C1-O11-P-O14
47	1h	201	PC1	O32-C31-O31-C3
47	1h	201	PC1	C32-C31-O31-C3
51	1N	402	CDL	OB5-CB3-CB4-OB6
51	1r	201	CDL	CA3-OA5-PA1-OA3
51	1r	201	CDL	CB3-OB5-PB2-OB4
52	1O	401	GTP	C5'-O5'-PA-O3A
54	1P	501	NDP	C5D-O5D-PN-O1N
56	1W	201	EHZ	S1-C10-C11-N1
56	1W	201	EHZ	C16-C17-C20-O6
56	1W	201	EHZ	C18-C17-C20-O6
56	1W	201	EHZ	C19-C17-C20-O6
56	1W	201	EHZ	O2-C9-S1-C10
56	1W	201	EHZ	C8-C9-S1-C10
56	1n	201	EHZ	C15-C16-C17-C18
56	1n	201	EHZ	C15-C16-C17-C20
56	1n	201	EHZ	O5-C16-C17-C18
56	1n	201	EHZ	O5-C16-C17-C20
56	1n	201	EHZ	O2-C9-S1-C10
56	1n	201	EHZ	C8-C9-S1-C10
57	1Y	201	PGT	C32-C31-O2-C2
57	1Y	201	PGT	C1-O3P-P-O1P
57	1Y	201	PGT	C4-O4P-P-O3P
57	1Y	201	PGT	C4-O4P-P-O1P
57	1Y	201	PGT	C4-O4P-P-O2P
57	1Y	201	PGT	C5-C4-O4P-P
57	1Y	201	PGT	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
57	1Y	201	PGT	O31-C31-O2-C2
54	1P	501	NDP	O4D-C1D-N1N-C6N
57	1Y	201	PGT	C15-C16-C17-C18
47	1D	501	PC1	C24-C25-C26-C27
57	1Y	201	PGT	C40-C41-C42-C43
57	1Y	201	PGT	O5-C5-C6-O6
57	1Y	201	PGT	C12-C13-C14-C15
57	1Y	201	PGT	C14-C15-C16-C17
47	1I	203	PC1	C36-C37-C38-C39
45	1Y	202	3PE	C3C-C3D-C3E-C3F
57	1Y	201	PGT	C35-C36-C37-C38
45	1L	701	3PE	C33-C34-C35-C36
45	1A	201	3PE	O21-C2-C3-O31
51	1r	201	CDL	OB6-CB4-CB6-OB8
57	1Y	201	PGT	C32-C33-C34-C35
57	1Y	201	PGT	C21-C22-C23-C24
51	1N	402	CDL	C75-C76-C77-C78
45	1Y	202	3PE	O11-C1-C2-C3
45	1L	703	3PE	O11-C1-C2-O21
45	1Y	202	3PE	C35-C36-C37-C38
51	1N	402	CDL	OA6-CA4-CA6-OA8
56	1n	201	EHZ	O5-C16-C17-C19
45	1N	401	3PE	C3A-C3B-C3C-C3D
52	1O	401	GTP	C4'-C5'-O5'-PA
45	1N	401	3PE	O31-C31-C32-C33
45	1N	401	3PE	C34-C35-C36-C37
45	1A	201	3PE	C1-C2-C3-O31
47	1I	203	PC1	C1-C2-C3-O31
51	1N	402	CDL	CA3-CA4-CA6-OA8
45	1Y	202	3PE	O11-C1-C2-O21
45	1L	701	3PE	C32-C33-C34-C35
47	1D	501	PC1	O31-C31-C32-C33
51	1r	201	CDL	CB2-C1-CA2-OA2
51	1N	402	CDL	OB5-CB3-CB4-CB6
51	1r	201	CDL	C52-C51-CB5-OB6
45	1L	701	3PE	C22-C23-C24-C25
57	1Y	201	PGT	C1-C2-C3-O3
45	1Y	202	3PE	C12-C11-O13-P
47	1J	201	PC1	O13-C11-C12-N
49	1F	501	FMN	N10-C1'-C2'-O2'
57	1Y	201	PGT	C22-C23-C24-C25
45	1N	401	3PE	C2-C3-O31-C31

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Mol	Chain	Res	Type	Atoms
45	1N	401	3PE	C2-C1-O11-P
54	1P	501	NDP	C4B-C5B-O5B-PA
57	1Y	201	PGT	C31-C32-C33-C34
51	1r	201	CDL	CB3-CB4-CB6-OB8
56	1W	201	EHZ	C10-C11-N1-C12
45	1A	201	3PE	C1-O11-P-O12
45	1L	701	3PE	C1-O11-P-O14
45	1N	401	3PE	C11-O13-P-O14
47	1D	501	PC1	C1-O11-P-O14
47	1I	203	PC1	C11-O13-P-O14
47	1J	201	PC1	C1-O11-P-O14
47	1M	501	PC1	C11-O13-P-O14
47	1M	501	PC1	C1-O11-P-O13
47	1h	201	PC1	C11-O13-P-O14
51	1r	201	CDL	CB3-OB5-PB2-OB2
51	1r	201	CDL	CB3-OB5-PB2-OB3
52	1O	401	GTP	C5'-O5'-PA-O1A
54	1P	501	NDP	C5D-O5D-PN-O3
54	1P	501	NDP	C5D-O5D-PN-O2N
47	1D	501	PC1	C23-C24-C25-C26
51	1r	201	CDL	CA4-CA3-OA5-PA1
51	1r	201	CDL	CB4-CB3-OB5-PB2
47	1M	501	PC1	O11-C1-C2-C3
45	1L	702	3PE	O21-C2-C3-O31
45	1L	701	3PE	C38-C39-C3A-C3B
45	1L	702	3PE	C32-C33-C34-C35
56	1n	201	EHZ	S1-C10-C11-N1
45	1N	401	3PE	O21-C2-C3-O31
56	1n	201	EHZ	C1-C2-C3-C4
47	1h	201	PC1	C2-C1-O11-P
47	1D	501	PC1	O32-C31-C32-C33
47	1M	501	PC1	C1-C2-C3-O31
47	1D	501	PC1	C3D-C3E-C3F-C3G
45	1L	703	3PE	C1-C2-O21-C21
47	1D	501	PC1	C3E-C3F-C3G-C3H
45	1N	401	3PE	O11-C1-C2-O21
51	1N	402	CDL	CA7-C31-C32-C33
47	1J	201	PC1	O21-C2-C3-O31
54	1P	501	NDP	C2N-C3N-C7N-N7N
57	1Y	201	PGT	C37-C38-C39-C40
57	1Y	201	PGT	C2-C1-O3P-P
57	1Y	201	PGT	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
45	1A	201	3PE	C33-C34-C35-C36
51	1N	402	CDL	C72-C71-CB7-OB8
56	1n	201	EHZ	C15-C16-C17-C19
45	1A	201	3PE	O21-C21-C22-C23
51	1r	201	CDL	C12-C13-C14-C15
49	1F	501	FMN	N10-C1'-C2'-C3'
45	1N	401	3PE	O32-C31-C32-C33
45	1A	201	3PE	O22-C21-C22-C23
47	1M	501	PC1	O31-C31-C32-C33
51	1r	201	CDL	C17-C18-C19-C20
54	1P	501	NDP	C3B-C2B-O2B-P2B
57	1Y	201	PGT	C17-C18-C19-C20
51	1N	402	CDL	C72-C71-CB7-OB9
47	1D	501	PC1	C3A-C3B-C3C-C3D
51	1N	402	CDL	C32-C33-C34-C35
51	1r	201	CDL	C52-C51-CB5-OB7
51	1N	402	CDL	C55-C56-C57-C58

There are no ring outliers.

25 monomers are involved in 86 short contacts:

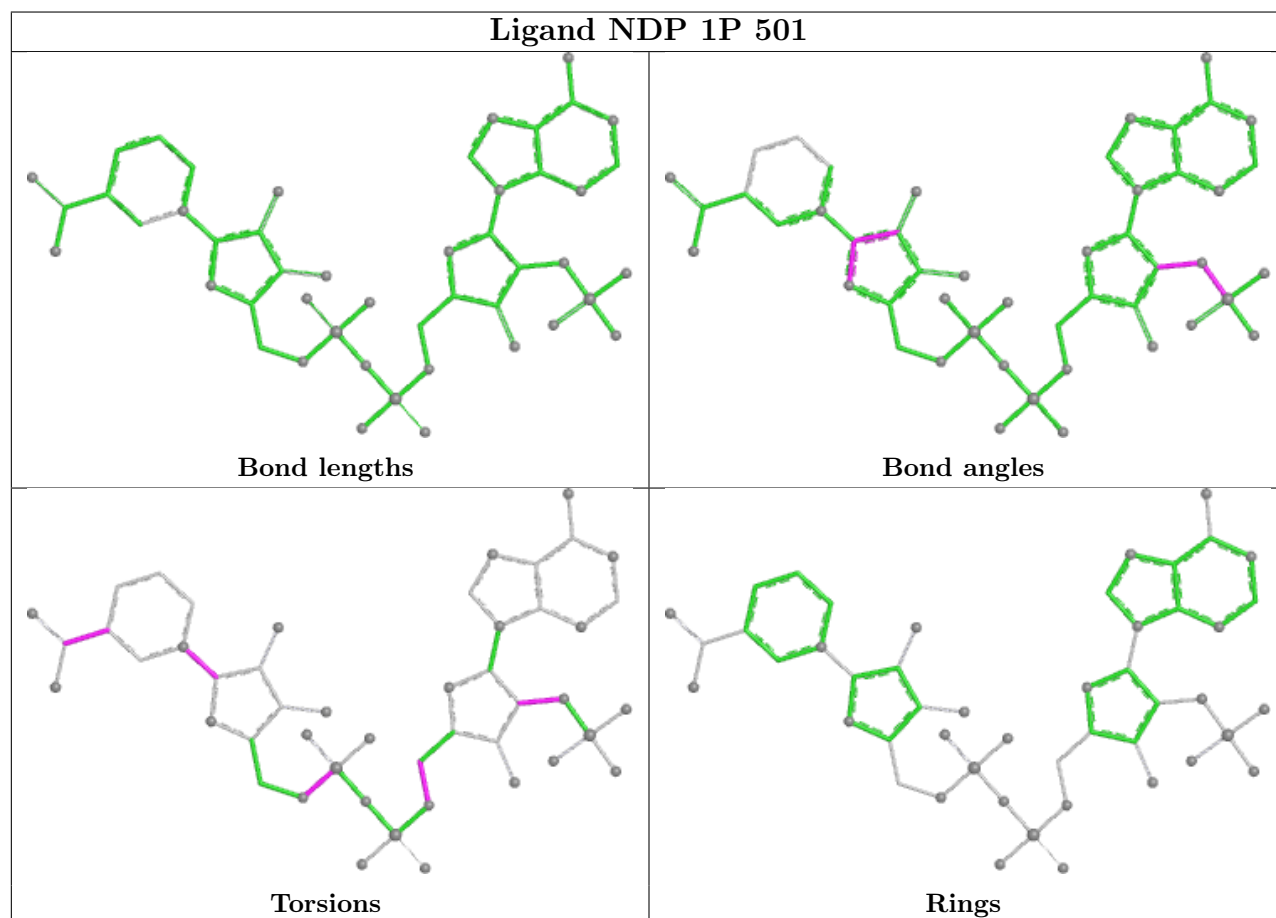
Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	1P	501	NDP	3	0
47	1h	201	PC1	2	0
45	1L	702	3PE	4	0
47	1D	501	PC1	7	0
51	1r	201	CDL	6	0
57	1Y	201	PGT	9	0
45	1L	701	3PE	4	0
49	1F	501	FMN	3	0
47	1I	203	PC1	9	0
45	1N	401	3PE	3	0
46	1G	802	SF4	1	0
46	1I	201	SF4	1	0
47	1J	201	PC1	4	0
56	1n	201	EHZ	2	0
46	1F	502	SF4	3	0
58	1l	201	MYR	1	0
46	1I	202	SF4	1	0
45	1L	703	3PE	1	0
51	1N	402	CDL	4	0
47	1M	501	PC1	6	0

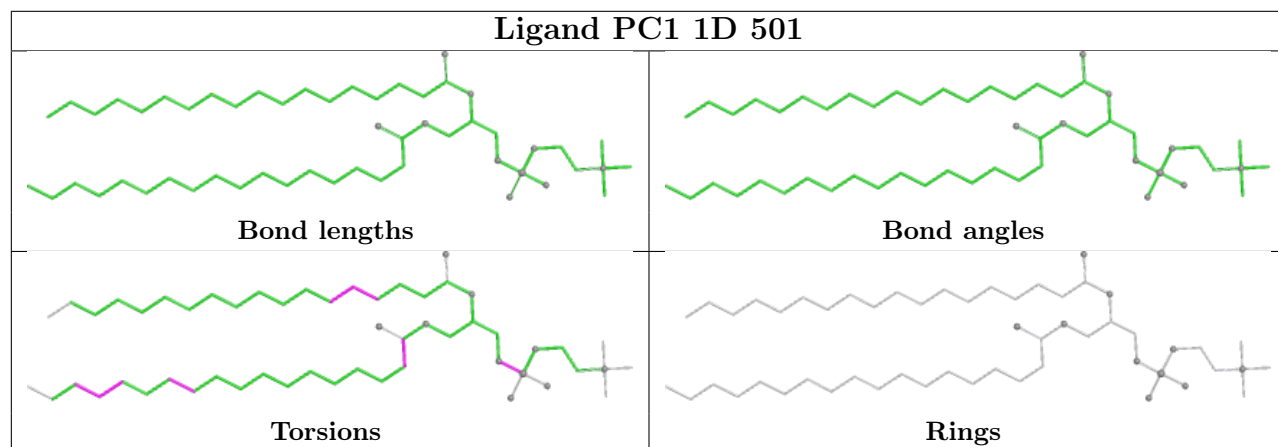
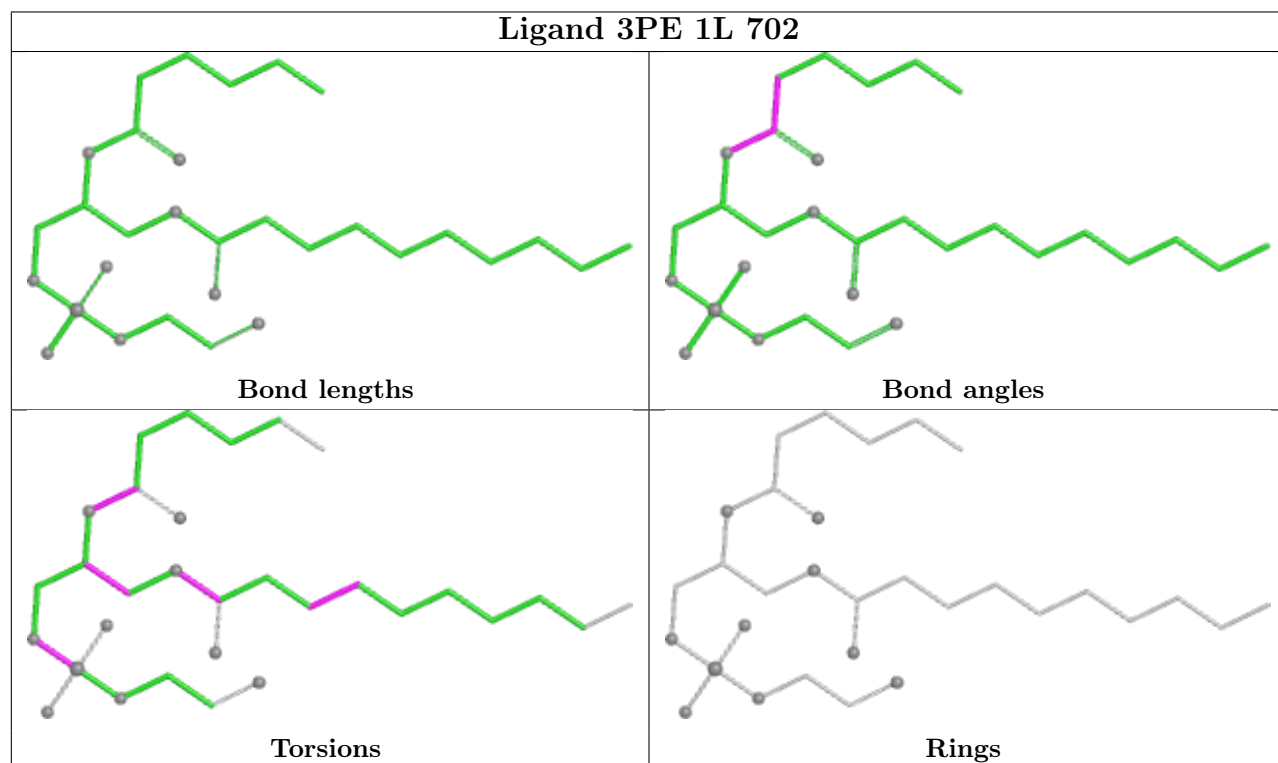
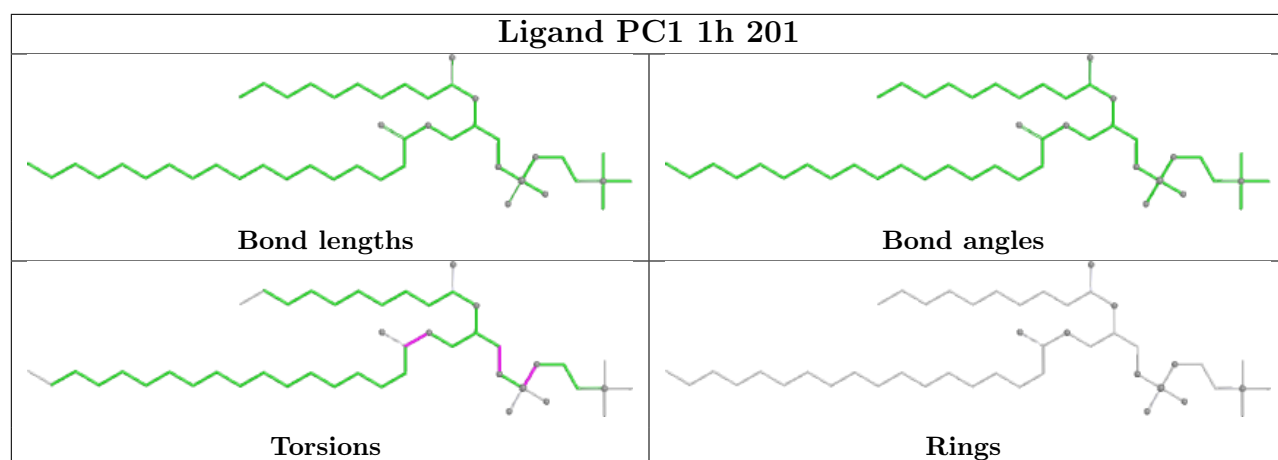
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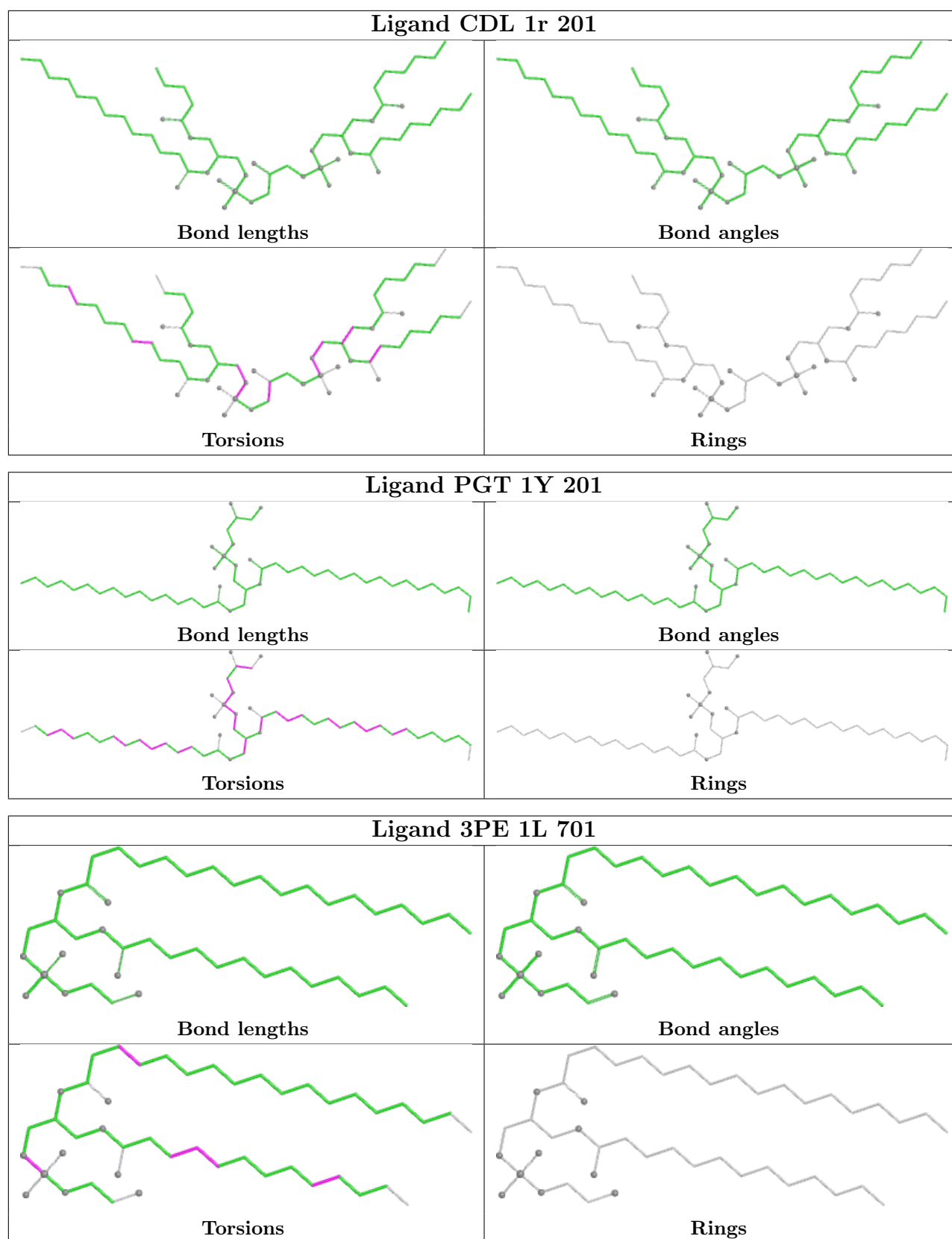
Continued from previous page...

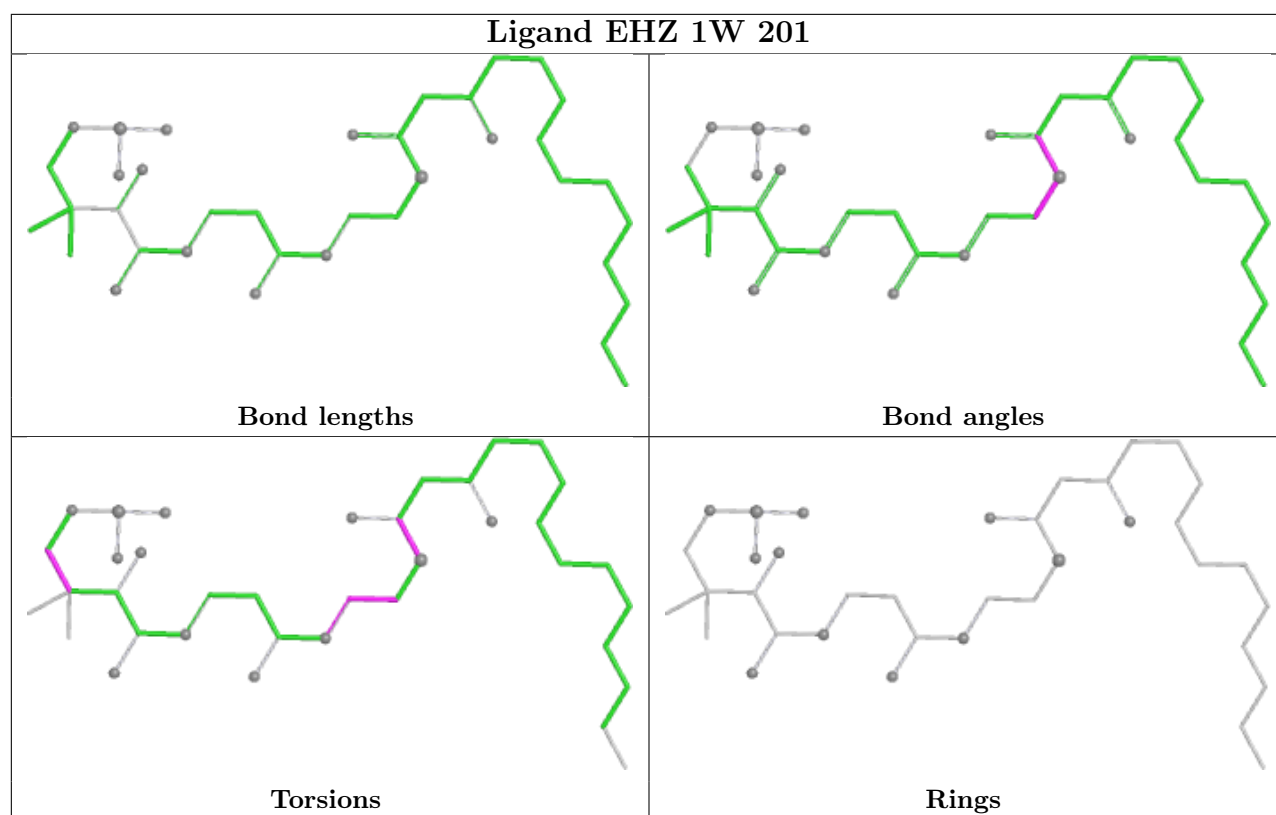
Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	1B	201	SF4	2	0
45	1A	201	3PE	3	0
52	1O	401	GTP	3	0
45	1Y	202	3PE	2	0
48	1E	301	FES	2	0

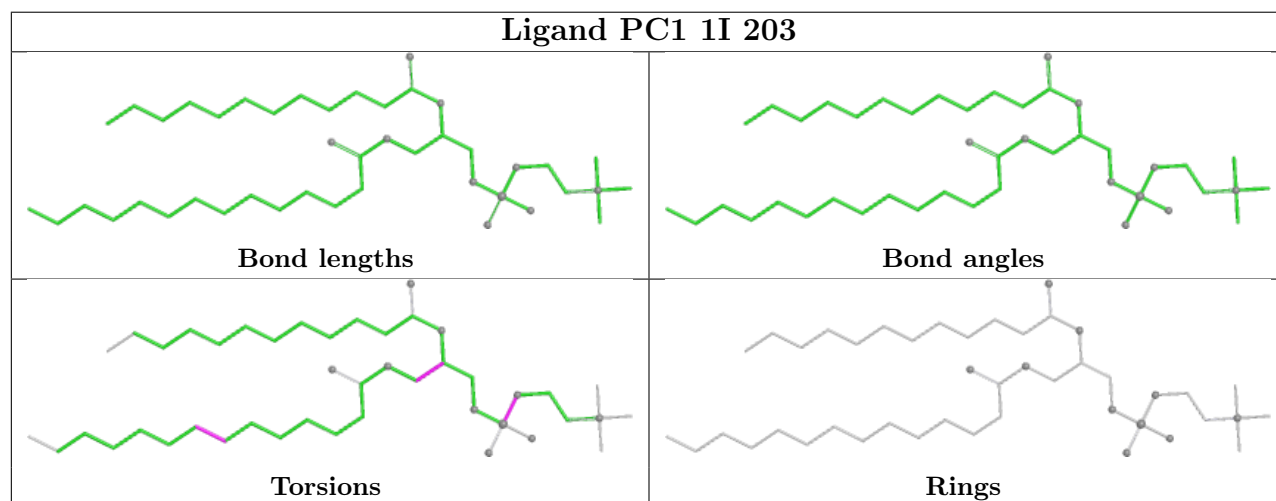
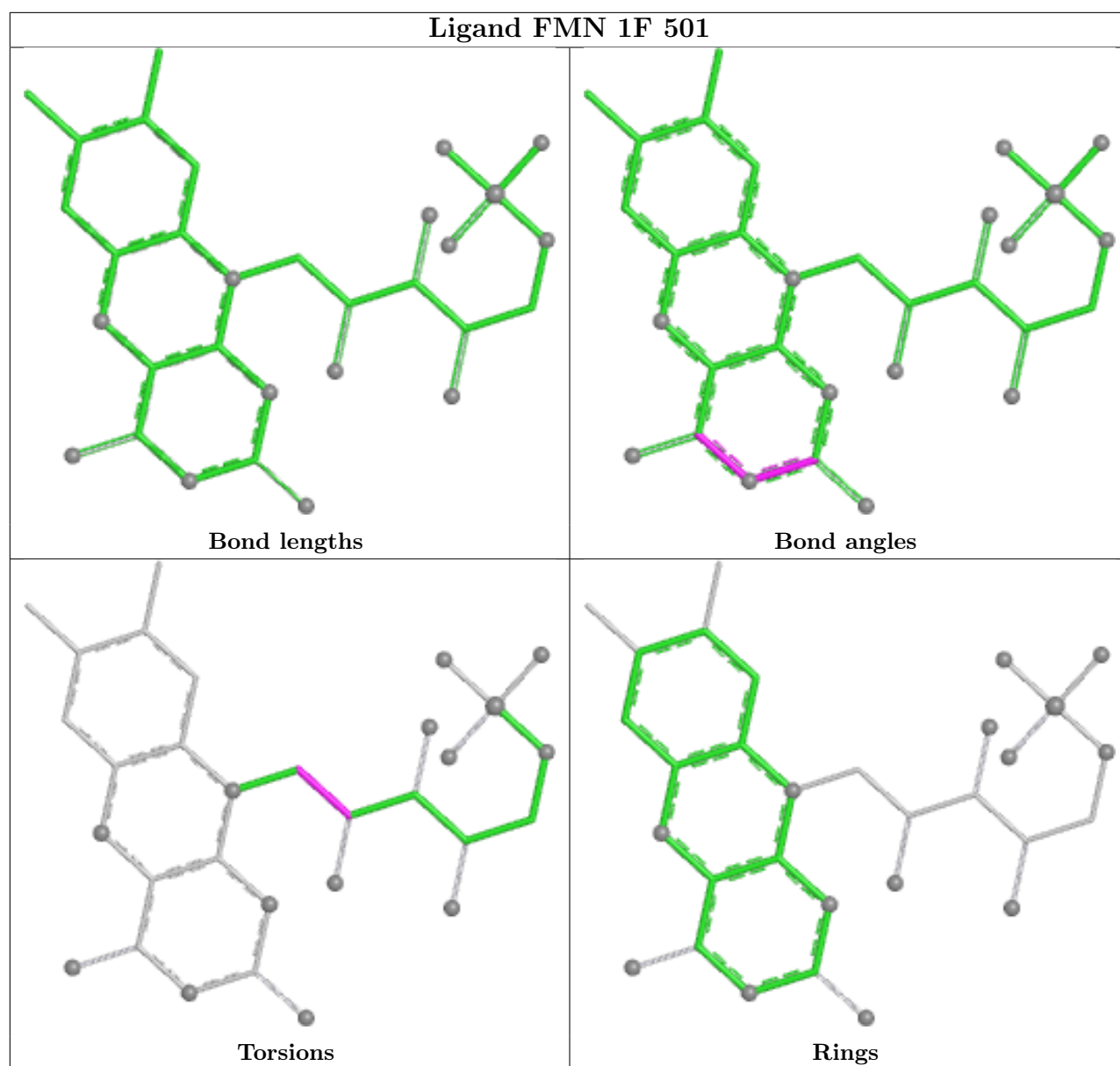
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

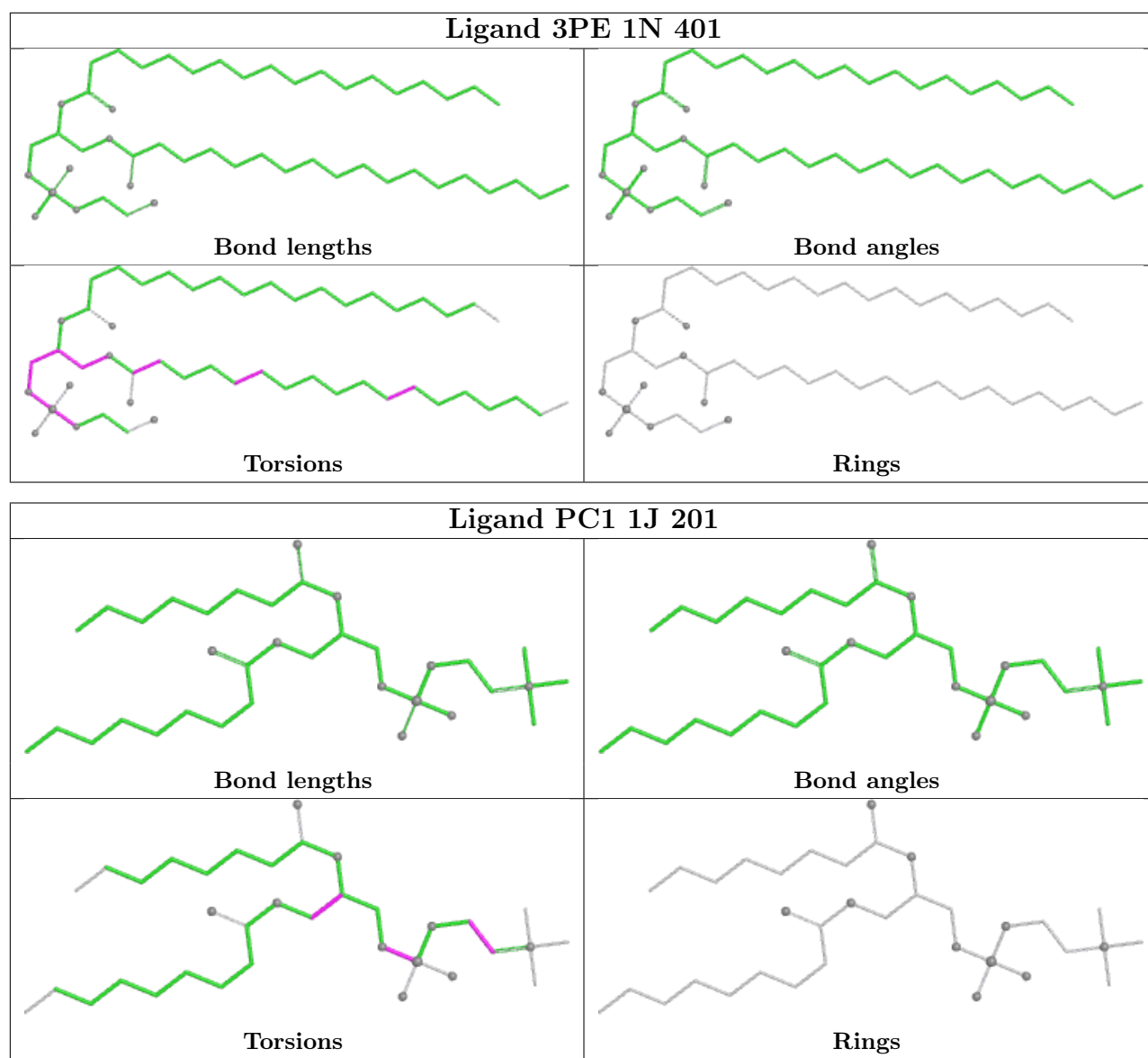


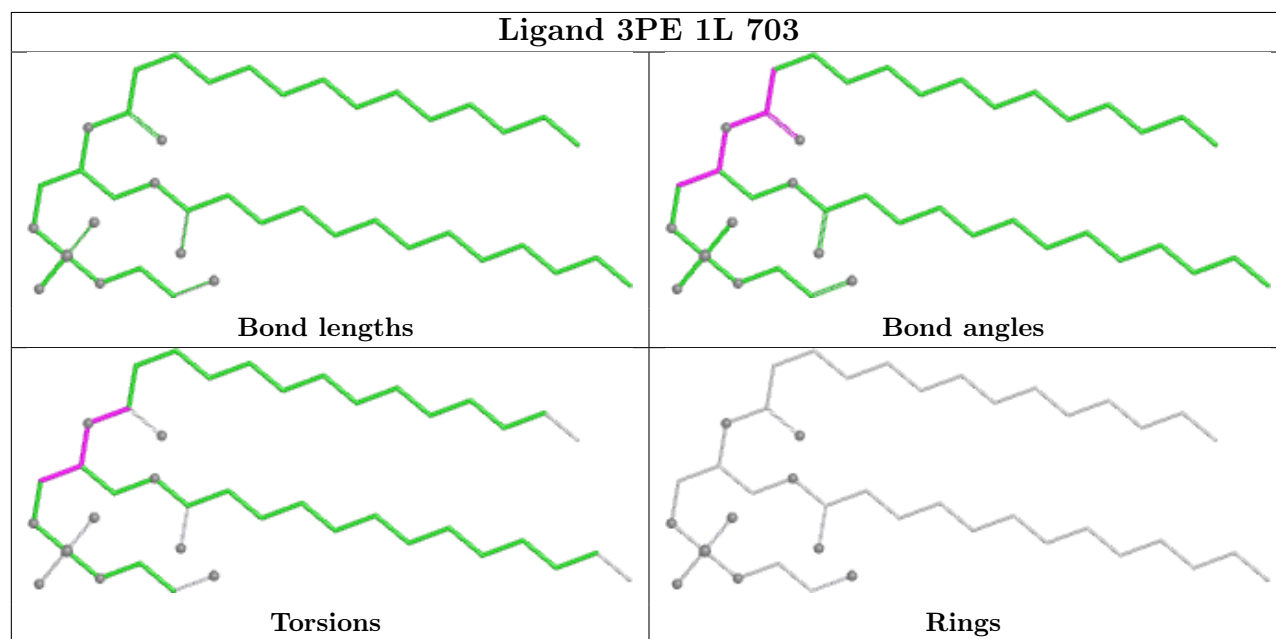
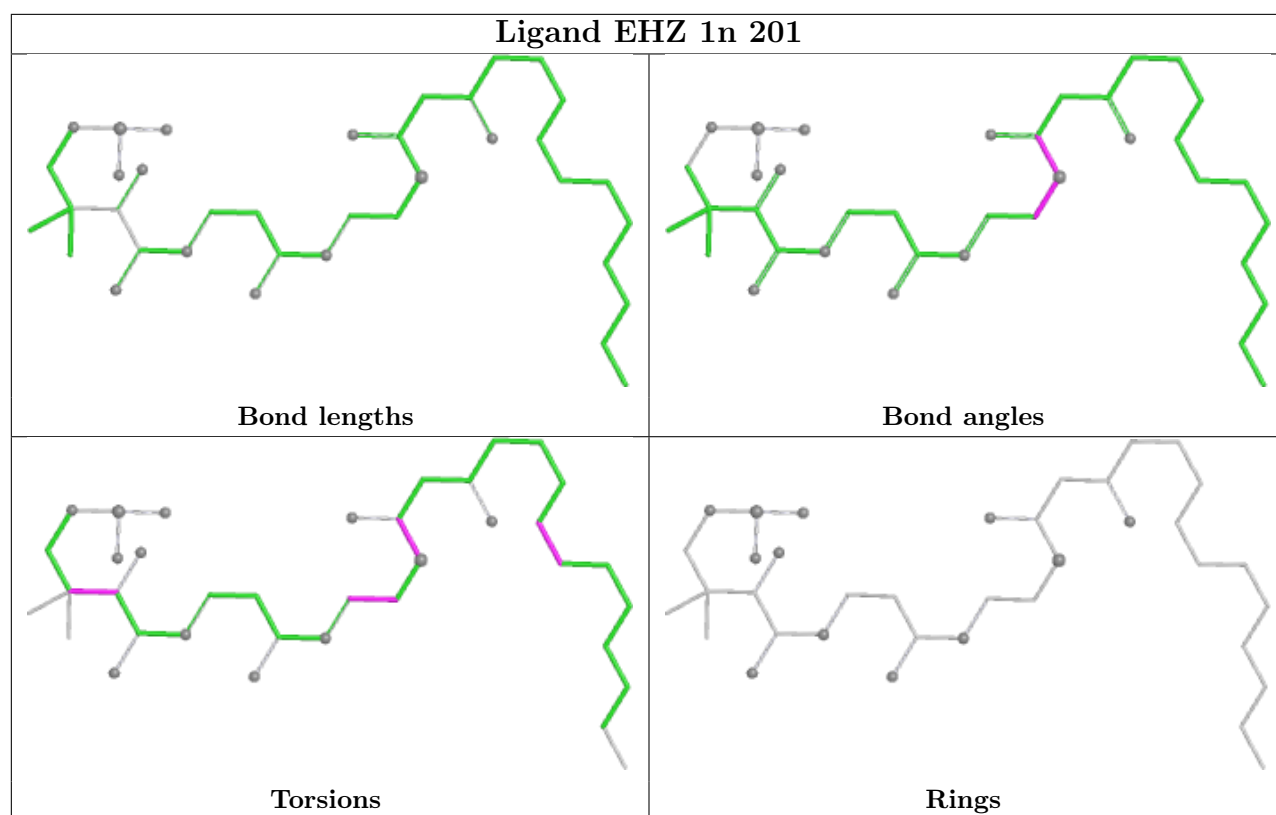


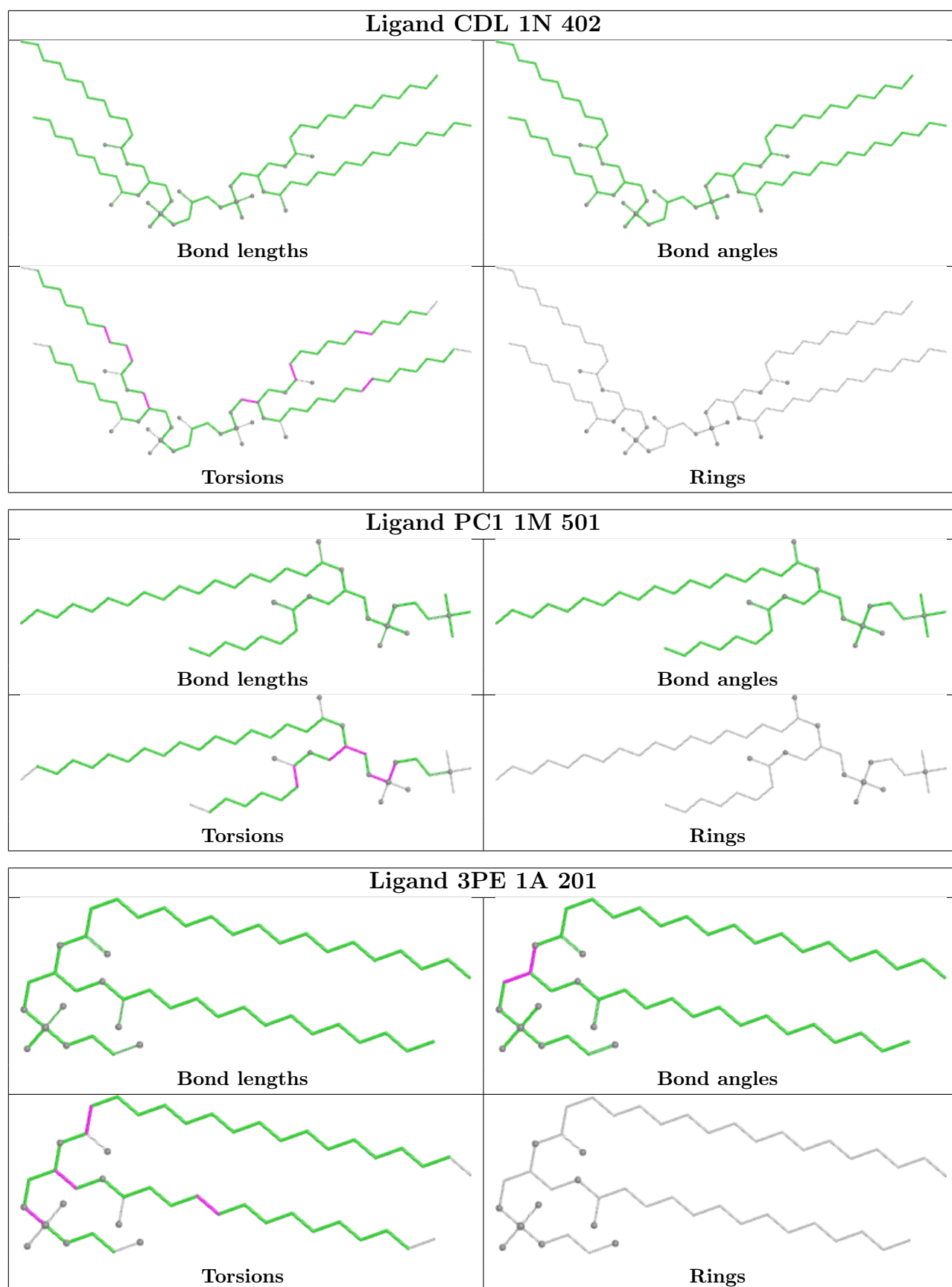


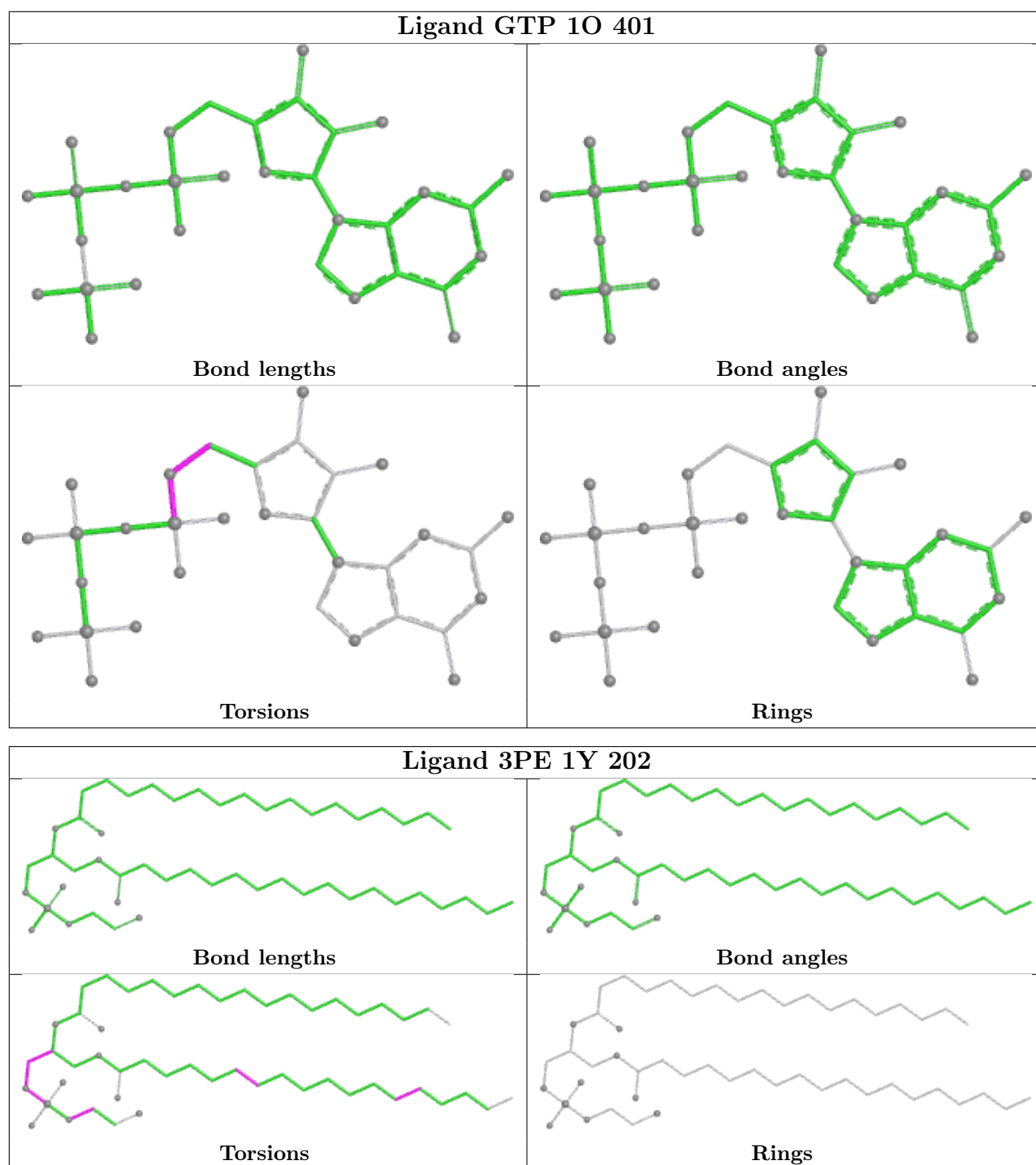












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1i	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	3.58
1	1r	1:ALA	C	2:SER	N	3.18

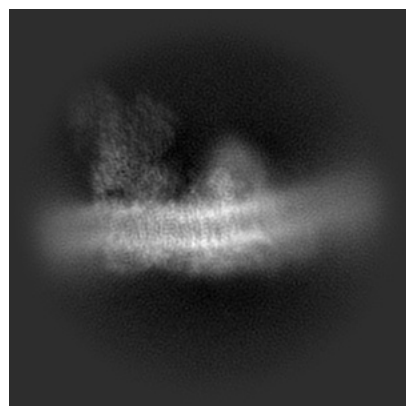
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42174. These allow visual inspection of the internal detail of the map and identification of artifacts.

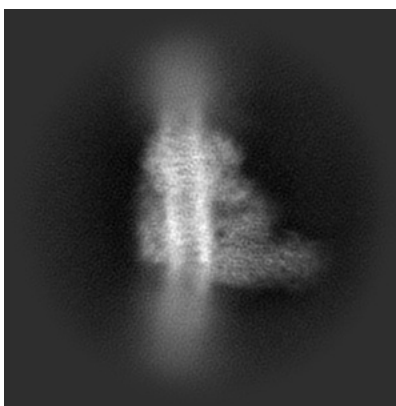
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

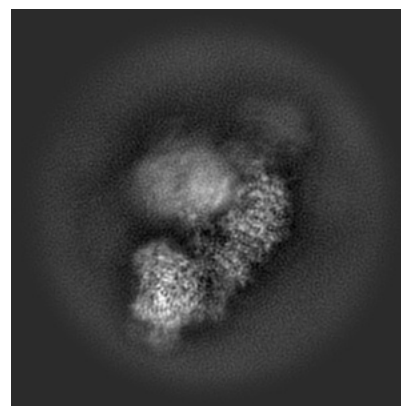
6.1.1 Primary map



X

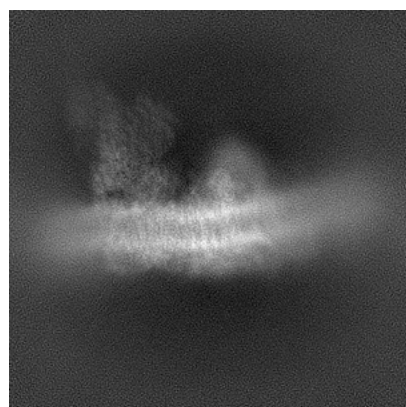


Y

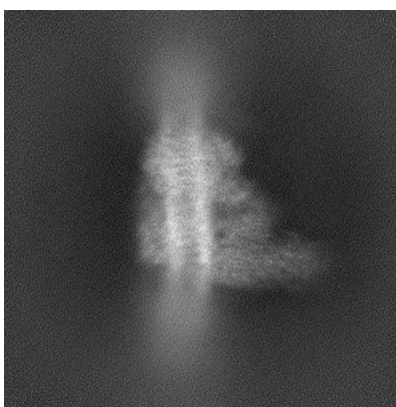


Z

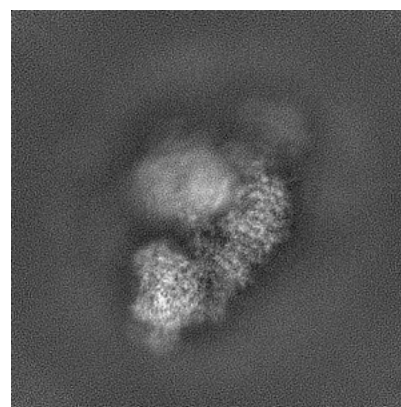
6.1.2 Raw map



X



Y

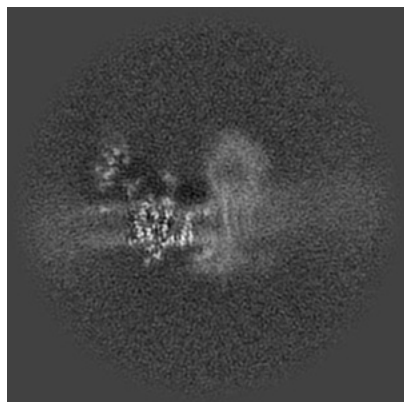


Z

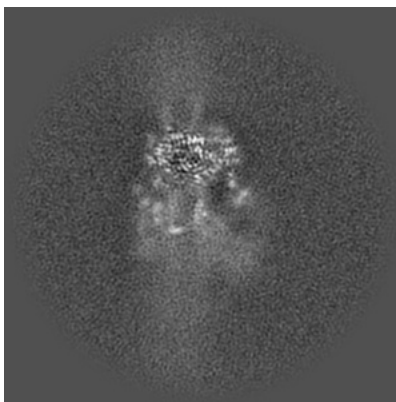
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

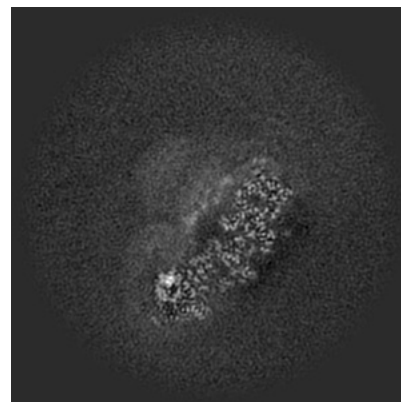
6.2.1 Primary map



X Index: 160



Y Index: 160

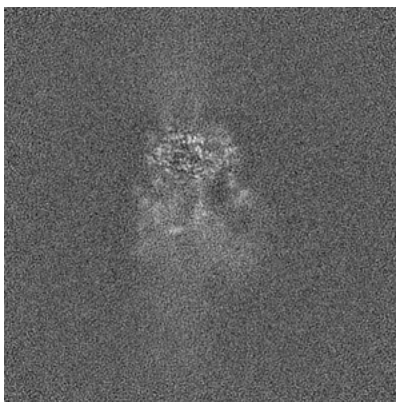


Z Index: 160

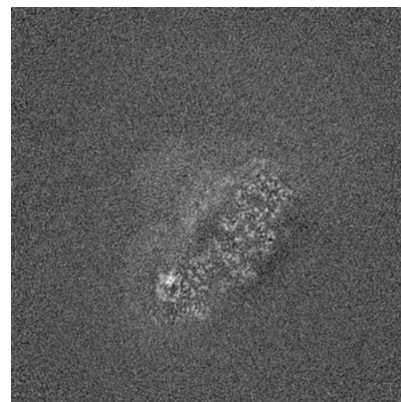
6.2.2 Raw map



X Index: 160



Y Index: 160

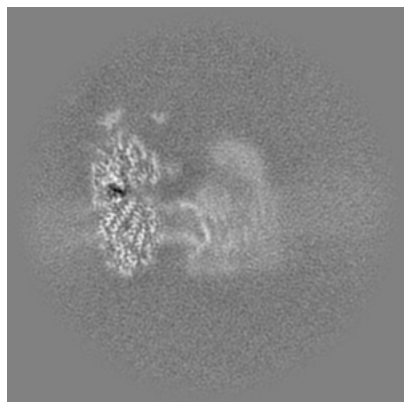


Z Index: 160

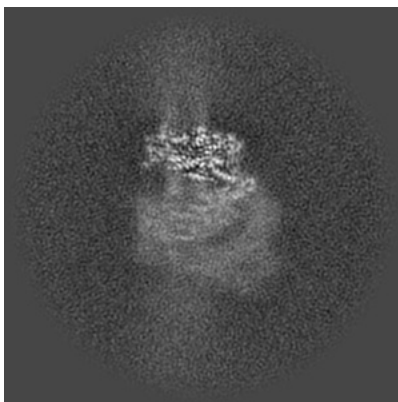
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

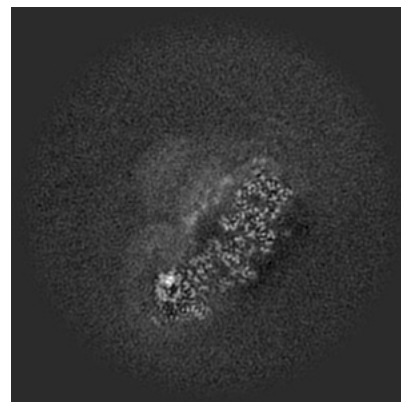
6.3.1 Primary map



X Index: 140

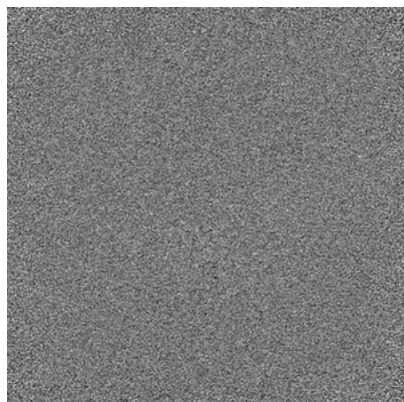


Y Index: 173

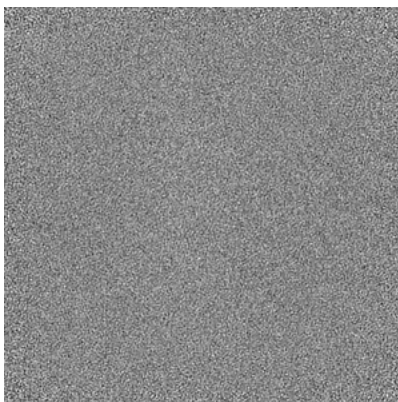


Z Index: 160

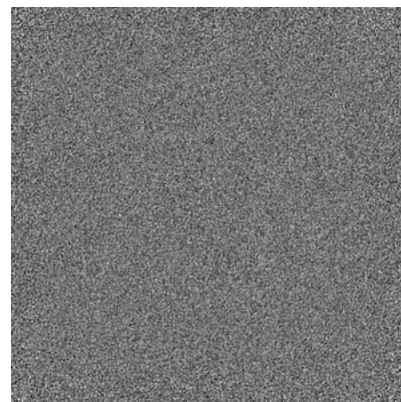
6.3.2 Raw map



X Index: 0



Y Index: 0

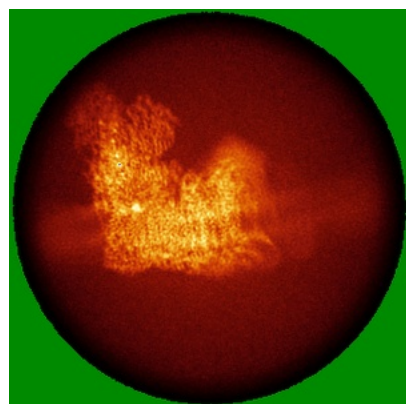


Z Index: 0

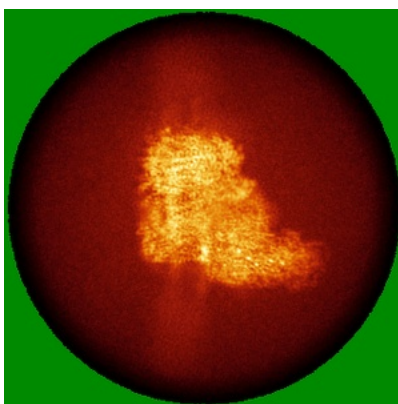
The images above show the largest variance slices of the map in three orthogonal directions.

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

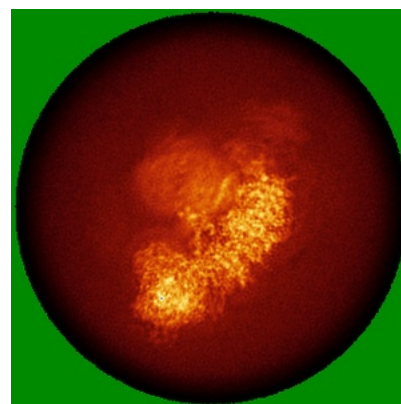
6.4.1 Primary map



X

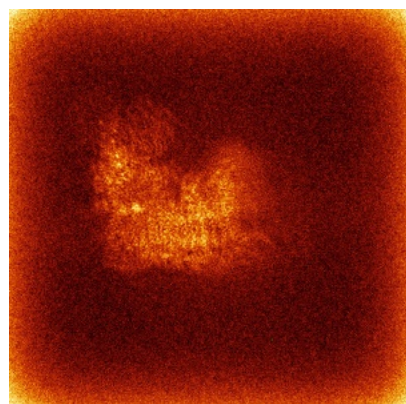


Y

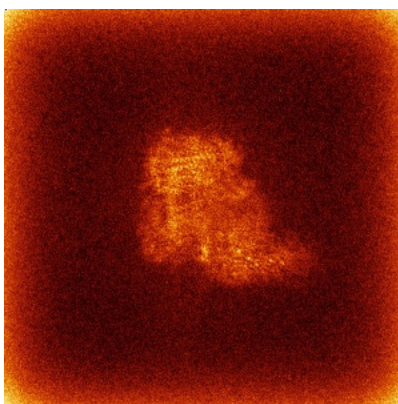


Z

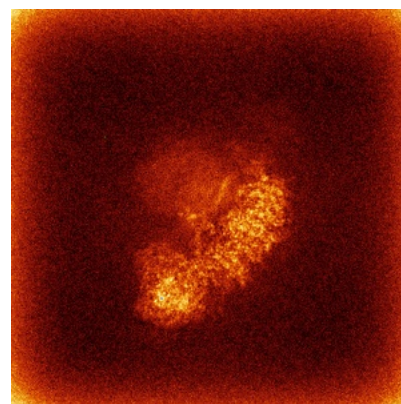
6.4.2 Raw map



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.

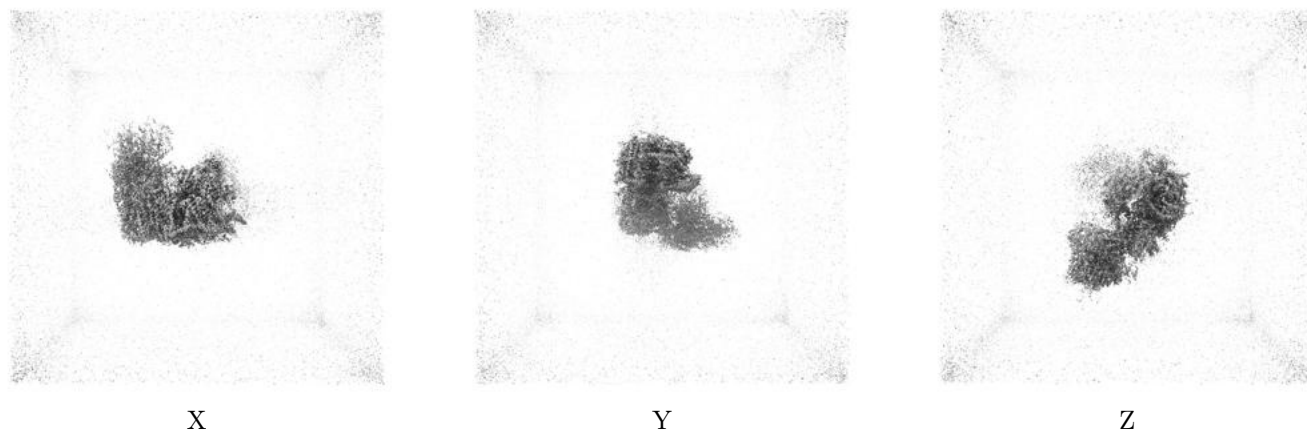
6.5 Orthogonal surface views [i](#)

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.

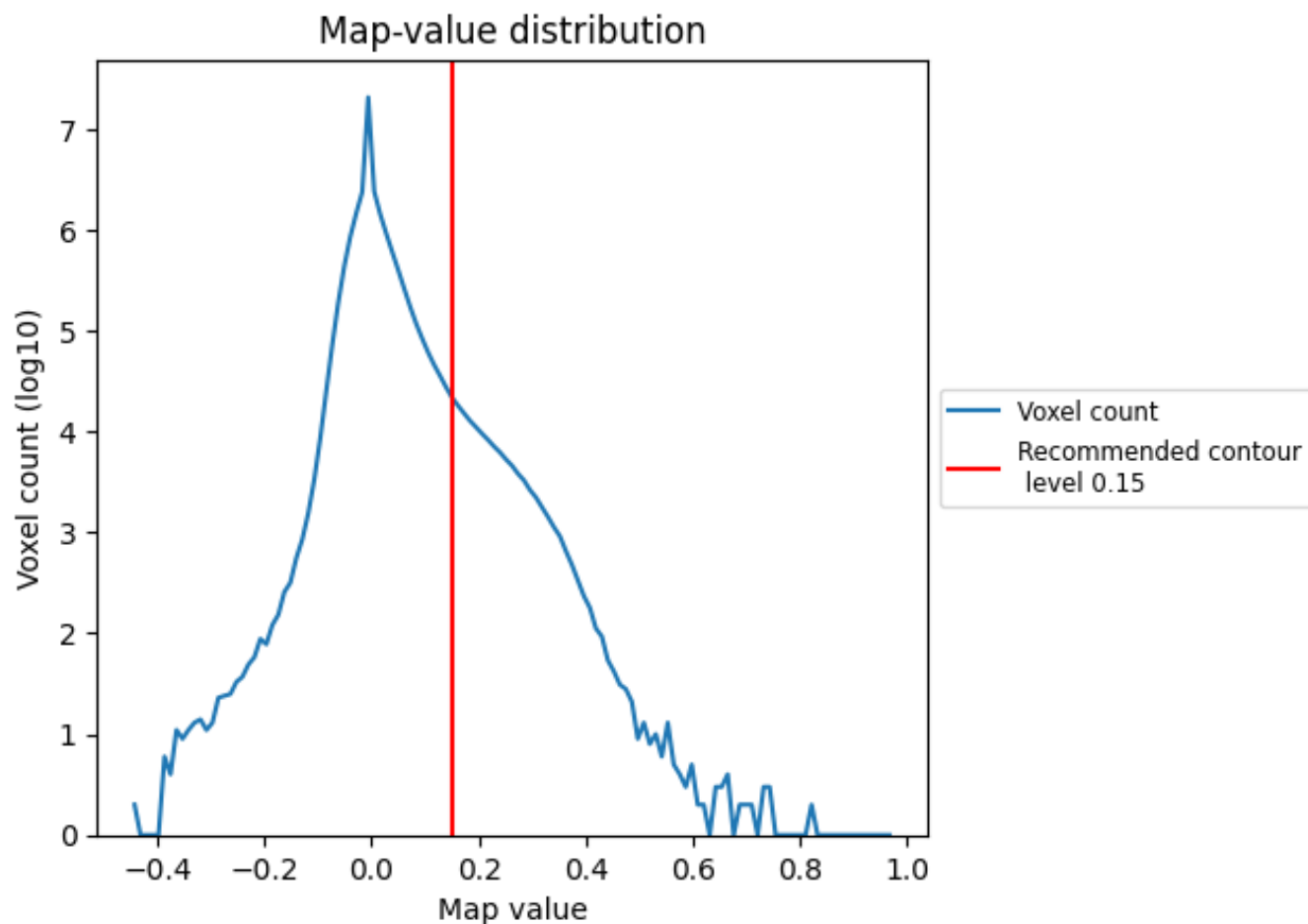
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

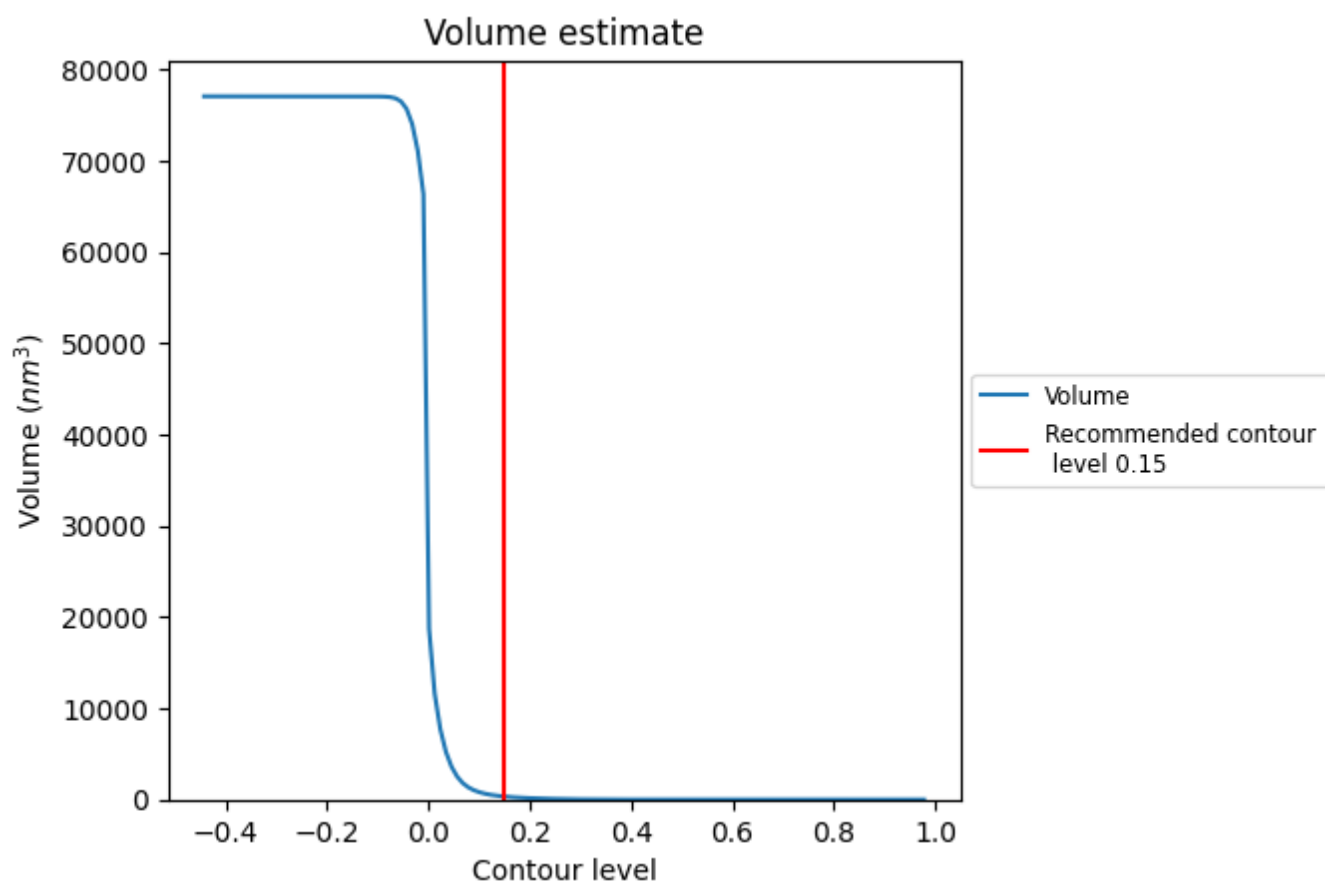
This section contains the results of statistical analysis of the map.

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.

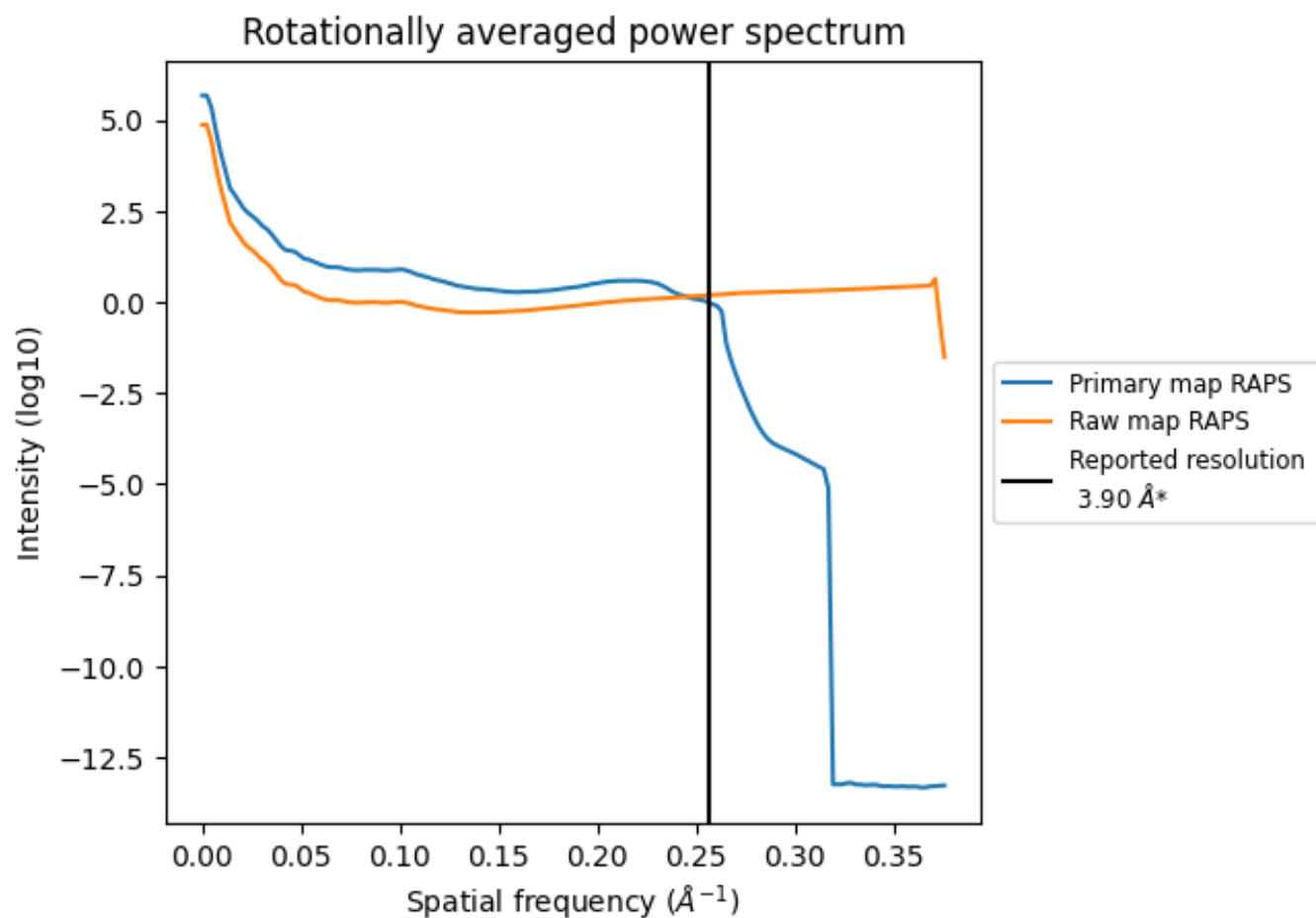
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 331 nm³; this corresponds to an approximate mass of 299 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 ⓘ

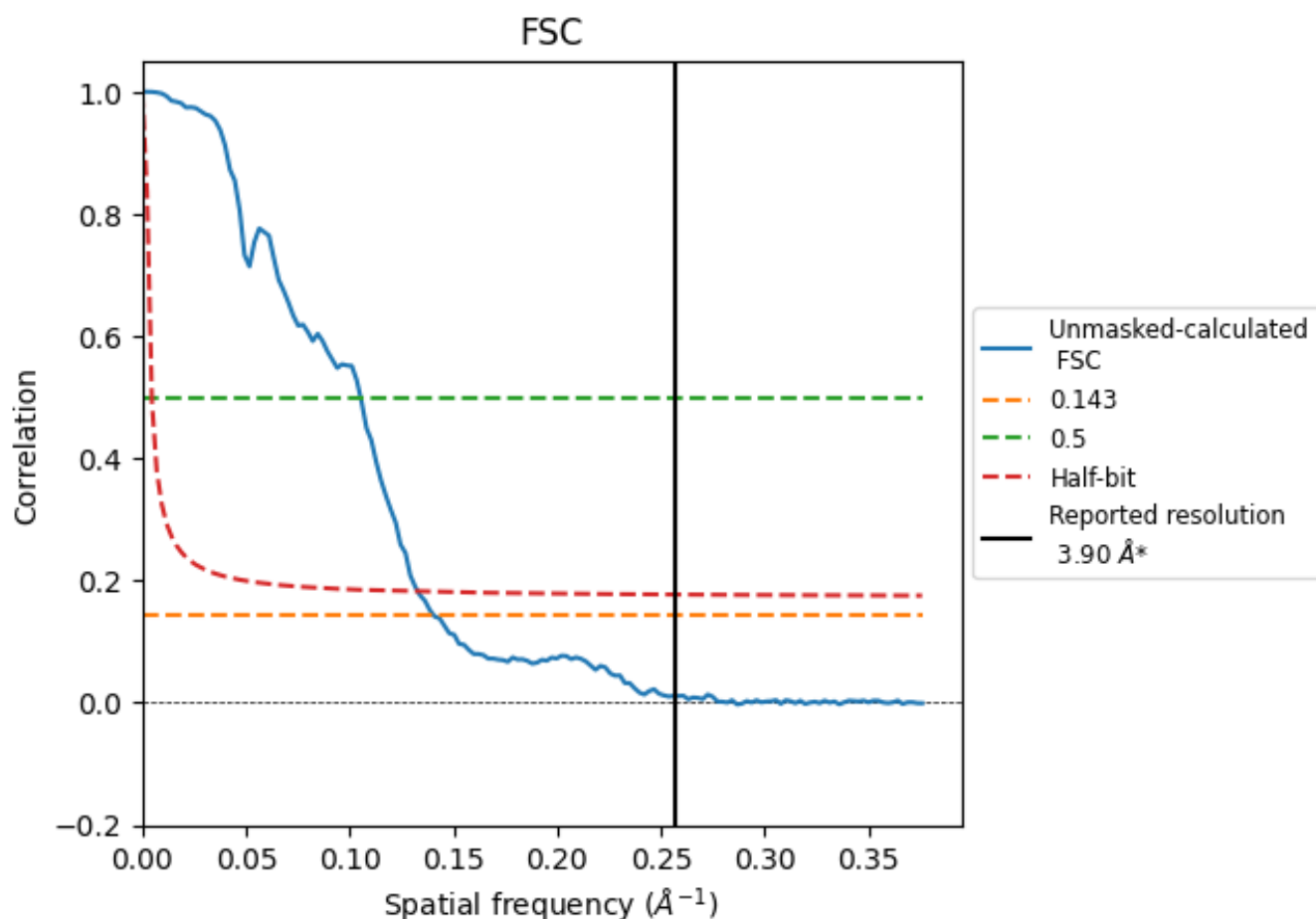


*Reported resolution corresponds to spatial frequency of 0.256 Å⁻¹

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 0.256 Å⁻¹

8.2 Resolution estimates [i](#)

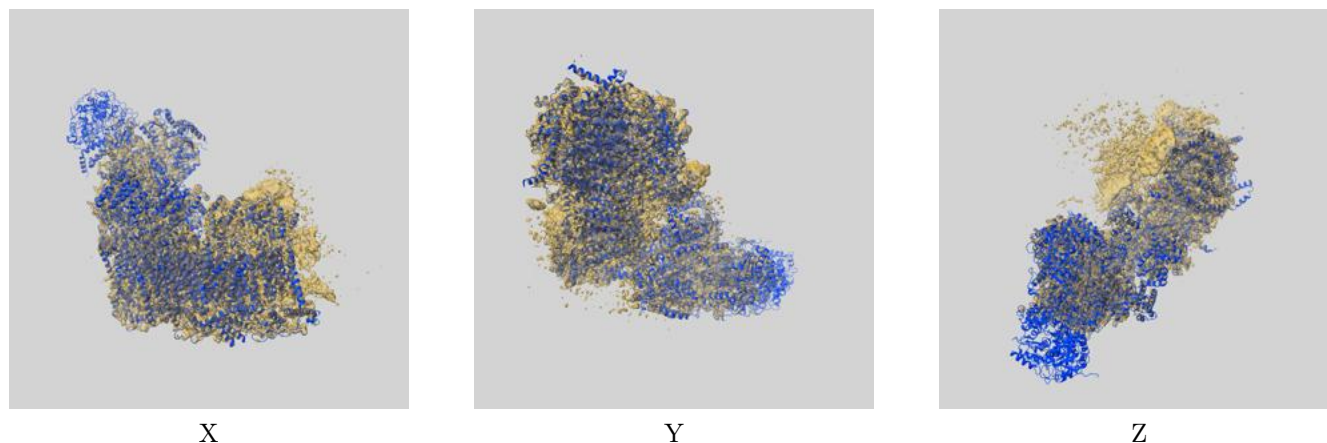
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.12	9.51	7.52

*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 7.12 differs from the reported value 3.9 by more than 10 %

9 Map-model fit [i](#)

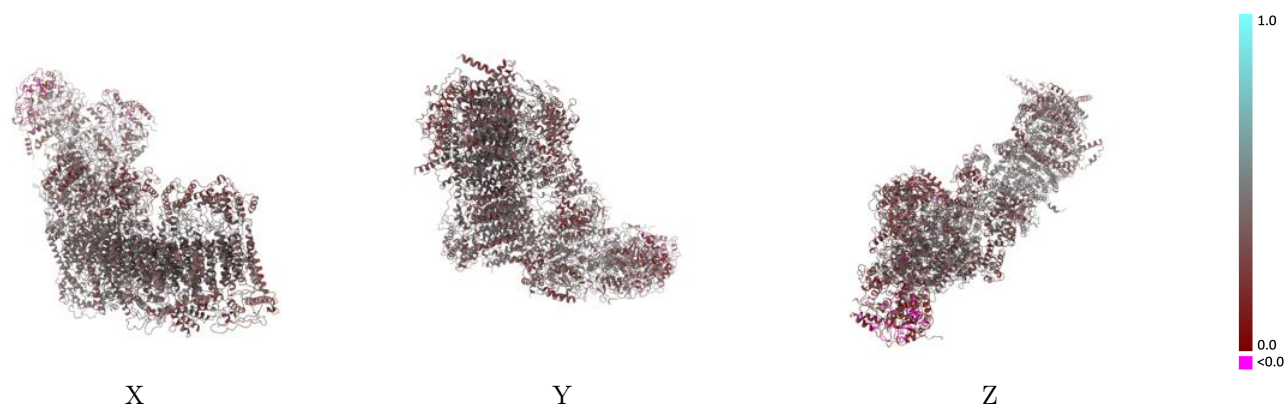
This section contains information regarding the fit between EMDB map EMD-42174 and PDB model 8UEX. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



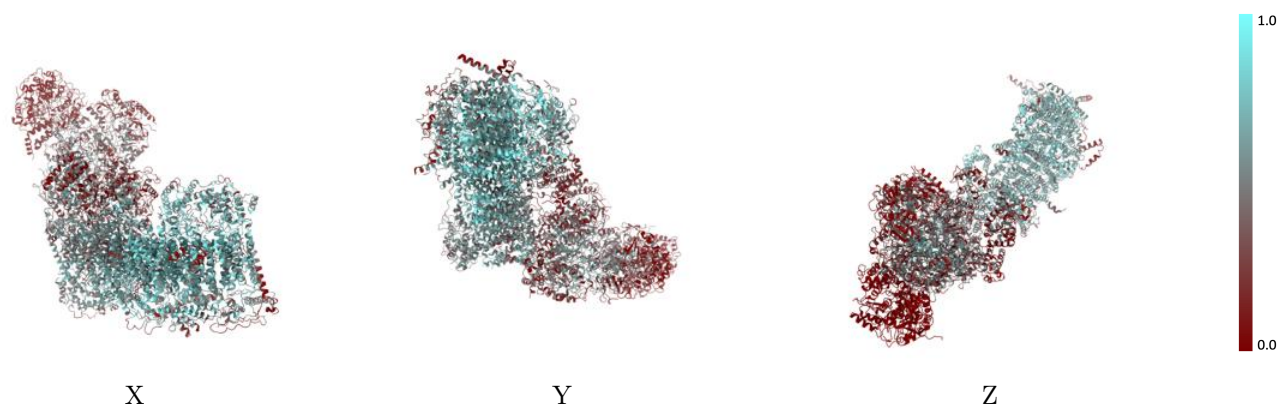
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



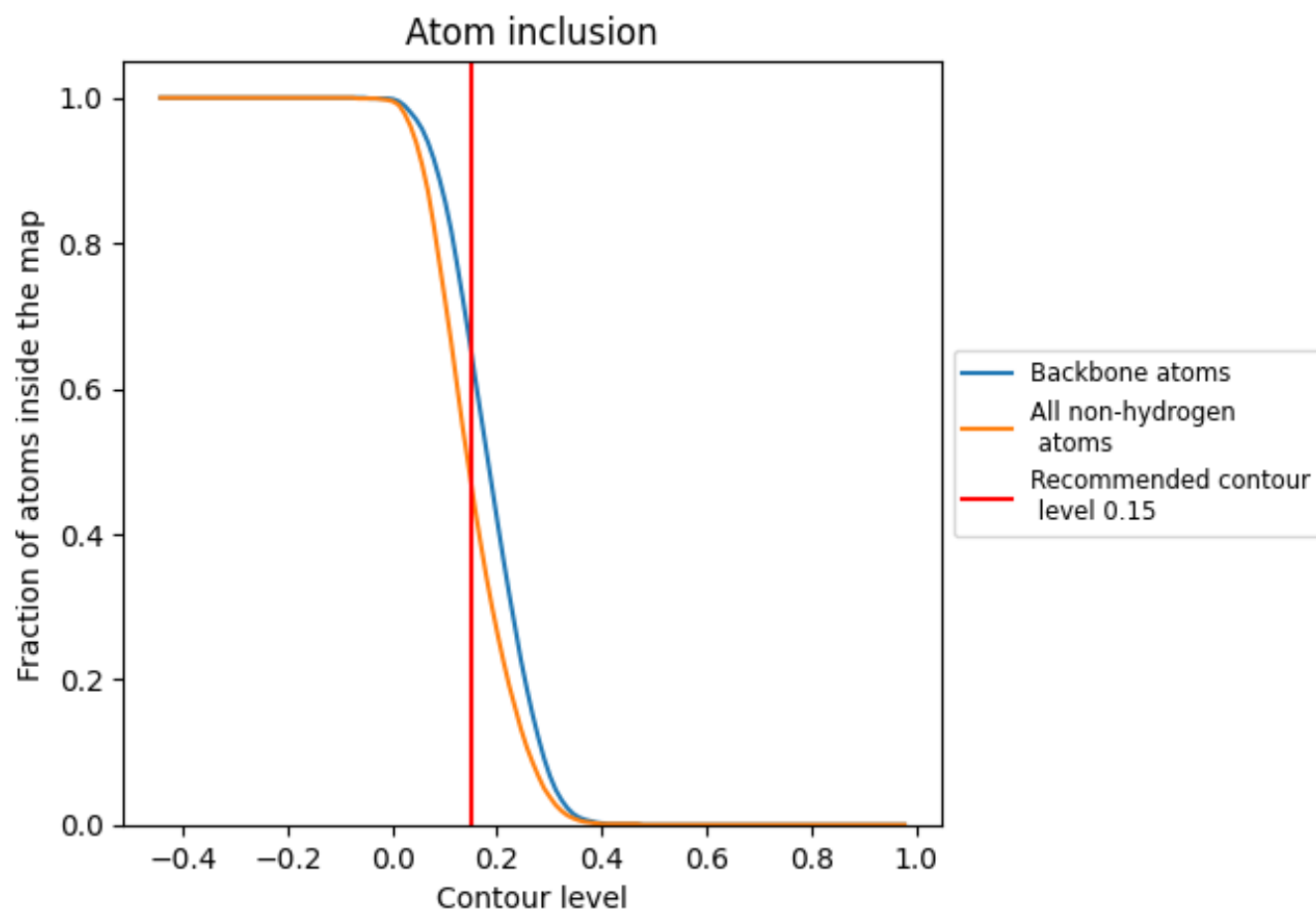
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 65% of all backbone atoms, 47% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	 0.4720	 0.3720
1A	 0.5230	 0.3860
1B	 0.5070	 0.4180
1C	 0.3860	 0.3970
1D	 0.4800	 0.3900
1E	 0.0200	 0.2590
1F	 0.0300	 0.2470
1G	 0.2760	 0.3550
1H	 0.6170	 0.3910
1I	 0.5640	 0.4150
1J	 0.5120	 0.3720
1K	 0.6200	 0.3960
1L	 0.7050	 0.3970
1M	 0.7590	 0.4330
1N	 0.6660	 0.4170
1O	 0.3720	 0.3580
1P	 0.2920	 0.3370
1Q	 0.3110	 0.3830
1R	 0.2870	 0.4030
1S	 0.1400	 0.2810
1T	 0.2050	 0.2760
1U	 0.6050	 0.3560
1V	 0.1790	 0.3360
1W	 0.2980	 0.3280
1X	 0.5230	 0.3930
1Y	 0.6680	 0.3780
1Z	 0.5460	 0.4130
1a	 0.6710	 0.4070
1b	 0.5170	 0.4060
1c	 0.4410	 0.3610
1d	 0.6470	 0.4160
1e	 0.5950	 0.4230
1f	 0.5170	 0.3850
1g	 0.5870	 0.3580
1h	 0.6450	 0.4130



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Chain	Atom inclusion	Q-score
1i	 0.3990	 0.3520
1j	 0.5340	 0.3660
1k	 0.5230	 0.3610
1l	 0.6350	 0.3980
1m	 0.6920	 0.3720
1n	 0.6710	 0.3750
1o	 0.5000	 0.3220
1p	 0.5940	 0.3780
1q	 0.4270	 0.4070
1r	 0.3890	 0.4030
1s	 0.0030	 0.2060