



Full wwPDB EM Validation Report ⓘ

Aug 4, 2026 – 09:40 PM EDT

PDB ID : 8UEP / pdb_00008uep
EMDB ID : EMD-42166
Title : In-situ complex I, Active-Q10 (State-alpha)
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

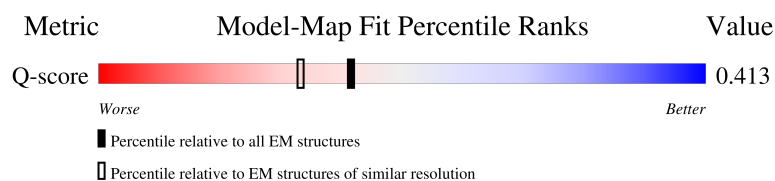
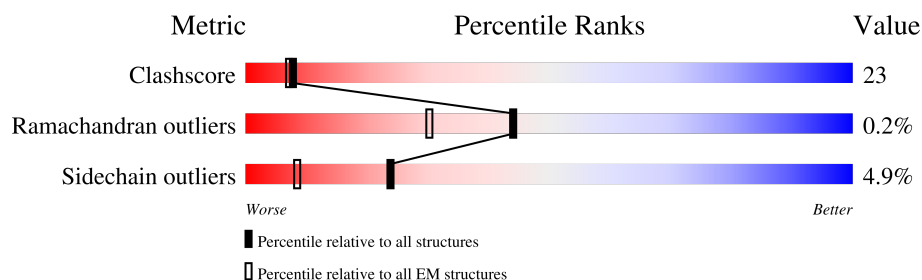
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.40 Å.

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



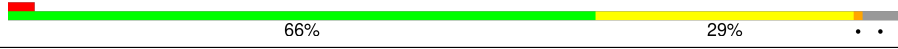
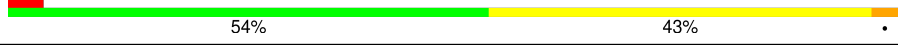
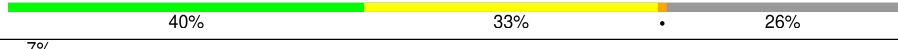
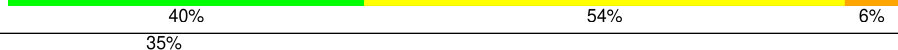
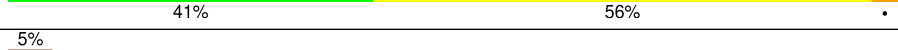
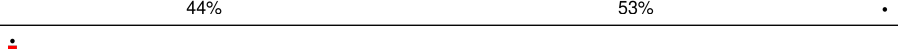
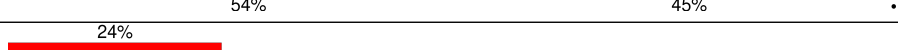
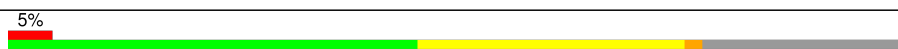
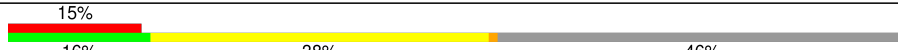
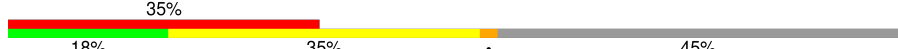
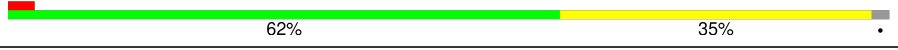
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

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

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

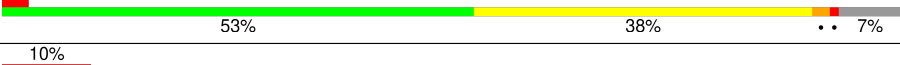
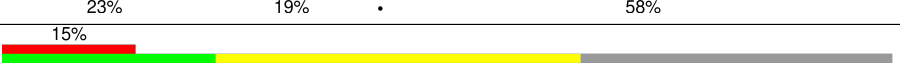
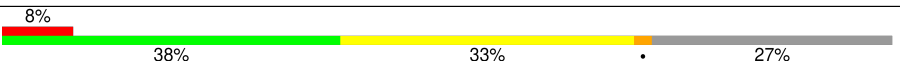
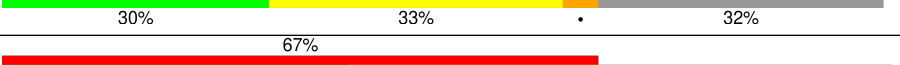
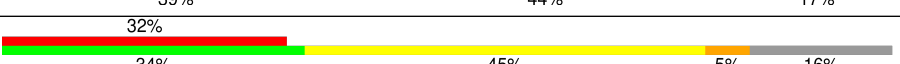
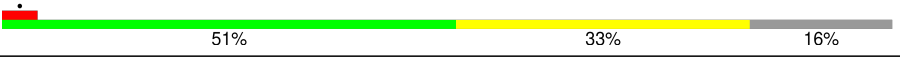
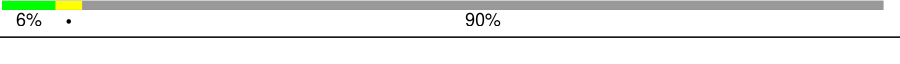
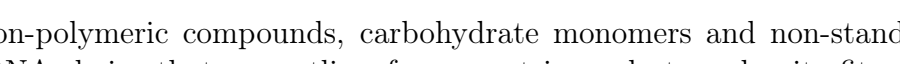
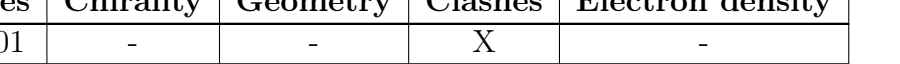
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Mol	Chain	Length	Quality of chain
5	1E	249	
6	1F	464	
7	1G	727	
8	1H	318	
9	1I	239	
10	1J	175	
11	1K	98	
12	1L	606	
13	1M	459	
14	1N	347	
15	1O	357	
16	1P	377	
17	1Q	175	
18	1R	123	
19	1S	99	
20	1T	156	
20	1U	156	
21	1V	116	
22	1W	128	
23	1X	172	
24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

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	SF4	1B	201	-	-	X	-
45	SF4	1I	201	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67436 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

There are 2 discrepancies between the modelled and reference sequences:

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

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

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

There are 29 discrepancies between the modelled and reference sequences:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

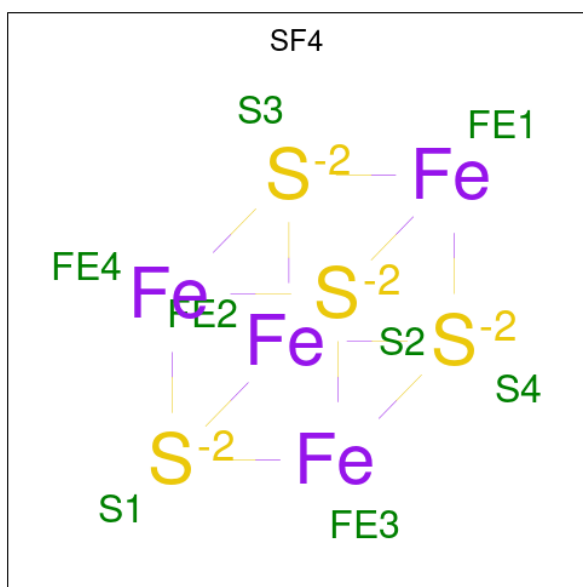
There is a discrepancy between the modelled and reference sequences:

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

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

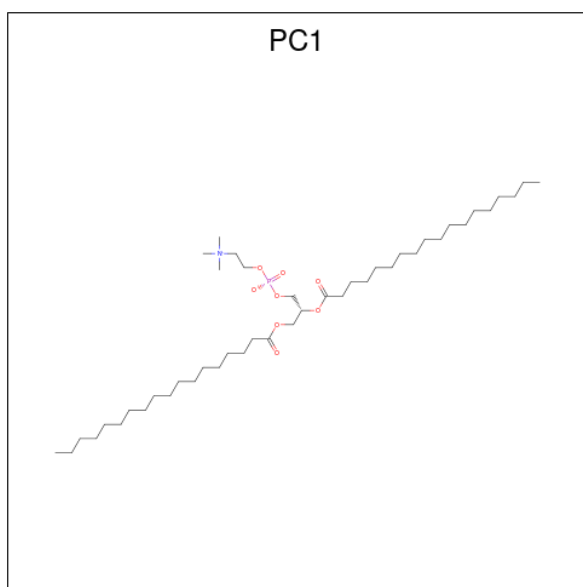
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



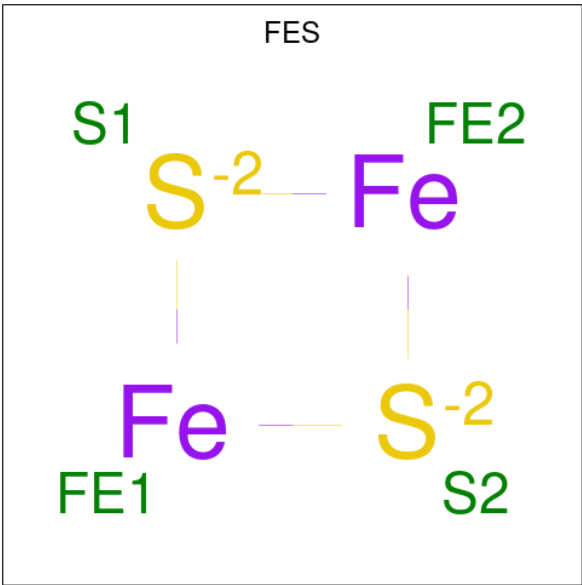
Mol	Chain	Residues	Atoms			AltConf
45	1B	1	Total	Fe	S	0
			8	4	4	
45	1F	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1G	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	
45	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $\text{C}_{44}\text{H}_{88}\text{NO}_8\text{P}$).



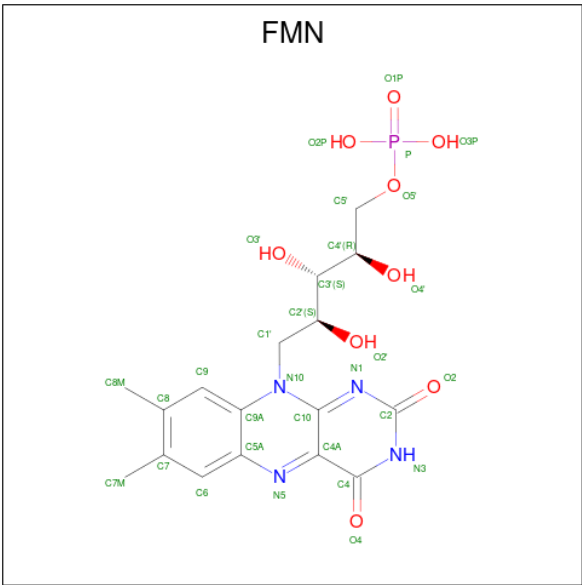
Mol	Chain	Residues	Atoms					AltConf
46	1B	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1M	1	Total	C	N	O	P	0
			35	25	1	8	1	
46	1Y	1	Total	C	N	O	P	0
			46	36	1	8	1	
46	1d	1	Total	C	N	O	P	0
			39	29	1	8	1	
46	1f	1	Total	C	N	O	P	0
			34	24	1	8	1	
46	1q	1	Total	C	N	O	P	0
			48	38	1	8	1	

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



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

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

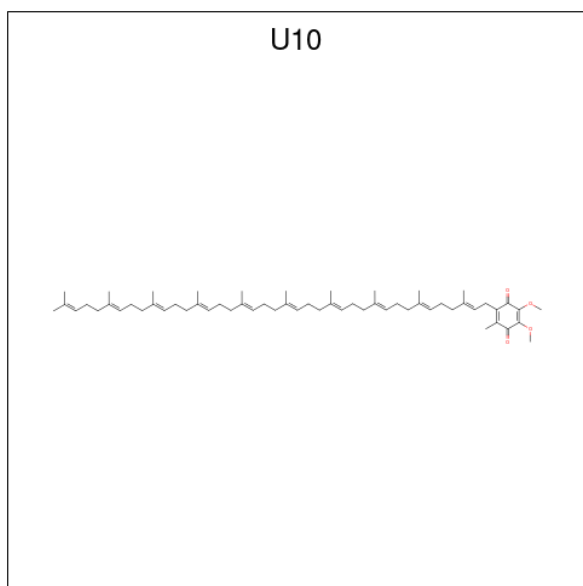


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

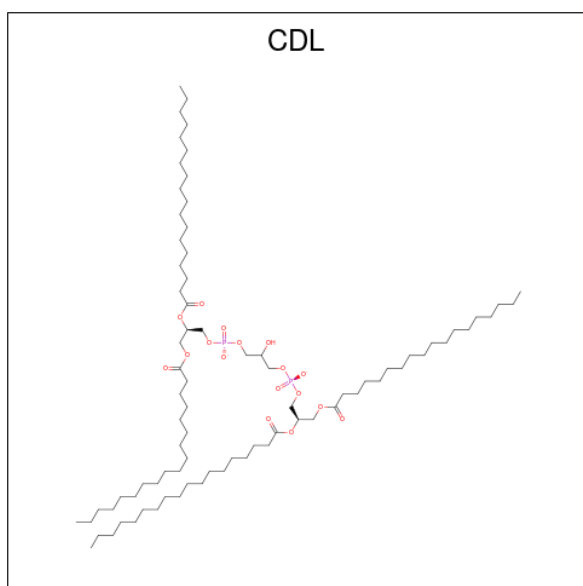
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

- Molecule 50 is UBIQUINONE-10 (CCD ID: U10) (formula: $C_{59}H_{90}O_4$).



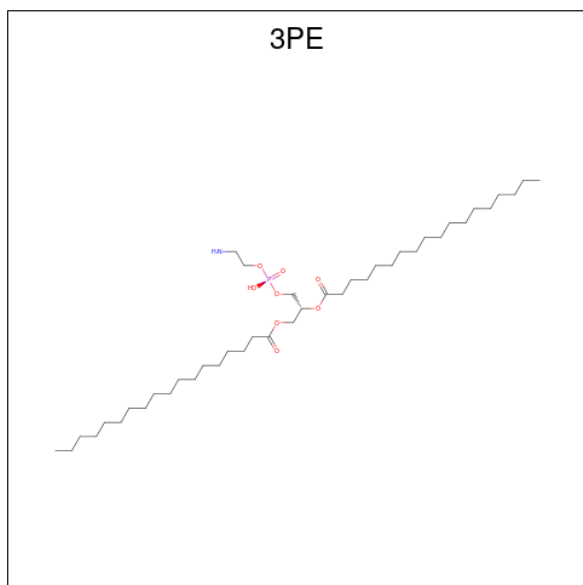
Mol	Chain	Residues	Atoms			AltConf
50	1H	1	Total	C	O	0
			63	59	4	

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



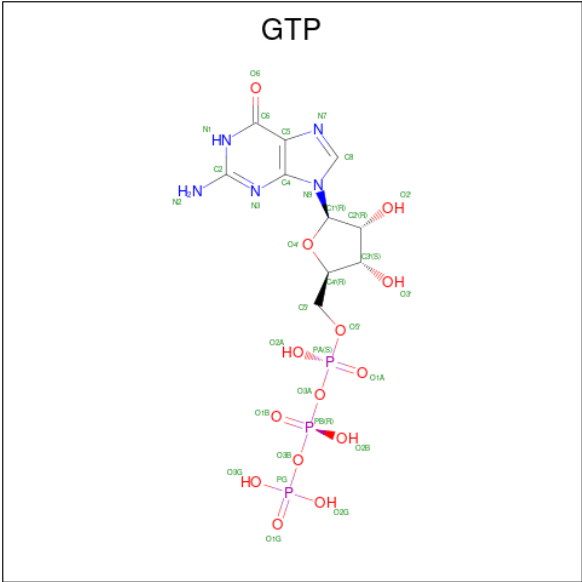
Mol	Chain	Residues	Atoms				AltConf
51	1H	1	Total	C	O	P	0
			51	32	17	2	
51	1N	1	Total	C	O	P	0
			67	48	17	2	
51	1a	1	Total	C	O	P	0
			61	42	17	2	

- Molecule 52 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
52	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
52	1N	1	Total	C	N	O	P	0
			38	28	1	8	1	
52	1Y	1	Total	C	N	O	P	0
			35	25	1	8	1	
52	1f	1	Total	C	N	O	P	0
			51	41	1	8	1	

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

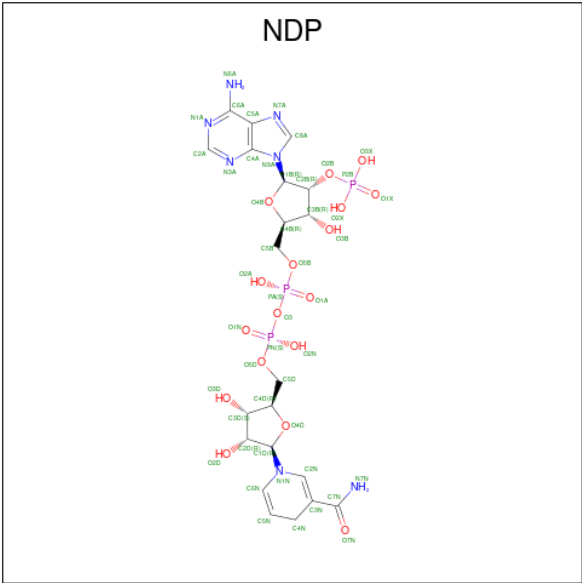


Mol	Chain	Residues	Atoms					AltConf
53	10	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

Mol	Chain	Residues	Atoms		AltConf
54	10	1	Total	Mg	0
			1	1	

- Molecule 55 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

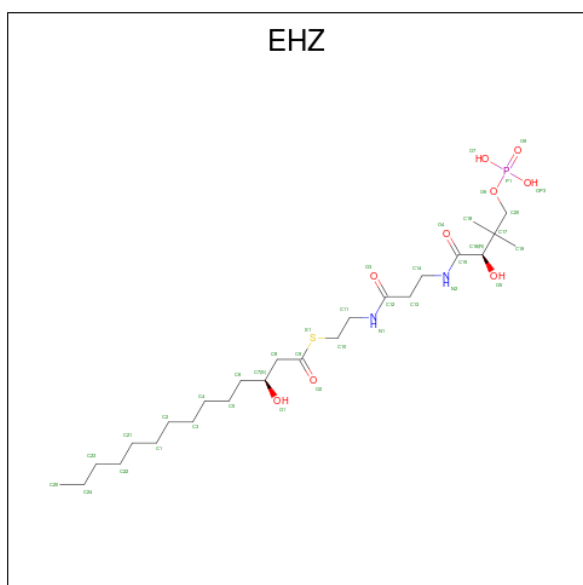


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

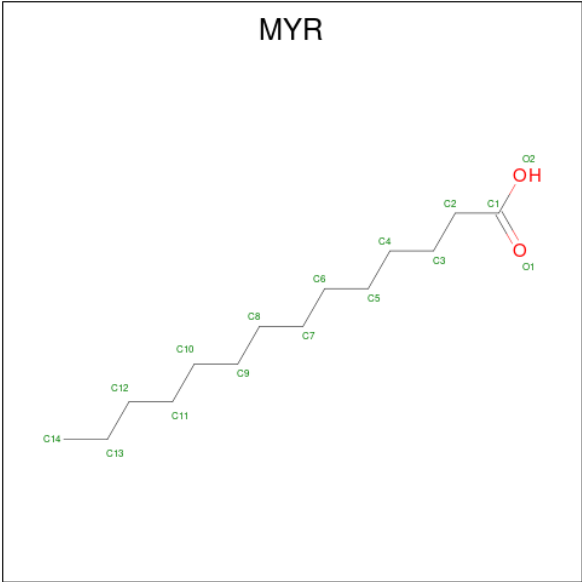
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

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

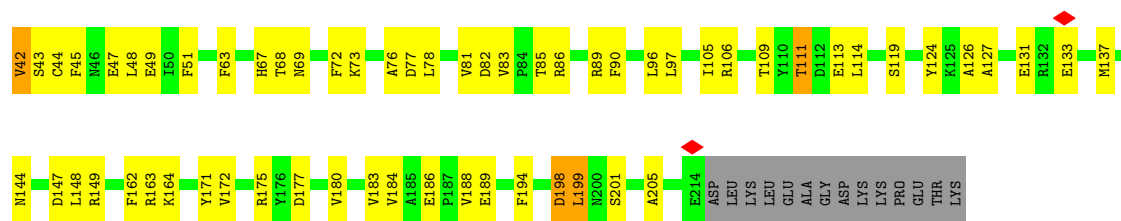


Mol	Chain	Residues	Atoms						AltConf
57	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

- Molecule 58 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).

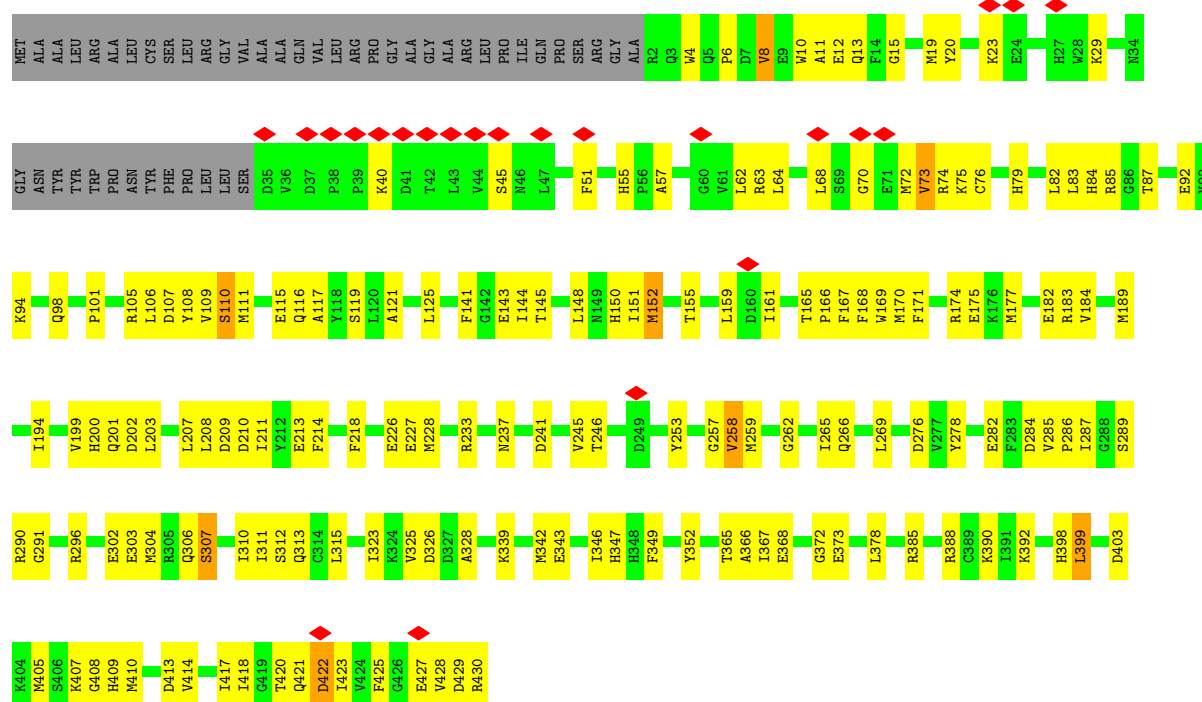


Mol	Chain	Residues	Atoms			AltConf
58	1l	1	Total	C	O	0
			15	14	1	



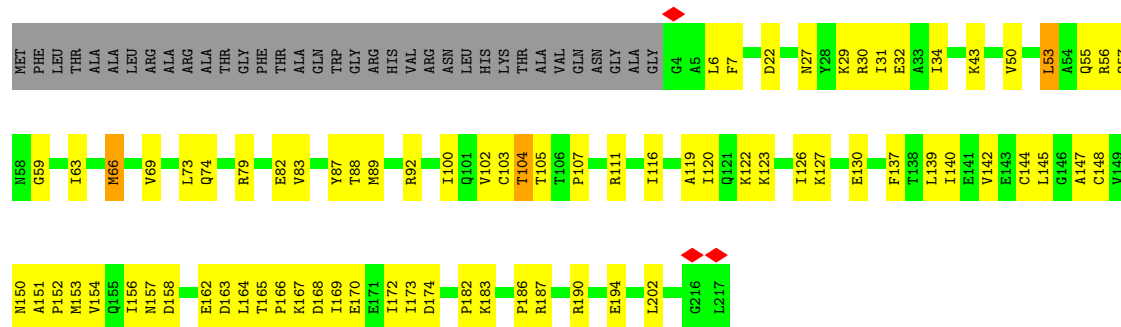
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain 1D: 5% 55% 34% 10%



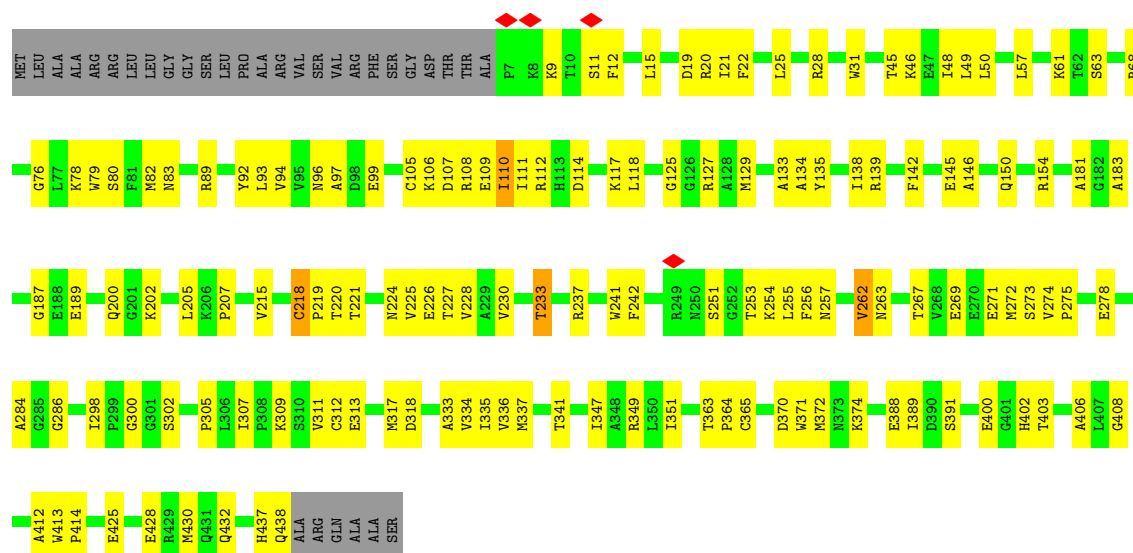
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain 1E: 55% 30% 14%



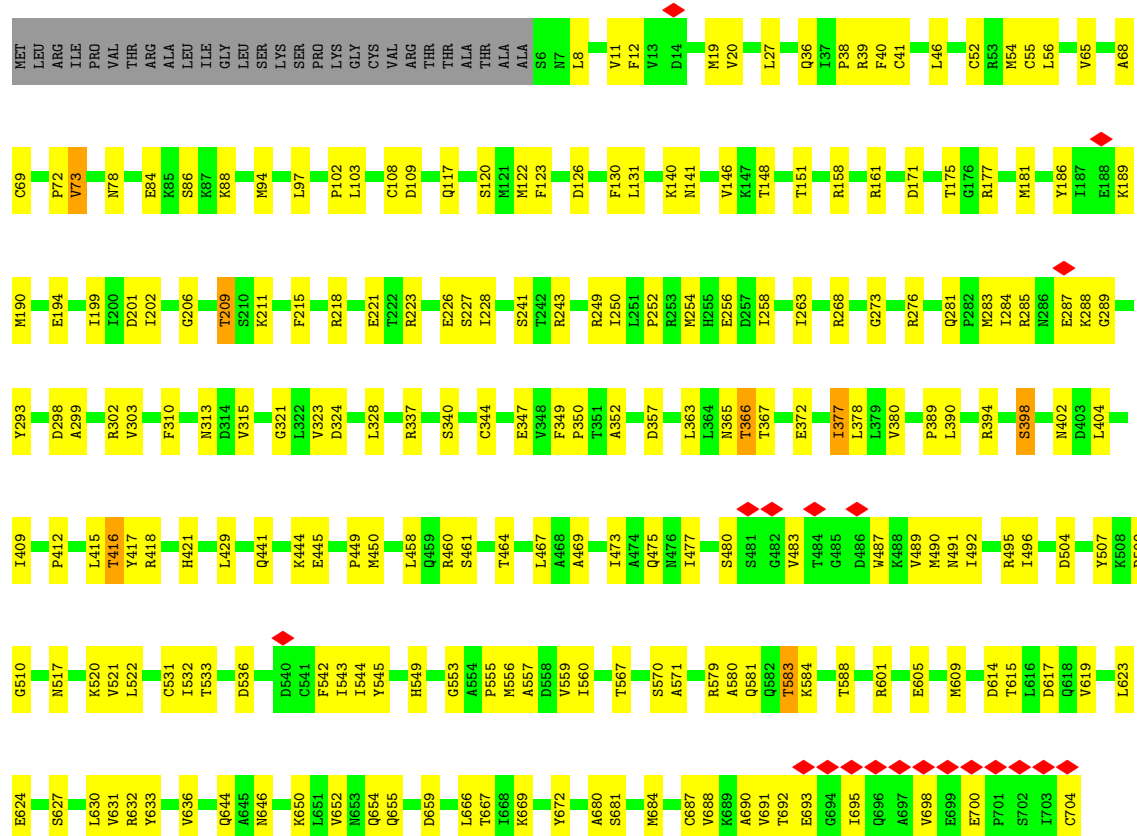
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain 1F: 62% 30% 7%



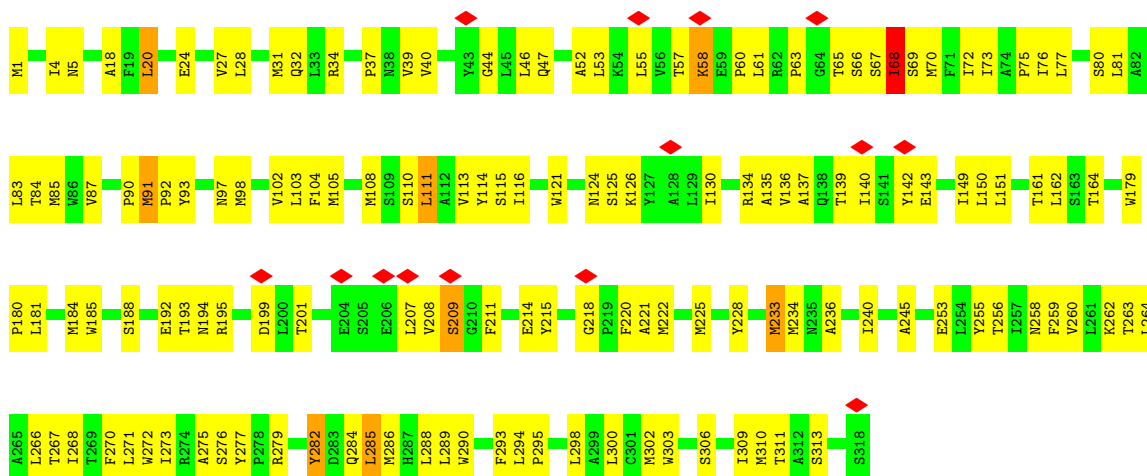
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain 1G: 66% 29%



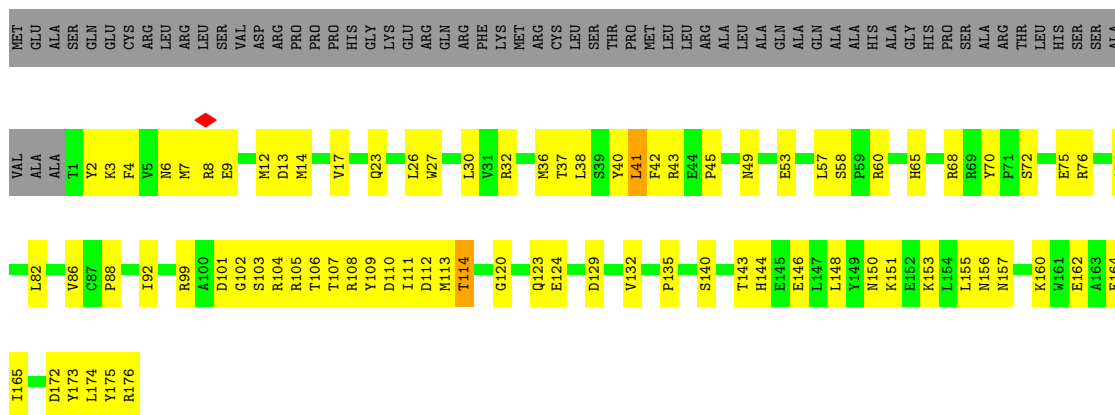
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain 1H: 54% 43%



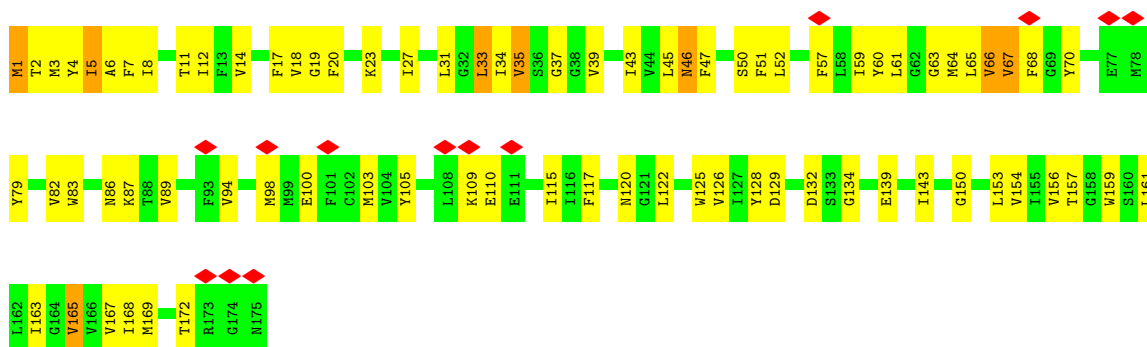
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain 1I: 40% 33% 26%



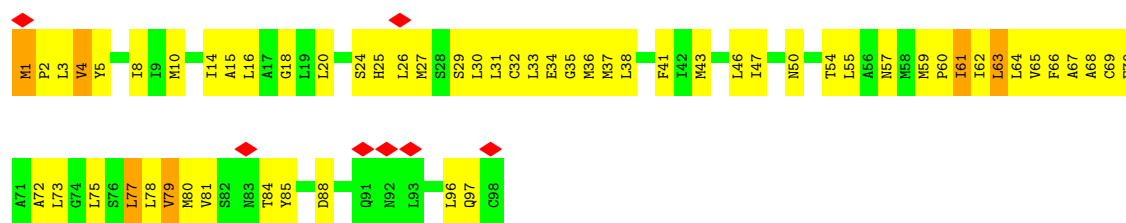
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain 1J: 7% 55% 41% 5%

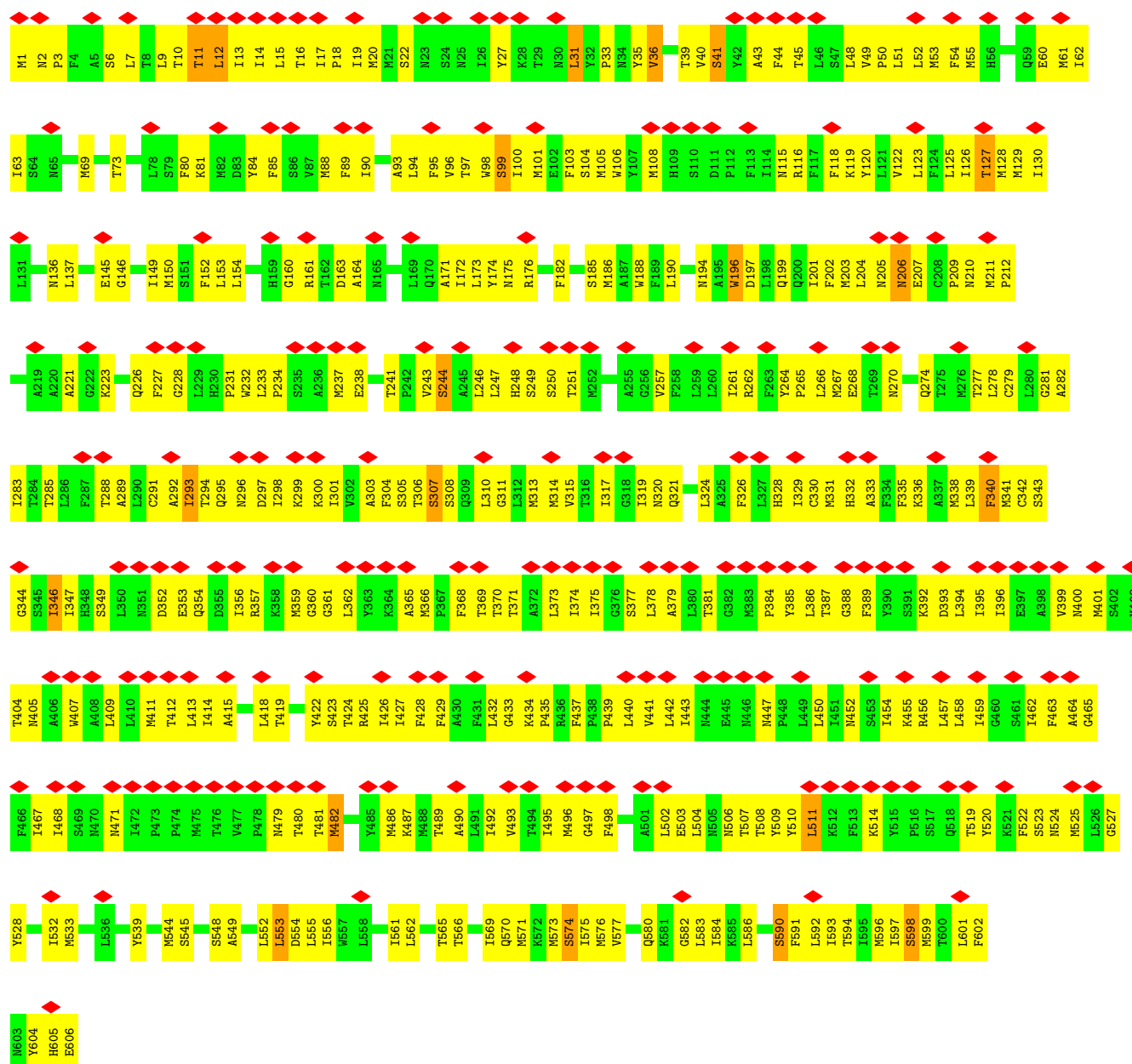


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain 1K: 7% 40% 54% 6%



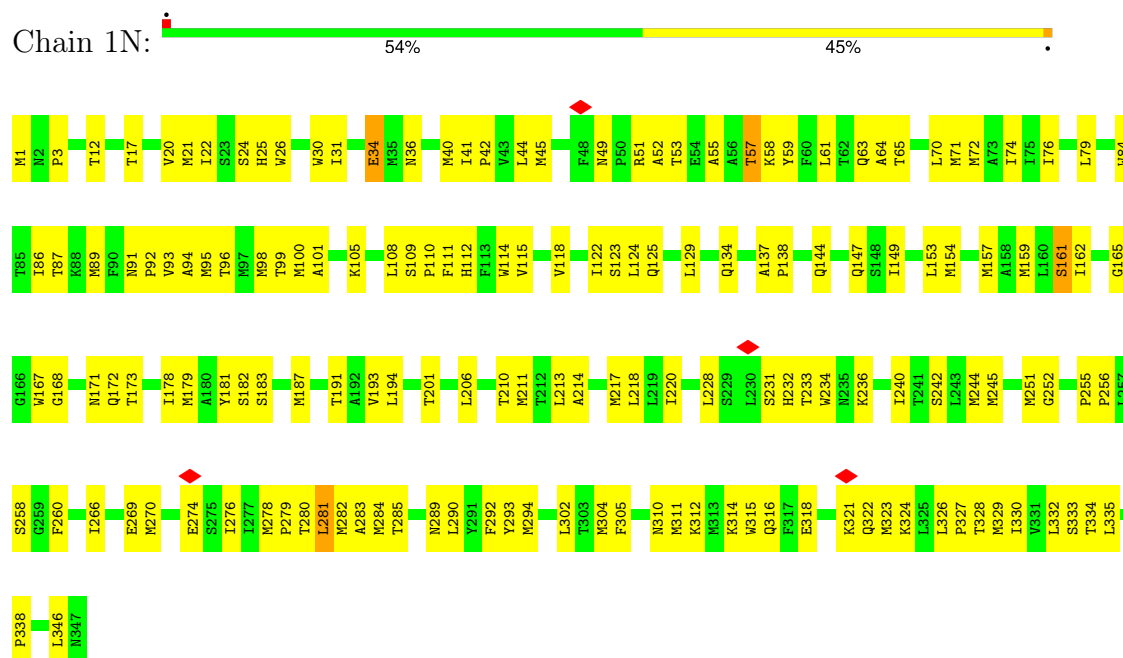
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



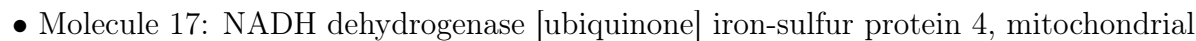
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

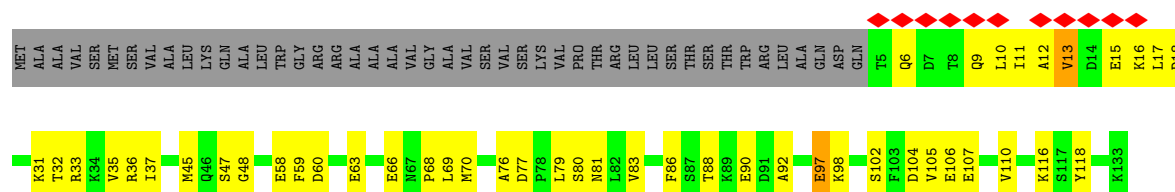


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

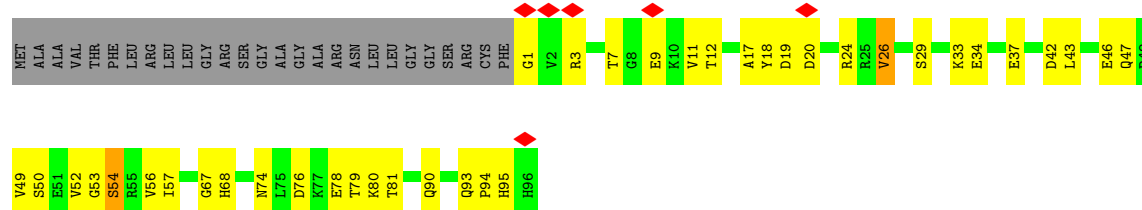


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial





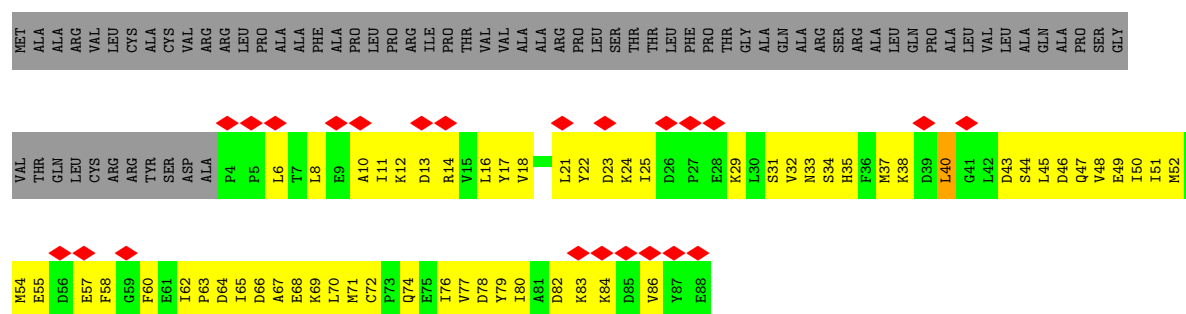
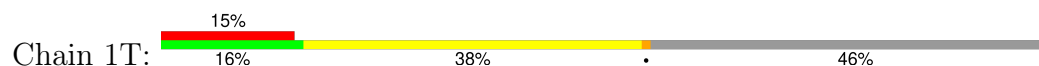
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



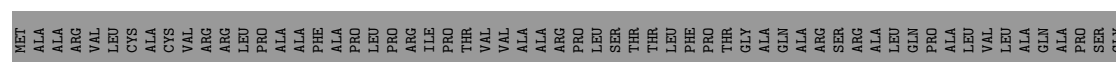
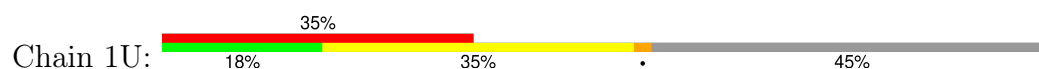
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

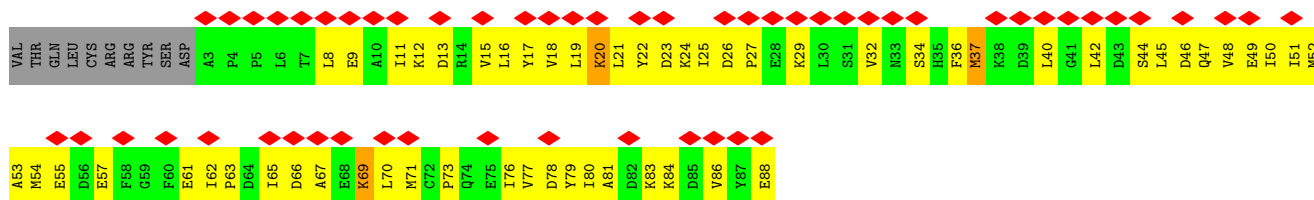


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

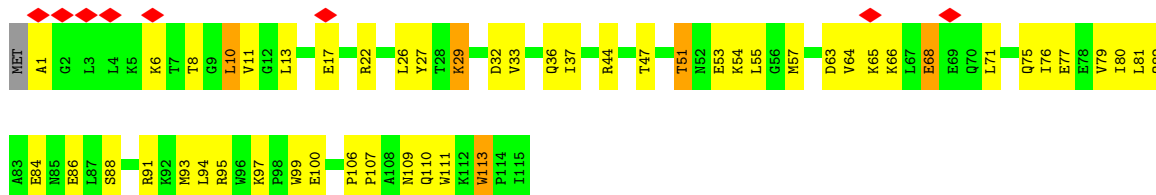


- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

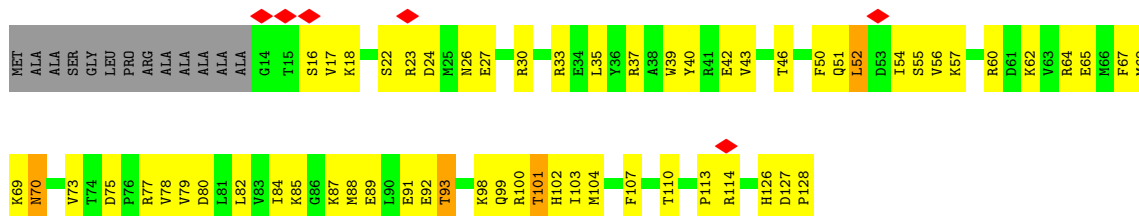
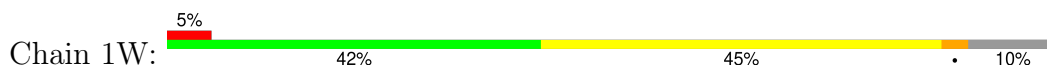




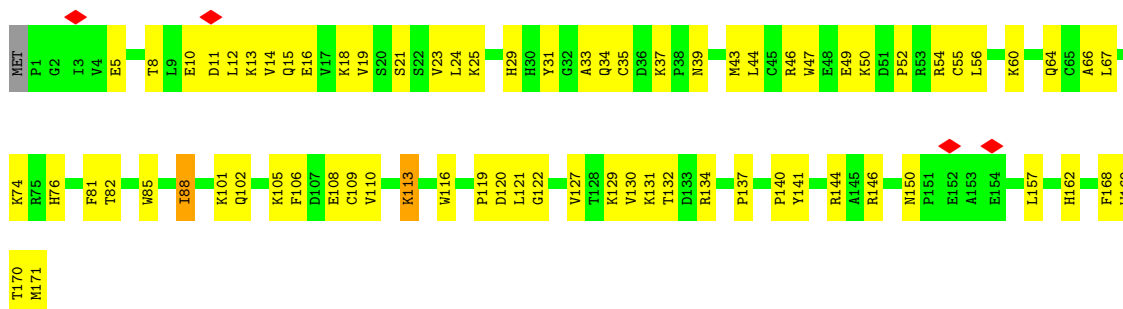
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1



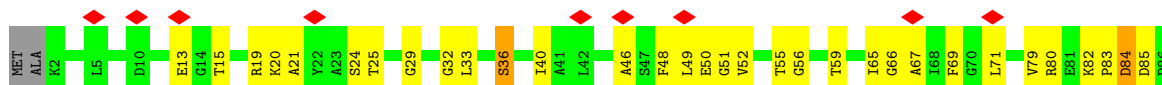
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

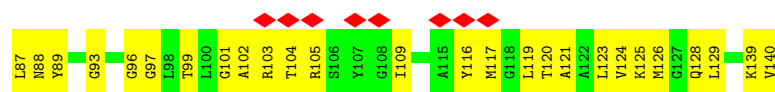


- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

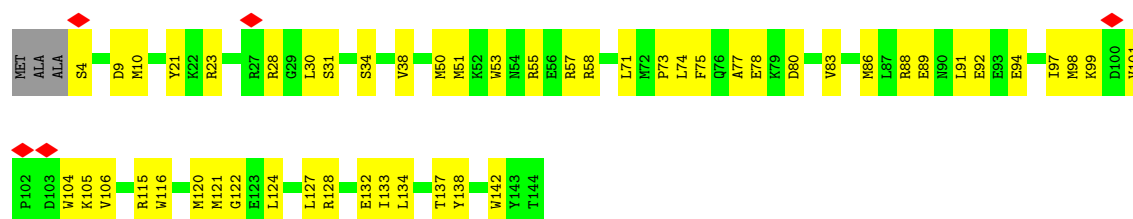


- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11





- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



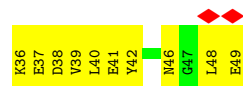
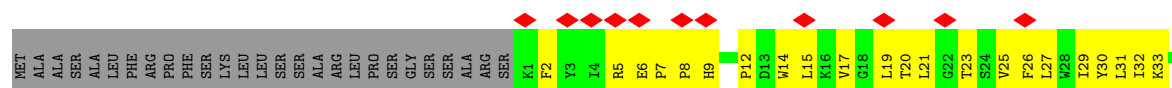
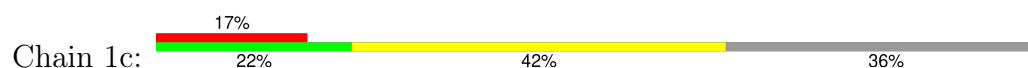
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



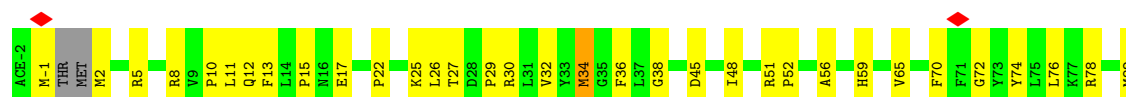
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

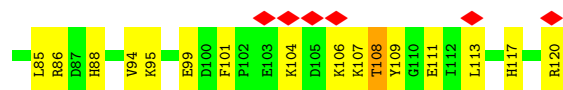


- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

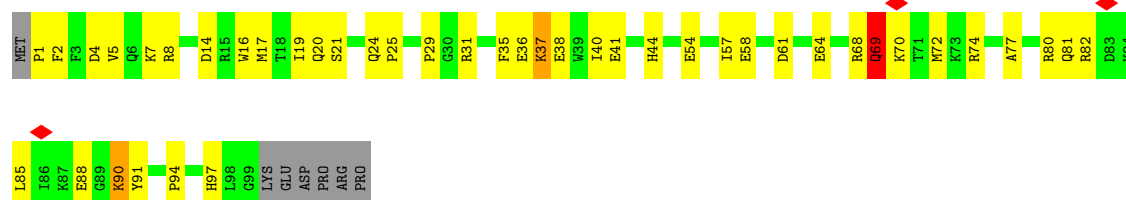


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

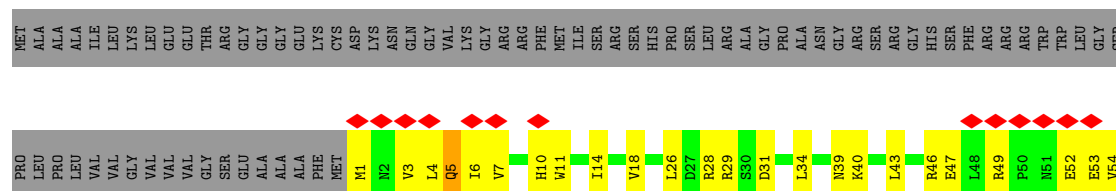




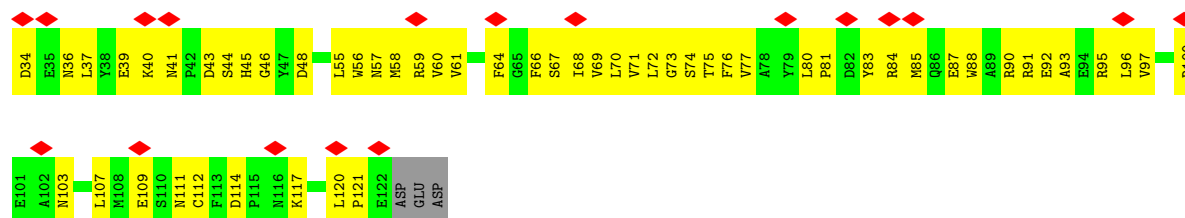
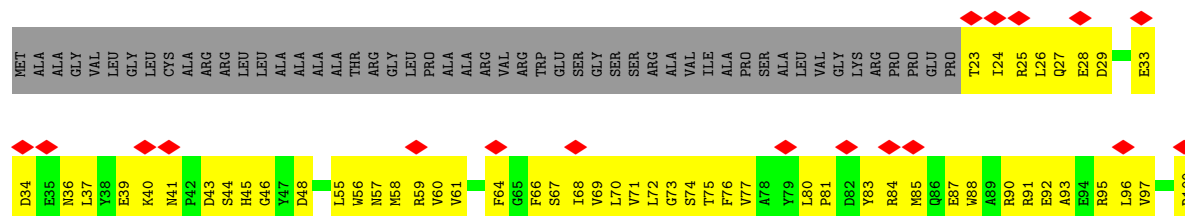
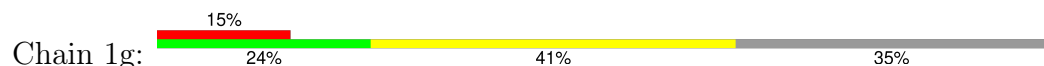
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



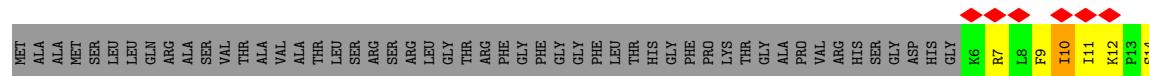
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]

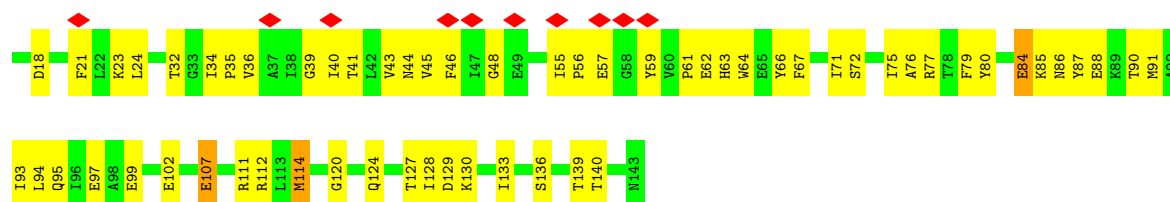


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

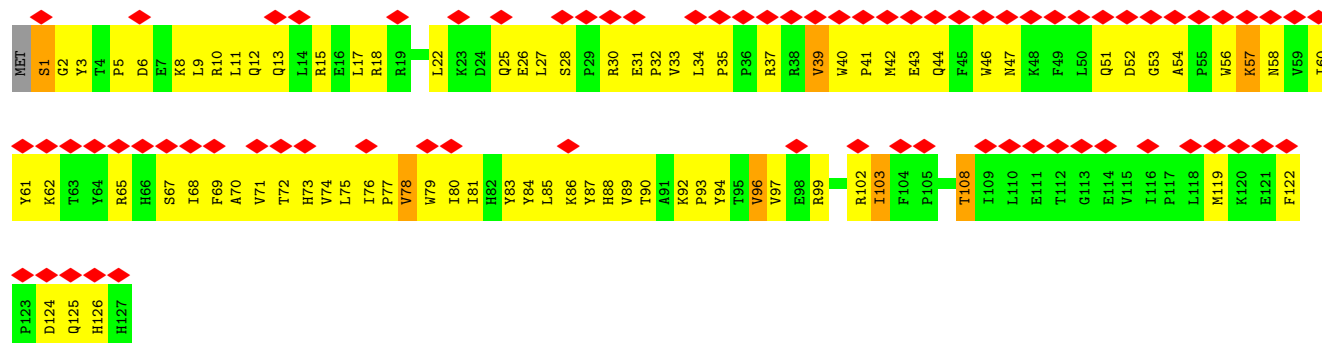


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

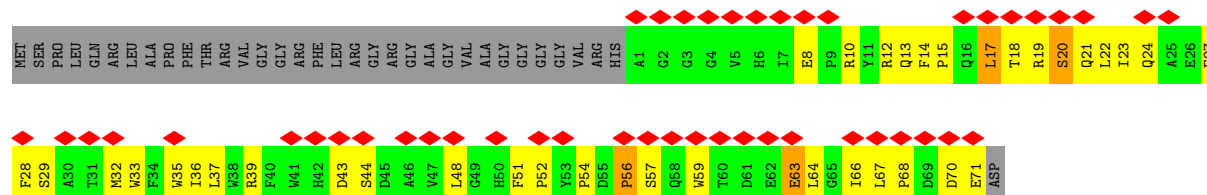




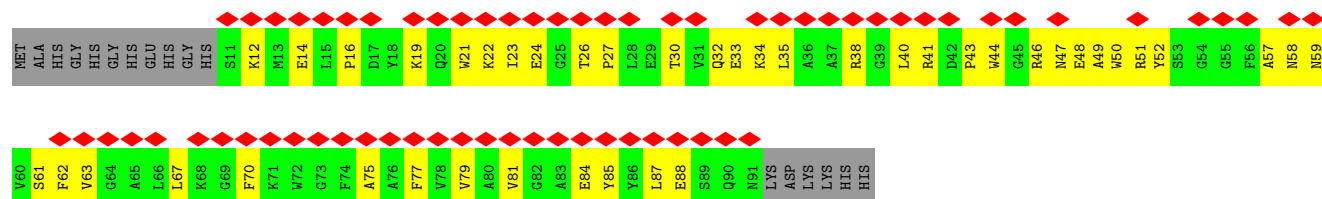
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2

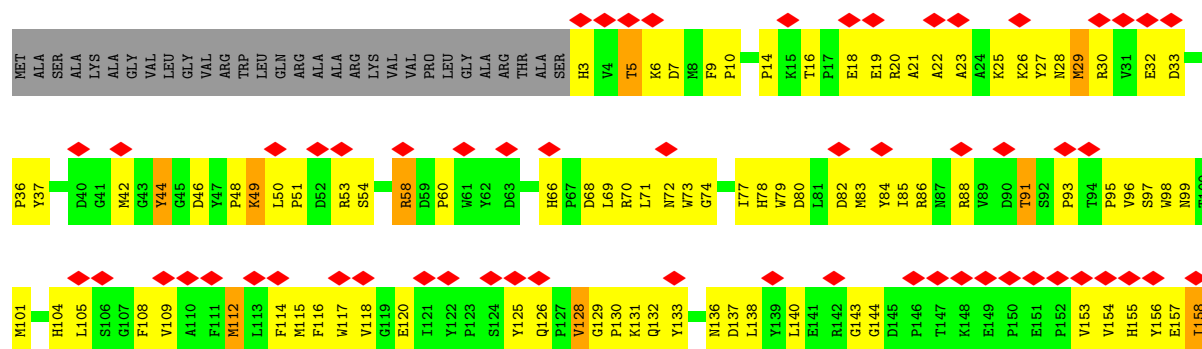


- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

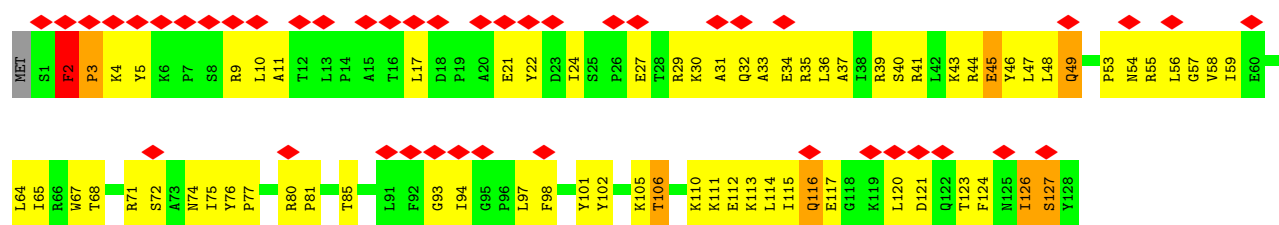
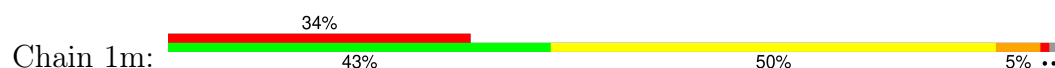


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

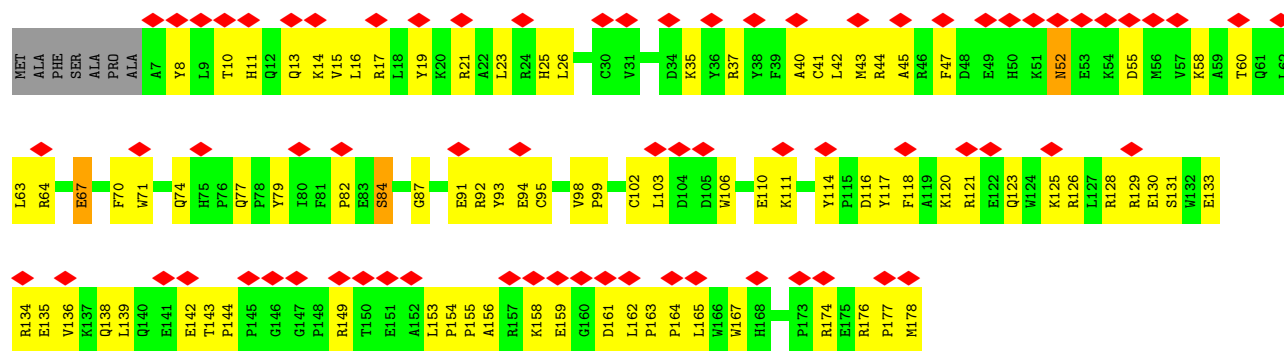
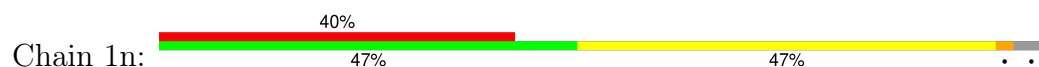




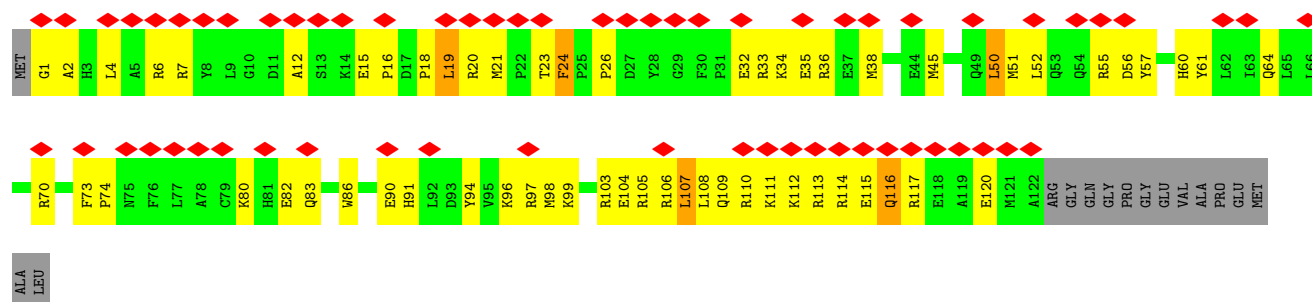
• Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



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



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





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.137	Depositor
Minimum map value	-0.300	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.019	Depositor
Recommended contour level	0.12	Depositor
Map size (Å)	556.0, 556.0, 556.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1A	0.23	0/930	0.55	0/1271
2	1B	0.21	0/1273	0.43	0/1722
3	1C	0.12	0/1791	0.32	0/2439
4	1D	0.16	0/3545	0.38	0/4806
5	1E	0.13	0/1698	0.36	0/2311
6	1F	0.12	0/3401	0.33	0/4595
7	1G	0.12	0/5451	0.33	0/7387
8	1H	0.19	0/2566	0.44	0/3509
9	1I	0.16	0/1443	0.37	0/1952
10	1J	0.18	0/1364	0.45	0/1850
11	1K	0.27	0/751	0.63	0/1018
12	1L	0.22	0/4939	0.58	0/6718
13	1M	0.19	0/3713	0.47	0/5063
14	1N	0.20	0/2765	0.49	0/3758
15	1O	0.17	0/2650	0.43	0/3588
16	1P	0.14	0/2828	0.41	2/3834 (0.1%)
17	1Q	0.18	0/1070	0.45	0/1446
18	1R	0.13	0/755	0.34	0/1018
19	1S	0.19	0/711	0.48	0/956
20	1T	0.30	0/701	0.69	0/946
20	1U	0.23	0/706	0.60	0/954
21	1V	0.19	0/946	0.43	0/1281
22	1W	0.20	0/995	0.51	0/1340
23	1X	0.12	0/1436	0.34	0/1938
24	1Y	0.23	0/1037	0.54	1/1404 (0.1%)
25	1Z	0.16	0/1199	0.36	0/1617
26	1a	0.22	0/577	0.47	1/777 (0.1%)
27	1b	0.16	0/664	0.45	0/912
28	1c	0.30	0/430	0.75	2/581 (0.3%)
29	1d	0.18	0/1024	0.43	0/1383
30	1e	0.20	0/836	0.56	2/1118 (0.2%)
31	1f	0.20	0/499	0.56	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.24	0/858	0.64	0/1165
33	1h	0.18	0/1184	0.48	0/1603
34	1i	0.26	0/1131	0.62	0/1541
35	1j	0.29	0/627	0.76	3/858 (0.3%)
36	1k	0.18	0/668	0.45	0/903
37	1l	0.22	0/1365	0.58	1/1867 (0.1%)
38	1m	0.92	2/1092 (0.2%)	1.15	5/1481 (0.3%)
39	1n	0.17	0/1549	0.43	0/2098
40	1o	0.18	0/1069	0.51	0/1430
41	1p	0.17	0/1481	0.49	0/1997
42	1q	0.25	0/1253	0.56	2/1704 (0.1%)
43	1r	0.17	0/782	0.40	0/1057
44	1s	0.11	0/394	0.31	0/533
All	All	0.22	2/68147 (0.0%)	0.48	19/92402 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	1H	0	1
21	1V	0	1
30	1e	0	2
37	1l	0	1
42	1q	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	1m	3	PRO	CB-CG	22.53	2.62	1.49
38	1m	3	PRO	CG-CD	-17.48	0.91	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	1m	3	PRO	CB-CG-CD	-33.15	0.01	106.10
38	1m	3	PRO	CA-N-CD	-13.43	93.20	112.00
38	1m	3	PRO	N-CA-CB	-11.96	91.83	103.19
38	1m	3	PRO	CA-CB-CG	-11.84	82.01	104.50
42	1q	9	ARG	CA-CB-CG	-9.27	95.56	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	1q	9	ARG	CB-CG-CD	8.78	131.50	111.30
35	1j	56	PRO	CA-N-CD	-8.25	100.44	112.00
16	1P	334	VAL	CA-C-N	7.64	131.34	120.49
16	1P	334	VAL	C-N-CA	7.64	131.34	120.49
30	1e	69	GLN	CA-CB-CG	7.12	128.34	114.10
26	1a	1	MET	CB-CG-SD	6.70	132.81	112.70
35	1j	52	PRO	N-CD-CG	-6.55	93.38	103.20
28	1c	7	PRO	N-CD-CG	-6.40	93.60	103.20
30	1e	69	GLN	N-CA-C	6.31	118.49	110.61
35	1j	52	PRO	CA-N-CD	-5.90	103.74	112.00
28	1c	7	PRO	CA-N-CD	-5.87	103.78	112.00
37	1l	112	MET	CB-CG-SD	5.87	130.30	112.70
24	1Y	128	GLN	CB-CG-CD	5.35	121.69	112.60
38	1m	2	PHE	C-N-CD	5.17	146.19	125.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1H	91	MET	Peptide
21	1V	113	TRP	Peptide
30	1e	69	GLN	Peptide,Sidechain
37	1l	50	LEU	Peptide
42	1q	9	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	63	0
2	1B	1242	0	1249	84	0
3	1C	1740	0	1691	52	0
4	1D	3452	0	3389	146	0
5	1E	1658	0	1662	61	0
6	1F	3325	0	3288	97	0
7	1G	5362	0	5389	150	0
8	1H	2504	0	2601	133	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	1I	1412	0	1366	83	0
10	1J	1339	0	1337	80	0
11	1K	750	0	797	66	0
12	1L	4818	0	4953	372	0
13	1M	3632	0	3836	242	0
14	1N	2712	0	2873	155	0
15	1O	2590	0	2556	116	0
16	1P	2751	0	2776	87	0
17	1Q	1047	0	1042	42	0
18	1R	741	0	704	28	0
19	1S	700	0	719	27	0
20	1T	689	0	687	62	0
20	1U	694	0	691	62	0
21	1V	927	0	972	44	0
22	1W	971	0	975	50	0
23	1X	1398	0	1378	60	0
24	1Y	1016	0	1019	48	0
25	1Z	1168	0	1161	61	0
26	1a	562	0	557	25	0
27	1b	643	0	645	20	0
28	1c	417	0	425	34	0
29	1d	996	0	989	54	0
30	1e	816	0	821	53	0
31	1f	487	0	497	20	0
32	1g	835	0	795	82	0
33	1h	1151	0	1164	73	0
34	1i	1100	0	1106	105	0
35	1j	601	0	546	45	0
36	1k	649	0	626	55	0
37	1l	1310	0	1204	104	0
38	1m	1062	0	1075	83	0
39	1n	1495	0	1434	115	0
40	1o	1045	0	1018	72	0
41	1p	1449	0	1416	103	0
42	1q	1212	0	1173	52	0
43	1r	767	0	791	35	0
44	1s	382	0	351	14	0
45	1B	8	0	0	2	0
45	1F	8	0	0	1	0
45	1G	16	0	0	0	0
45	1I	16	0	0	2	0
46	1B	34	0	42	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
46	1M	35	0	44	4	0
46	1Y	46	0	66	2	0
46	1d	39	0	51	6	0
46	1f	34	0	40	7	0
46	1q	48	0	68	1	0
47	1E	4	0	0	1	0
47	1G	4	0	0	0	0
48	1F	31	0	19	2	0
49	1G	1	0	0	0	0
50	1H	63	0	90	7	0
51	1H	51	0	46	2	0
51	1N	67	0	78	6	0
51	1a	61	0	62	9	0
52	1L	42	0	54	5	0
52	1N	38	0	50	8	0
52	1Y	35	0	42	6	0
52	1f	51	0	78	4	0
53	1O	32	0	12	0	0
54	1O	1	0	0	0	0
55	1P	48	0	26	5	0
56	1R	1	0	0	0	0
57	1W	37	0	0	2	0
57	1n	37	0	0	0	0
58	1l	15	0	27	2	0
All	All	67436	0	67589	3054	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 (3054) 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)
38:1m:3:PRO:CG	38:1m:3:PRO:N	1.86	1.35
38:1m:3:PRO:CD	38:1m:3:PRO:HG2	1.68	1.14
38:1m:3:PRO:CD	38:1m:3:PRO:HG3	1.68	1.11
38:1m:3:PRO:CG	38:1m:3:PRO:HD2	1.56	1.06
38:1m:3:PRO:CG	38:1m:3:PRO:HD3	1.56	1.03
12:1L:161:ARG:HA	39:1n:91:GLU:HG2	1.43	0.96
34:1i:9:LEU:HA	34:1i:12:GLN:HE22	1.31	0.93
11:1K:1:FME:O1	30:1e:69:GLN:HG3	1.68	0.93
22:1W:70:ASN:HD22	22:1W:82:LEU:HD22	1.34	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:135:ARG:HH12	52:1N:401:3PE:H342	1.33	0.92
38:1m:3:PRO:CG	38:1m:3:PRO:CD	0.91	0.91
11:1K:81:VAL:O	11:1K:85:TYR:HB2	1.71	0.90
13:1M:221:VAL:O	13:1M:340:ARG:NH2	2.03	0.90
42:1q:9:ARG:HA	42:1q:12:GLN:OE1	1.72	0.90
41:1p:109:LEU:HD13	41:1p:127:GLU:HB3	1.53	0.90
3:1C:194:PHE:O	17:1Q:81:ASN:ND2	2.06	0.89
20:1T:70:LEU:HB3	20:1T:76:ILE:HD12	1.55	0.88
8:1H:85:MET:HE2	8:1H:108:MET:HB2	1.54	0.88
34:1i:76:ILE:HD12	34:1i:77:PRO:HD3	1.54	0.87
40:1o:113:ARG:HA	40:1o:116:GLN:HE22	1.40	0.87
37:1l:129:GLY:HA2	40:1o:21:MET:HE1	1.57	0.85
2:1B:81:ARG:HE	8:1H:61:LEU:HD11	1.41	0.85
1:1A:67:LEU:HD11	11:1K:65:VAL:HA	1.58	0.85
1:1A:46:SER:HB2	1:1A:49:LEU:HD22	1.59	0.85
33:1h:10:ILE:HG13	33:1h:12:LYS:HD3	1.59	0.84
12:1L:49:VAL:HG12	12:1L:53:MET:HE1	1.60	0.84
2:1B:96:MET:HE2	4:1D:82:LEU:HD12	1.58	0.84
26:1a:57:VAL:HG13	26:1a:59:ARG:HG2	1.59	0.84
13:1M:94:LEU:HD22	13:1M:136:TRP:HH2	1.43	0.83
39:1n:138:GLN:HE22	39:1n:156:ALA:HA	1.43	0.83
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	1.57	0.83
34:1i:3:TYR:CD2	34:1i:8:LYS:HE3	2.14	0.83
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.61	0.82
2:1B:86:MET:HB2	2:1B:107:MET:HE1	1.61	0.82
4:1D:165:THR:HG22	8:1H:32:GLN:HG2	1.62	0.82
41:1p:48:ARG:HD2	41:1p:51:ILE:HD11	1.61	0.82
35:1j:56:PRO:HD2	35:1j:57:SER:H	1.44	0.81
12:1L:171:ALA:HA	12:1L:232:TRP:HB2	1.61	0.81
10:1J:163:ILE:HG12	14:1N:12:THR:HG21	1.63	0.81
7:1G:521:VAL:HG23	7:1G:542:PHE:HB3	1.63	0.81
20:1T:33:ASN:HA	20:1T:74:GLN:NE2	1.96	0.81
7:1G:570:SER:HA	7:1G:583:THR:O	1.79	0.81
12:1L:176:ARG:HG2	12:1L:176:ARG:HH11	1.44	0.80
1:1A:57:LEU:O	1:1A:61:THR:HG23	1.81	0.80
5:1E:120:ILE:HD11	5:1E:169:ILE:HG12	1.63	0.80
14:1N:162:ILE:HD12	14:1N:282:MET:HG2	1.63	0.80
20:1U:25:ILE:HG13	20:1U:40:LEU:HD12	1.64	0.80
8:1H:81:LEU:HD11	8:1H:111:LEU:HD22	1.64	0.80
14:1N:89:MET:HG3	14:1N:95:MET:HB2	1.64	0.80
30:1e:90:LYS:N	30:1e:90:LYS:HE2	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:33:GLU:OE1	32:1g:33:GLU:N	2.16	0.79
1:1A:61:THR:HG21	1:1A:105:GLU:OE2	1.80	0.79
2:1B:69:MET:HB3	2:1B:74:VAL:HG13	1.62	0.79
12:1L:60:GLU:HB2	34:1i:99:ARG:HD3	1.65	0.79
10:1J:172:THR:HA	11:1K:80:MET:HE2	1.65	0.79
12:1L:274:GLN:HE21	12:1L:320:ASN:HD21	1.28	0.78
34:1i:119:MET:HE2	34:1i:122:PHE:HE1	1.47	0.78
12:1L:573:MET:HB2	12:1L:576:MET:HE2	1.66	0.78
34:1i:92:LYS:HA	34:1i:92:LYS:HE3	1.65	0.78
34:1i:41:PRO:HA	34:1i:44:GLN:HG2	1.66	0.78
15:1O:232:GLU:OE2	15:1O:232:GLU:N	2.13	0.78
12:1L:305:SER:OG	12:1L:336:LYS:NZ	2.17	0.78
3:1C:28:TYR:HH	3:1C:67:HIS:HE2	1.32	0.77
15:1O:91:GLY:HA3	15:1O:281:GLU:HG2	1.66	0.77
15:1O:176:VAL:HG13	15:1O:177:PRO:HD3	1.66	0.77
26:1a:67:GLU:OE2	26:1a:67:GLU:N	2.18	0.77
12:1L:172:ILE:O	12:1L:176:ARG:NH1	2.18	0.77
3:1C:68:THR:HA	21:1V:82:GLN:HE21	1.50	0.77
12:1L:203:MET:HE3	41:1p:109:LEU:HG	1.66	0.77
32:1g:81:PRO:HB3	33:1h:67:PHE:CE2	2.20	0.77
12:1L:295:GLN:NE2	12:1L:523:SER:O	2.18	0.76
6:1F:112:ARG:HB3	6:1F:145:GLU:HG3	1.67	0.76
13:1M:216:LEU:HD21	13:1M:236:LEU:HD11	1.67	0.76
11:1K:43:MET:HE2	11:1K:43:MET:HA	1.68	0.76
15:1O:78:SER:H	15:1O:92:ASN:HD21	1.31	0.76
12:1L:295:GLN:HE22	12:1L:524:ASN:HA	1.51	0.76
10:1J:64:MET:HA	10:1J:64:MET:HE3	1.67	0.75
14:1N:44:LEU:HD11	14:1N:59:TYR:HD1	1.50	0.75
16:1P:145:TYR:HH	55:1P:501:NDP:HO2N	1.31	0.75
38:1m:102:TYR:O	38:1m:106:THR:OG1	2.05	0.75
1:1A:10:ASN:HD22	8:1H:83:LEU:HB3	1.50	0.75
14:1N:159:MET:HE1	14:1N:282:MET:HG3	1.68	0.75
1:1A:33:LYS:HE3	2:1B:108:PRO:HA	1.68	0.75
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.68	0.75
17:1Q:90:GLU:OE1	17:1Q:90:GLU:N	2.18	0.75
13:1M:393:ILE:O	13:1M:397:GLY:N	2.17	0.74
13:1M:427:LYS:HG2	32:1g:36:ASN:HD22	1.50	0.74
17:1Q:107:GLU:N	17:1Q:107:GLU:OE2	2.20	0.74
7:1G:556:MET:HA	42:1q:144:TYR:HE2	1.53	0.74
8:1H:85:MET:SD	8:1H:233:MET:HE2	2.27	0.74
9:1I:43:ARG:HH12	43:1r:19:LEU:HD22	1.52	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:312:LYS:NZ	15:1O:72:GLN:O	2.20	0.74
20:1U:12:LYS:HE3	20:1U:16:LEU:HD23	1.69	0.74
9:1I:92:ILE:HG13	9:1I:111:ILE:HG12	1.70	0.74
13:1M:141:GLU:OE1	13:1M:141:GLU:N	2.17	0.74
43:1r:29:GLU:OE2	43:1r:29:GLU:N	2.18	0.74
41:1p:111:ALA:O	41:1p:115:ARG:HG2	1.87	0.74
24:1Y:93:GLY:O	24:1Y:97:GLY:N	2.19	0.73
41:1p:109:LEU:HD21	41:1p:128:LEU:HA	1.70	0.73
6:1F:21:ILE:HG21	6:1F:230:VAL:HG12	1.69	0.73
12:1L:18:PRO:HG3	12:1L:39:THR:HG21	1.69	0.73
7:1G:285:ARG:NH1	7:1G:289:GLY:O	2.21	0.73
14:1N:255:PRO:HG3	14:1N:260:PHE:CG	2.23	0.73
20:1T:52:MET:HE1	22:1W:37:ARG:HA	1.70	0.73
2:1B:139:ILE:HG22	2:1B:140:VAL:HG13	1.70	0.73
39:1n:178:MET:HE2	39:1n:178:MET:H	1.51	0.73
14:1N:159:MET:HA	14:1N:159:MET:HE2	1.70	0.73
37:1l:30:ARG:NH2	38:1m:31:ALA:O	2.22	0.73
20:1T:47:GLN:HA	20:1T:50:ILE:HG12	1.69	0.73
13:1M:334:TYR:O	13:1M:338:HIS:N	2.22	0.73
29:1d:12:GLN:HB3	30:1e:8:ARG:HH21	1.52	0.73
29:1d:34:MET:HE3	29:1d:72:GLY:HA2	1.71	0.73
38:1m:30:LYS:HA	38:1m:30:LYS:HE2	1.70	0.73
12:1L:422:TYR:HA	12:1L:425:ARG:HB2	1.71	0.72
39:1n:103:LEU:HA	39:1n:106:TRP:CD1	2.24	0.72
5:1E:31:ILE:HD12	5:1E:50:VAL:HG22	1.70	0.72
12:1L:173:LEU:HD12	13:1M:405:LEU:HD21	1.70	0.72
12:1L:161:ARG:HG3	39:1n:91:GLU:OE2	1.89	0.72
13:1M:425:ASN:HB2	38:1m:57:GLY:HA2	1.71	0.72
13:1M:453:MET:HE3	13:1M:453:MET:HA	1.72	0.72
51:1H:702:CDL:H722	51:1H:702:CDL:H521	1.70	0.72
22:1W:78:VAL:O	22:1W:82:LEU:HD12	1.89	0.72
3:1C:175:ARG:HD2	16:1P:13:ARG:HD2	1.70	0.72
13:1M:325:MET:HE1	13:1M:441:ILE:HB	1.72	0.72
34:1i:8:LYS:HA	34:1i:8:LYS:HE2	1.70	0.72
6:1F:28:ARG:NH1	44:1s:35:ASN:O	2.22	0.72
28:1c:33:LYS:NZ	28:1c:37:GLU:HB2	2.05	0.72
6:1F:189:GLU:N	6:1F:189:GLU:OE1	2.23	0.71
8:1H:67:SER:O	8:1H:69:SER:N	2.23	0.71
14:1N:129:LEU:HD13	51:1N:402:CDL:H532	1.72	0.71
20:1T:43:ASP:OD1	20:1T:44:SER:N	2.23	0.71
20:1U:36:PHE:HB2	20:1U:71:MET:SD	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:66:PHE:HA	32:1g:70:LEU:HB2	1.72	0.71
16:1P:244:TYR:HB2	16:1P:337:ALA:HB2	1.69	0.71
27:1b:51:ASN:HB3	33:1h:139:THR:HG22	1.70	0.71
40:1o:16:PRO:HB3	40:1o:104:GLU:HG2	1.72	0.71
2:1B:62:MET:HE3	2:1B:156:LEU:HG	1.72	0.71
12:1L:243:VAL:HG13	12:1L:247:LEU:HD13	1.71	0.71
9:1I:9:GLU:N	9:1I:9:GLU:OE2	2.23	0.71
20:1T:38:LYS:HA	20:1T:38:LYS:HE3	1.72	0.71
12:1L:411:MET:N	12:1L:411:MET:SD	2.64	0.71
14:1N:124:LEU:HB3	14:1N:220:ILE:HD11	1.72	0.71
20:1U:21:LEU:HD11	36:1k:47:ASN:HA	1.72	0.71
39:1n:139:LEU:O	39:1n:143:THR:OG1	2.08	0.71
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.73	0.71
9:1I:65:HIS:CD2	45:1I:201:SF4:S3	2.84	0.71
12:1L:506:ASN:HA	12:1L:509:TYR:HD2	1.54	0.71
20:1U:78:ASP:OD1	34:1i:15:ARG:NE	2.23	0.71
12:1L:482:MET:HE1	12:1L:487:LYS:HB2	1.72	0.71
30:1e:88:GLU:HG2	30:1e:90:LYS:HE3	1.73	0.71
39:1n:21:ARG:O	39:1n:25:HIS:ND1	2.24	0.71
18:1R:19:ASP:OD1	18:1R:20:ASP:N	2.23	0.70
20:1U:20:LYS:HE2	20:1U:27:PRO:HG3	1.71	0.70
8:1H:75:PRO:HG3	8:1H:215:TYR:HE2	1.54	0.70
32:1g:85:MET:H	32:1g:85:MET:HE2	1.56	0.70
39:1n:103:LEU:HD23	39:1n:121:ARG:HD3	1.72	0.70
51:1a:101:CDL:HB32	42:1q:6:VAL:HG11	1.73	0.70
1:1A:102:LEU:HD22	8:1H:294:LEU:HD12	1.72	0.70
12:1L:378:LEU:HD13	12:1L:386:LEU:HD22	1.72	0.70
13:1M:108:MET:HB2	13:1M:121:LEU:HG	1.74	0.70
13:1M:312:ALA:O	13:1M:316:MET:HG3	1.91	0.70
18:1R:37:GLU:OE1	18:1R:37:GLU:N	2.23	0.70
29:1d:99:GLU:N	29:1d:99:GLU:OE2	2.25	0.70
2:1B:69:MET:HB3	2:1B:74:VAL:CG1	2.21	0.70
29:1d:-1:MET:HB2	29:1d:2:MET:HG3	1.72	0.70
35:1j:21:GLN:HA	35:1j:24:GLN:OE1	1.91	0.70
23:1X:102:GLN:OE1	23:1X:102:GLN:N	2.25	0.70
24:1Y:126:MET:HA	24:1Y:129:LEU:HG	1.74	0.70
13:1M:129:THR:HG21	13:1M:235:LEU:HD11	1.72	0.70
14:1N:232:HIS:HB3	14:1N:311:MET:HE1	1.74	0.70
21:1V:6:LYS:H	21:1V:6:LYS:HE2	1.55	0.70
6:1F:129:MET:HE1	6:1F:221:THR:HB	1.74	0.69
11:1K:47:ILE:HD13	14:1N:79:LEU:HB2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:90:LYS:HE2	30:1e:90:LYS:H	1.54	0.69
6:1F:365:CYS:HB2	45:1F:502:SF4:S2	2.32	0.69
10:1J:20:PHE:HE1	11:1K:32:CYS:HA	1.57	0.69
32:1g:83:TYR:CZ	32:1g:84:ARG:HD3	2.26	0.69
7:1G:349:PHE:HB3	7:1G:509:PRO:HB2	1.75	0.69
7:1G:357:ASP:OD2	19:1S:44:LYS:NZ	2.25	0.69
22:1W:114:ARG:HA	22:1W:114:ARG:NH1	2.07	0.69
31:1f:10:HIS:HB3	52:1f:102:3PE:H3E1	1.73	0.69
40:1o:20:ARG:HG3	40:1o:23:THR:HG22	1.73	0.69
5:1E:145:LEU:HD12	5:1E:153:MET:HE1	1.73	0.69
7:1G:285:ARG:HD2	42:1q:145:LYS:HD3	1.74	0.69
12:1L:480:THR:O	12:1L:482:MET:HG3	1.92	0.69
14:1N:63:GLN:HE22	14:1N:105:LYS:HA	1.56	0.69
29:1d:5:ARG:HB2	29:1d:8:ARG:HD2	1.74	0.69
32:1g:39:GLU:N	32:1g:39:GLU:OE2	2.23	0.69
2:1B:79:SER:OG	2:1B:82:GLN:OE1	2.09	0.69
12:1L:313:MET:HE1	12:1L:328:HIS:HB3	1.75	0.69
38:1m:22:TYR:HD2	39:1n:64:ARG:HG2	1.55	0.69
41:1p:59:ARG:NH1	41:1p:59:ARG:O	2.26	0.69
15:1O:43:ALA:HB2	15:1O:123:VAL:HG21	1.72	0.69
20:1U:52:MET:HE1	39:1n:23:LEU:HB3	1.74	0.69
28:1c:19:LEU:O	28:1c:23:THR:HG23	1.93	0.69
32:1g:93:ALA:O	32:1g:97:VAL:HG23	1.93	0.69
30:1e:70:LYS:HE2	30:1e:70:LYS:HA	1.75	0.69
1:1A:115:GLU:HG3	4:1D:72:MET:SD	2.33	0.68
7:1G:226:GLU:OE1	17:1Q:36:ARG:NH2	2.26	0.68
4:1D:151:ILE:HG12	4:1D:170:MET:HE2	1.75	0.68
36:1k:84:GLU:HA	36:1k:87:LEU:HG	1.73	0.68
42:1q:49:TYR:CE1	42:1q:63:ILE:HG12	2.28	0.68
12:1L:129:MET:HA	12:1L:129:MET:HE3	1.75	0.68
28:1c:23:THR:O	28:1c:27:LEU:HD23	1.94	0.68
13:1M:16:TRP:NE1	13:1M:97:THR:OG1	2.27	0.68
14:1N:25:HIS:HE2	30:1e:17:MET:HG2	1.58	0.68
24:1Y:123:LEU:HB2	52:1Y:202:3PE:H292	1.75	0.68
4:1D:72:MET:HE3	4:1D:408:GLY:O	1.93	0.68
12:1L:199:GLN:O	12:1L:203:MET:HB3	1.92	0.68
12:1L:504:LEU:O	12:1L:507:THR:OG1	2.09	0.68
13:1M:406:TYR:HA	13:1M:409:TYR:HB3	1.76	0.68
16:1P:203:GLN:HG2	16:1P:231:VAL:HB	1.76	0.68
42:1q:49:TYR:HE1	42:1q:63:ILE:HG12	1.57	0.68
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:292:ALA:HB2	12:1L:304:PHE:HB2	1.76	0.68
37:1l:80:ASP:HB3	37:1l:83:MET:HB3	1.75	0.68
12:1L:561:ILE:HD12	46:1Y:201:PC1:H2A2	1.76	0.68
15:1O:42:ILE:HG22	15:1O:235:VAL:HG12	1.76	0.68
1:1A:8:LEU:O	1:1A:12:THR:HG23	1.94	0.67
7:1G:298:ASP:OD1	7:1G:302:ARG:NH1	2.27	0.67
8:1H:65:THR:O	8:1H:124:ASN:ND2	2.24	0.67
20:1U:23:ASP:OD2	36:1k:46:ARG:NH2	2.27	0.67
22:1W:80:ASP:O	22:1W:84:ILE:HG12	1.94	0.67
6:1F:309:LYS:NZ	6:1F:313:GLU:OE2	2.27	0.67
7:1G:54:MET:HE1	7:1G:94:MET:HB2	1.74	0.67
8:1H:130:ILE:O	8:1H:134:ARG:HG3	1.94	0.67
11:1K:55:LEU:HG	30:1e:25:PRO:HD3	1.75	0.67
25:1Z:99:LYS:HE2	25:1Z:99:LYS:HA	1.74	0.67
29:1d:12:GLN:HE22	29:1d:15:PRO:HB3	1.59	0.67
29:1d:104:LYS:HZ1	29:1d:107:LYS:HG2	1.60	0.67
13:1M:225:ILE:HD13	13:1M:331:ASN:HB2	1.74	0.67
43:1r:104:GLU:N	43:1r:104:GLU:OE2	2.27	0.67
35:1j:56:PRO:HD2	35:1j:57:SER:N	2.09	0.67
12:1L:12:LEU:HD23	12:1L:129:MET:HB3	1.77	0.67
12:1L:104:SER:O	12:1L:108:MET:N	2.26	0.67
13:1M:225:ILE:O	13:1M:229:MET:HG2	1.95	0.67
40:1o:109:GLN:HB2	40:1o:113:ARG:HH21	1.59	0.67
14:1N:44:LEU:HB3	14:1N:122:ILE:HG21	1.76	0.67
21:1V:37:ILE:O	21:1V:44:ARG:NH1	2.27	0.67
34:1i:53:GLY:H	34:1i:57:LYS:HE3	1.58	0.67
8:1H:4:ILE:HD12	8:1H:4:ILE:H	1.60	0.67
12:1L:63:ILE:HG22	34:1i:96:VAL:HG12	1.77	0.67
29:1d:106:LYS:HD2	41:1p:77:GLU:HB3	1.76	0.67
4:1D:409:HIS:HB3	4:1D:413:ASP:HB2	1.75	0.66
21:1V:6:LYS:HE2	21:1V:6:LYS:N	2.10	0.66
2:1B:54:CYS:HB3	4:1D:108:TYR:HB3	1.77	0.66
12:1L:264:TYR:CD1	12:1L:265:PRO:HD3	2.30	0.66
13:1M:17:MET:HE3	31:1f:11:TRP:CZ2	2.30	0.66
24:1Y:13:GLU:N	24:1Y:13:GLU:OE1	2.28	0.66
6:1F:300:GLY:HA2	6:1F:333:ALA:H	1.59	0.66
13:1M:222:GLU:N	13:1M:222:GLU:OE2	2.27	0.66
20:1U:26:ASP:OD1	20:1U:29:LYS:HG2	1.96	0.66
23:1X:82:THR:HA	23:1X:85:TRP:CD1	2.30	0.66
41:1p:29:VAL:O	41:1p:33:THR:HG23	1.95	0.66
24:1Y:109:ILE:HD13	46:1Y:201:PC1:H321	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:124:VAL:HG21	52:1Y:202:3PE:H342	1.77	0.66
14:1N:244:MET:HE2	14:1N:244:MET:HA	1.76	0.66
15:1O:97:GLN:HG2	15:1O:135:LEU:HD23	1.76	0.66
27:1b:56:LEU:HD11	27:1b:65:VAL:HG11	1.76	0.66
15:1O:61:SER:HA	15:1O:66:GLY:HA2	1.77	0.66
5:1E:107:PRO:HG3	6:1F:335:ILE:HD13	1.78	0.66
34:1i:76:ILE:HD12	34:1i:77:PRO:CD	2.25	0.66
42:1q:34:ARG:HH21	42:1q:54:GLN:HG3	1.60	0.66
4:1D:227:GLU:OE2	9:1I:32:ARG:NH2	2.29	0.66
12:1L:182:PHE:O	12:1L:186:MET:HG3	1.96	0.66
4:1D:4:TRP:HE3	13:1M:140:THR:HA	1.61	0.65
39:1n:138:GLN:NE2	39:1n:156:ALA:HA	2.11	0.65
35:1j:10:ARG:HE	35:1j:15:PRO:HA	1.61	0.65
37:1l:18:GLU:OE1	37:1l:18:GLU:N	2.26	0.65
7:1G:365:ASN:ND2	7:1G:490:MET:O	2.30	0.65
16:1P:264:ARG:NH1	16:1P:285:GLU:OE2	2.27	0.65
24:1Y:79:VAL:HG12	24:1Y:80:ARG:HE	1.61	0.65
10:1J:4:TYR:O	10:1J:6:ALA:N	2.30	0.65
13:1M:237:LYS:HD2	13:1M:316:MET:HB3	1.78	0.65
29:1d:2:MET:HE1	29:1d:85:LEU:HB3	1.78	0.65
36:1k:48:GLU:HB3	36:1k:51:ARG:HD2	1.77	0.65
41:1p:30:THR:O	41:1p:34:LYS:HD2	1.97	0.65
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.14	0.65
8:1H:311:THR:HB	25:1Z:51:MET:HE2	1.78	0.65
14:1N:114:TRP:O	14:1N:118:VAL:HG22	1.97	0.65
16:1P:198:LYS:HA	16:1P:237:LEU:HD11	1.77	0.65
2:1B:166:LYS:C	2:1B:166:LYS:HD3	2.22	0.65
12:1L:93:ALA:O	12:1L:97:THR:HG23	1.96	0.65
20:1T:23:ASP:OD1	20:1T:24:LYS:N	2.29	0.65
21:1V:8:THR:OG1	21:1V:13:LEU:O	2.15	0.65
25:1Z:120:MET:HE2	30:1e:68:ARG:HD3	1.79	0.65
14:1N:318:GLU:OE2	14:1N:318:GLU:N	2.17	0.65
36:1k:46:ARG:HE	36:1k:46:ARG:H	1.41	0.65
3:1C:175:ARG:NH1	3:1C:186:GLU:OE2	2.29	0.65
6:1F:20:ARG:NH1	6:1F:269:GLU:O	2.30	0.65
34:1i:5:PRO:HA	34:1i:8:LYS:HG2	1.79	0.65
12:1L:55:MET:HA	12:1L:55:MET:HE3	1.78	0.64
12:1L:313:MET:HE3	12:1L:329:ILE:HG23	1.77	0.64
12:1L:343:SER:O	12:1L:347:ILE:HG12	1.97	0.64
20:1T:18:VAL:HG11	20:1T:57:GLU:HG2	1.80	0.64
33:1h:36:VAL:O	33:1h:40:ILE:HG13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:117:TYR:HA	39:1n:120:LYS:HD2	1.80	0.64
42:1q:58:ARG:HD3	43:1r:1:ALA:HB2	1.79	0.64
9:1I:75:GLU:O	9:1I:105:ARG:NH1	2.29	0.64
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.32	0.64
12:1L:89:PHE:HB2	12:1L:326:PHE:HZ	1.62	0.64
14:1N:323:MET:HE2	14:1N:323:MET:HA	1.79	0.64
32:1g:88:TRP:HD1	41:1p:65:ARG:HB3	1.62	0.64
39:1n:126:ARG:HH22	39:1n:130:GLU:HB3	1.61	0.64
41:1p:27:ASN:O	41:1p:30:THR:OG1	2.15	0.64
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	1.80	0.64
33:1h:44:ASN:O	41:1p:55:HIS:NE2	2.28	0.64
20:1T:54:MET:O	20:1T:58:PHE:HB2	1.98	0.64
34:1i:52:ASP:HB3	34:1i:57:LYS:HD3	1.78	0.64
34:1i:76:ILE:O	34:1i:80:ILE:HG12	1.97	0.64
41:1p:159:LYS:O	41:1p:163:LEU:HD22	1.96	0.64
8:1H:236:ALA:HA	8:1H:263:THR:HG22	1.79	0.64
38:1m:32:GLN:HE21	39:1n:8:TYR:HA	1.62	0.64
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.31	0.64
19:1S:87:THR:O	19:1S:91:GLU:HG2	1.97	0.64
24:1Y:99:THR:O	24:1Y:103:ARG:N	2.31	0.64
29:1d:78:ARG:HH12	46:1d:201:PC1:H222	1.62	0.64
30:1e:88:GLU:HG2	30:1e:90:LYS:CE	2.28	0.64
12:1L:452:ASN:OD1	12:1L:455:LYS:NZ	2.31	0.64
16:1P:139:ILE:H	16:1P:139:ILE:HD12	1.63	0.64
35:1j:39:ARG:NH2	35:1j:43:ASP:OD2	2.31	0.64
12:1L:400:ASN:O	37:1l:126:GLN:NE2	2.31	0.64
13:1M:96:ILE:O	13:1M:100:ILE:HD12	1.97	0.64
37:1l:42:MET:HA	37:1l:42:MET:HE3	1.77	0.64
14:1N:206:LEU:O	14:1N:210:THR:HG23	1.98	0.64
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.80	0.64
2:1B:62:MET:HG2	2:1B:156:LEU:HD23	1.78	0.64
7:1G:276:ARG:NH1	7:1G:680:ALA:O	2.31	0.64
9:1I:156:ASN:ND2	18:1R:34:GLU:OE1	2.31	0.64
12:1L:433:GLY:O	36:1k:59:ASN:ND2	2.26	0.64
52:1L:701:3PE:O12	52:1L:701:3PE:N	2.30	0.64
15:1O:30:ASN:O	15:1O:35:LYS:NZ	2.30	0.64
24:1Y:13:GLU:HA	24:1Y:20:LYS:HE3	1.79	0.64
20:1U:50:ILE:HG22	36:1k:44:TRP:HZ2	1.63	0.63
21:1V:53:GLU:O	21:1V:57:MET:HG3	1.97	0.63
37:1l:30:ARG:HG3	37:1l:32:GLU:H	1.62	0.63
6:1F:94:VAL:HG22	6:1F:135:TYR:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.79	0.63
8:1H:142:TYR:OH	8:1H:285:LEU:HB2	1.98	0.63
12:1L:123:LEU:HB2	12:1L:150:MET:HE2	1.81	0.63
12:1L:411:MET:HA	12:1L:414:ILE:HG22	1.79	0.63
13:1M:459:TYR:O	32:1g:84:ARG:NH2	2.32	0.63
8:1H:91:MET:HE1	26:1a:19:PRO:HB2	1.79	0.63
13:1M:225:ILE:HD13	13:1M:331:ASN:CB	2.29	0.63
35:1j:35:TRP:CZ3	35:1j:39:ARG:HG3	2.34	0.63
4:1D:107:ASP:OD2	4:1D:110:SER:OG	2.17	0.63
32:1g:91:ARG:HH22	41:1p:64:HIS:HA	1.62	0.63
38:1m:33:ALA:O	39:1n:149:ARG:NH2	2.29	0.63
1:1A:40:GLY:HA2	2:1B:103:VAL:HG23	1.80	0.63
3:1C:68:THR:HG23	21:1V:86:GLU:HG3	1.81	0.63
8:1H:28:LEU:O	8:1H:32:GLN:HG3	1.98	0.63
14:1N:328:THR:O	14:1N:332:LEU:HD12	1.98	0.63
20:1U:81:ALA:HA	20:1U:86:VAL:HB	1.80	0.63
46:1f:101:PC1:H361	32:1g:76:PHE:CE2	2.34	0.63
33:1h:114:MET:SD	33:1h:120:GLY:HA3	2.39	0.63
7:1G:140:LYS:O	7:1G:148:THR:OG1	2.13	0.63
12:1L:128:MET:HE3	12:1L:251:THR:HB	1.79	0.63
25:1Z:89:GLU:HB3	30:1e:97:HIS:HE1	1.63	0.63
29:1d:86:ARG:NH1	33:1h:107:GLU:OE2	2.32	0.63
34:1i:10:ARG:HD3	39:1n:153:LEU:HG	1.80	0.63
3:1C:183:VAL:O	22:1W:101:THR:OG1	2.13	0.63
7:1G:632:ARG:HG2	7:1G:632:ARG:HH11	1.64	0.63
10:1J:60:TYR:HE1	11:1K:38:LEU:HB2	1.63	0.63
37:1l:97:SER:HA	38:1m:5:TYR:CD1	2.33	0.63
5:1E:111:ARG:HB2	5:1E:152:PRO:HD3	1.81	0.63
8:1H:233:MET:HE1	8:1H:234:MET:SD	2.39	0.63
23:1X:144:ARG:NH2	30:1e:54:GLU:O	2.32	0.63
4:1D:10:TRP:O	4:1D:13:GLN:NE2	2.32	0.62
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.81	0.62
25:1Z:94:GLU:HA	25:1Z:97:ILE:HG22	1.80	0.62
6:1F:254:LYS:HB2	6:1F:272:MET:HE2	1.81	0.62
8:1H:135:ALA:O	8:1H:139:THR:HG23	1.98	0.62
11:1K:26:LEU:HB3	11:1K:78:LEU:HD12	1.81	0.62
12:1L:51:LEU:HD21	12:1L:88:MET:HB2	1.81	0.62
37:1l:73:TRP:CD1	38:1m:46:TYR:HB2	2.34	0.62
38:1m:22:TYR:CD2	39:1n:64:ARG:HG2	2.34	0.62
7:1G:252:PRO:HG3	7:1G:263:ILE:HG12	1.81	0.62
12:1L:570:GLN:OE1	14:1N:167:TRP:NE1	2.25	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:22:MET:HE1	52:1f:102:3PE:H252	1.81	0.62
17:1Q:15:GLU:N	17:1Q:15:GLU:OE1	2.31	0.62
22:1W:68:MET:HE2	22:1W:68:MET:HA	1.81	0.62
23:1X:24:LEU:HB3	25:1Z:71:LEU:HD21	1.80	0.62
5:1E:194:GLU:OE2	6:1F:28:ARG:NH2	2.27	0.62
8:1H:104:PHE:O	8:1H:108:MET:HG2	1.98	0.62
37:1l:93:PRO:HA	38:1m:11:ALA:HB1	1.80	0.62
12:1L:349:SER:HB2	12:1L:443:ILE:HA	1.81	0.62
20:1T:32:VAL:O	20:1T:74:GLN:NE2	2.32	0.62
35:1j:33:TRP:HE3	35:1j:36:ILE:HD11	1.63	0.62
4:1D:94:LYS:HB3	4:1D:98:GLN:HB3	1.82	0.62
13:1M:348:LEU:H	13:1M:415:GLN:HA	1.64	0.62
23:1X:146:ARG:NH1	30:1e:41:GLU:OE1	2.32	0.62
8:1H:181:LEU:HG	8:1H:300:LEU:HD13	1.82	0.62
12:1L:90:ILE:O	12:1L:94:LEU:HG	1.99	0.62
13:1M:78:MET:HA	13:1M:81:GLN:HE22	1.63	0.62
13:1M:305:THR:HG22	13:1M:308:SER:H	1.65	0.62
15:1O:320:LYS:HA	28:1c:12:PRO:HB3	1.81	0.62
37:1l:140:LEU:HA	37:1l:144:GLY:HA3	1.82	0.62
7:1G:352:ALA:HB1	7:1G:652:VAL:HG21	1.82	0.62
12:1L:119:LYS:O	12:1L:123:LEU:HD22	1.99	0.62
37:1l:131:LYS:NZ	40:1o:56:ASP:HB2	2.15	0.62
10:1J:110:GLU:O	30:1e:80:ARG:NH2	2.33	0.62
12:1L:80:PHE:HE2	12:1L:130:ILE:HG22	1.64	0.62
13:1M:294:MET:HE2	13:1M:294:MET:HA	1.82	0.62
20:1T:72:CYS:SG	20:1T:74:GLN:NE2	2.72	0.62
7:1G:313:ASN:OD1	7:1G:517:ASN:ND2	2.33	0.62
11:1K:1:FME:CN	30:1e:69:GLN:HG3	2.30	0.62
20:1U:11:ILE:HG12	20:1U:80:ILE:HG21	1.81	0.62
22:1W:56:VAL:O	22:1W:60:ARG:HG3	1.99	0.62
23:1X:129:LYS:HB2	27:1b:58:ASP:HB2	1.81	0.62
24:1Y:126:MET:SD	24:1Y:129:LEU:HD12	2.40	0.62
39:1n:131:SER:HB3	39:1n:162:LEU:HD23	1.82	0.62
12:1L:161:ARG:NH2	39:1n:87:GLY:O	2.32	0.61
27:1b:73:GLN:N	27:1b:73:GLN:OE1	2.30	0.61
12:1L:10:THR:HG21	34:1i:78:VAL:HG13	1.82	0.61
31:1f:57:LYS:HE2	31:1f:57:LYS:HA	1.82	0.61
41:1p:27:ASN:HD21	41:1p:30:THR:HG23	1.65	0.61
42:1q:6:VAL:HA	42:1q:9:ARG:HD2	1.80	0.61
6:1F:114:ASP:HB3	6:1F:117:LYS:HD2	1.81	0.61
7:1G:477:ILE:HD11	7:1G:489:VAL:HG11	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:195:ARG:HH22	8:1H:271:LEU:HD13	1.65	0.61
12:1L:161:ARG:HG2	12:1L:164:ALA:H	1.63	0.61
12:1L:319:ILE:O	12:1L:321:GLN:NE2	2.32	0.61
14:1N:87:THR:O	14:1N:147:GLN:NE2	2.33	0.61
15:1O:133:VAL:HG11	15:1O:206:TYR:CD2	2.36	0.61
20:1T:47:GLN:NE2	20:1T:67:ALA:O	2.34	0.61
24:1Y:46:ALA:N	24:1Y:50:GLU:OE2	2.33	0.61
33:1h:34:ILE:HG12	33:1h:35:PRO:HD3	1.80	0.61
40:1o:50:LEU:O	40:1o:55:ARG:NE	2.29	0.61
2:1B:47:PRO:HD2	2:1B:75:VAL:O	1.99	0.61
5:1E:22:ASP:O	5:1E:57:GLN:NE2	2.33	0.61
8:1H:276:SER:HB3	9:1I:37:THR:HG21	1.81	0.61
12:1L:36:VAL:HG11	12:1L:118:PHE:HB3	1.80	0.61
12:1L:294:THR:HG22	52:1L:701:3PE:H222	1.83	0.61
15:1O:151:HIS:HD2	15:1O:277:VAL:HG21	1.65	0.61
23:1X:29:HIS:HB3	23:1X:119:PRO:HD2	1.82	0.61
25:1Z:104:TRP:HZ2	30:1e:74:ARG:HG3	1.65	0.61
32:1g:43:ASP:N	32:1g:43:ASP:OD1	2.32	0.61
32:1g:68:ILE:HD12	32:1g:69:VAL:HG23	1.82	0.61
36:1k:22:LYS:HB3	36:1k:24:GLU:CD	2.25	0.61
7:1G:372:GLU:O	7:1G:402:ASN:ND2	2.34	0.61
9:1I:164:GLU:OE2	42:1q:88:ARG:N	2.33	0.61
16:1P:248:VAL:O	16:1P:322:ARG:NH1	2.34	0.61
29:1d:25:LYS:HG2	29:1d:27:THR:H	1.64	0.61
34:1i:54:ALA:HB3	34:1i:57:LYS:HG2	1.83	0.61
37:1l:16:THR:OG1	37:1l:18:GLU:OE1	2.10	0.61
41:1p:14:ARG:NH2	41:1p:15:ARG:O	2.22	0.61
5:1E:74:GLN:OE1	5:1E:74:GLN:N	2.33	0.61
11:1K:73:LEU:HD11	14:1N:41:ILE:HG13	1.81	0.61
15:1O:169:VAL:HB	15:1O:214:MET:HE2	1.83	0.61
40:1o:116:GLN:O	40:1o:120:GLU:HG2	1.99	0.61
12:1L:592:LEU:HD13	12:1L:596:MET:HE1	1.83	0.61
23:1X:49:GLU:HG3	23:1X:134:ARG:HH21	1.65	0.61
31:1f:53:GLU:N	31:1f:53:GLU:OE2	2.33	0.61
37:1l:5:THR:OG1	37:1l:6:LYS:N	2.33	0.61
7:1G:337:ARG:NH1	7:1G:337:ARG:HB2	2.16	0.61
11:1K:61:ILE:HG22	11:1K:62:ILE:HD13	1.83	0.61
13:1M:207:MET:HG3	13:1M:298:ILE:HG12	1.82	0.61
13:1M:346:ARG:NE	37:1l:68:ASP:OD2	2.34	0.61
14:1N:57:THR:HG22	14:1N:61:LEU:HD11	1.83	0.61
20:1U:19:LEU:HD12	20:1U:20:LYS:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:36:SER:O	24:1Y:40:ILE:HG13	2.00	0.61
28:1c:49:GLU:OE1	28:1c:49:GLU:N	2.34	0.61
35:1j:33:TRP:CE3	35:1j:36:ILE:HD11	2.35	0.61
10:1J:150:GLY:O	10:1J:154:VAL:HG23	2.00	0.61
20:1T:70:LEU:HB3	20:1T:76:ILE:CD1	2.30	0.61
29:1d:108:THR:HA	41:1p:77:GLU:HA	1.82	0.61
11:1K:43:MET:O	11:1K:47:ILE:HG13	2.00	0.61
12:1L:464:ALA:O	12:1L:468:ILE:HG12	2.00	0.61
34:1i:76:ILE:HA	34:1i:79:TRP:CD1	2.35	0.61
39:1n:55:ASP:HB3	39:1n:58:LYS:HB2	1.82	0.61
4:1D:328:ALA:HB3	7:1G:126:ASP:HB2	1.82	0.60
13:1M:23:ILE:HG13	13:1M:24:TRP:N	2.16	0.60
15:1O:105:LEU:HA	15:1O:128:ILE:HD11	1.82	0.60
28:1c:33:LYS:HZ2	28:1c:37:GLU:HB2	1.66	0.60
31:1f:14:ILE:O	31:1f:18:VAL:HG12	2.01	0.60
34:1i:37:ARG:HB3	34:1i:37:ARG:NH1	2.15	0.60
35:1j:71:GLU:O	40:1o:114:ARG:NH1	2.34	0.60
15:1O:111:ALA:HB1	15:1O:122:VAL:HG11	1.83	0.60
6:1F:125:GLY:O	6:1F:129:MET:HG3	2.02	0.60
3:1C:85:THR:HB	17:1Q:86:PHE:HA	1.84	0.60
5:1E:105:THR:OG1	47:1E:301:FES:S2	2.59	0.60
12:1L:237:MET:CE	12:1L:244:SER:HB3	2.32	0.60
13:1M:263:MET:HE1	38:1m:97:LEU:HD13	1.82	0.60
13:1M:434:ASN:HB3	33:1h:21:PHE:CE2	2.36	0.60
34:1i:53:GLY:N	34:1i:57:LYS:HE3	2.15	0.60
2:1B:45:LEU:O	2:1B:74:VAL:HG23	2.02	0.60
4:1D:286:PRO:HG2	4:1D:303:GLU:HG2	1.81	0.60
8:1H:233:MET:SD	8:1H:233:MET:C	2.85	0.60
12:1L:539:TYR:HA	37:1l:83:MET:HE1	1.83	0.60
14:1N:98:MET:HA	14:1N:101:ALA:HB3	1.82	0.60
16:1P:169:SER:HB3	16:1P:231:VAL:HG12	1.83	0.60
20:1T:13:ASP:OD1	20:1T:14:ARG:N	2.34	0.60
20:1U:37:MET:HE1	20:1U:44:SER:N	2.16	0.60
29:1d:2:MET:HE3	29:1d:5:ARG:HD2	1.84	0.60
7:1G:347:GLU:OE2	7:1G:495:ARG:NH1	2.34	0.60
7:1G:556:MET:HA	42:1q:144:TYR:CE2	2.37	0.60
8:1H:18:ALA:HB2	50:1H:701:U10:H453	1.84	0.60
12:1L:324:LEU:H	12:1L:324:LEU:HD12	1.66	0.60
13:1M:243:MET:O	13:1M:247:THR:HG23	2.00	0.60
20:1T:49:GLU:OE2	20:1T:49:GLU:N	2.30	0.60
20:1U:73:PRO:HA	20:1U:76:ILE:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.01	0.60
39:1n:37:ARG:NH2	39:1n:41:CYS:SG	2.75	0.60
14:1N:108:LEU:HB2	14:1N:161:SER:HB3	1.84	0.60
37:1l:138:LEU:HD21	40:1o:55:ARG:HB3	1.84	0.60
6:1F:21:ILE:HG13	6:1F:233:THR:HG21	1.81	0.60
8:1H:193:THR:HG23	8:1H:234:MET:HG3	1.82	0.60
12:1L:10:THR:O	12:1L:14:ILE:HG12	2.02	0.60
25:1Z:97:ILE:HD11	30:1e:85:LEU:HD11	1.83	0.60
6:1F:437:HIS:O	6:1F:438:GLN:NE2	2.34	0.60
20:1T:18:VAL:HA	20:1T:21:LEU:HD23	1.84	0.60
35:1j:18:THR:O	35:1j:21:GLN:NE2	2.35	0.60
3:1C:42:VAL:HG22	3:1C:48:LEU:HD13	1.84	0.60
9:1I:106:THR:OG1	9:1I:151:LYS:NZ	2.30	0.60
24:1Y:99:THR:HA	24:1Y:102:ALA:HB3	1.84	0.60
46:1f:101:PC1:H361	32:1g:76:PHE:HE2	1.67	0.60
32:1g:37:LEU:HD13	32:1g:40:LYS:HZ2	1.66	0.60
10:1J:23:LYS:NZ	11:1K:18:GLY:O	2.30	0.59
25:1Z:105:LYS:NZ	25:1Z:106:VAL:O	2.33	0.59
14:1N:252:GLY:HA3	14:1N:290:LEU:HD13	1.83	0.59
37:1l:16:THR:HG23	37:1l:19:GLU:H	1.67	0.59
8:1H:267:THR:O	8:1H:271:LEU:HD22	2.02	0.59
13:1M:81:GLN:OE1	13:1M:81:GLN:N	2.29	0.59
13:1M:126:LEU:HD21	13:1M:153:THR:HG21	1.85	0.59
17:1Q:45:MET:HE2	17:1Q:45:MET:HA	1.84	0.59
20:1U:70:LEU:HD12	20:1U:76:ILE:HA	1.84	0.59
28:1c:15:LEU:O	28:1c:19:LEU:HD12	2.02	0.59
37:1l:28:ASN:ND2	37:1l:74:GLY:O	2.30	0.59
38:1m:9:ARG:HG3	38:1m:10:LEU:HD12	1.84	0.59
4:1D:398:HIS:HB3	4:1D:421:GLN:HG2	1.84	0.59
30:1e:64:GLU:O	30:1e:68:ARG:N	2.34	0.59
40:1o:7:ARG:HB2	40:1o:15:GLU:HB2	1.84	0.59
40:1o:61:TYR:HB2	40:1o:86:TRP:CD1	2.38	0.59
42:1q:48:TYR:HD1	42:1q:86:TRP:CE3	2.21	0.59
3:1C:32:ILE:HG22	3:1C:33:LEU:HG	1.83	0.59
4:1D:226:GLU:OE1	25:1Z:23:ARG:NH2	2.35	0.59
6:1F:49:LEU:HD13	6:1F:127:ARG:HG3	1.83	0.59
14:1N:234:TRP:CD2	14:1N:304:MET:HB3	2.38	0.59
15:1O:189:PRO:HA	15:1O:192:MET:HG2	1.83	0.59
15:1O:287:HIS:ND1	32:1g:28:GLU:OE2	2.35	0.59
17:1Q:80:SER:OG	17:1Q:81:ASN:OD1	2.20	0.59
33:1h:63:HIS:NE2	33:1h:76:ALA:O	2.26	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:86:LYS:HD2	34:1i:87:TYR:CZ	2.37	0.59
6:1F:89:ARG:HE	6:1F:219:PRO:HD3	1.66	0.59
12:1L:211:MET:N	12:1L:211:MET:SD	2.75	0.59
13:1M:94:LEU:HD13	52:1N:401:3PE:H351	1.83	0.59
18:1R:3:ARG:HB3	18:1R:3:ARG:NH1	2.16	0.59
33:1h:85:LYS:HE2	33:1h:85:LYS:HA	1.84	0.59
7:1G:315:VAL:O	7:1G:340:SER:OG	2.18	0.59
13:1M:244:MET:HE1	13:1M:316:MET:SD	2.42	0.59
14:1N:213:LEU:HD11	51:1N:402:CDL:H581	1.85	0.59
24:1Y:89:TYR:HB3	24:1Y:121:ALA:HB1	1.85	0.59
32:1g:83:TYR:CE1	32:1g:84:ARG:HD3	2.37	0.59
6:1F:138:ILE:HG21	6:1F:146:ALA:HB2	1.85	0.59
7:1G:310:PHE:HE1	7:1G:520:LYS:HD2	1.67	0.59
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.33	0.59
23:1X:21:SER:OG	26:1a:51:ASP:OD2	2.21	0.59
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.84	0.59
43:1r:91:LYS:HE2	43:1r:91:LYS:N	2.17	0.59
1:1A:109:LYS:NZ	10:1J:169:MET:HE1	2.17	0.59
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.85	0.59
6:1F:107:ASP:O	6:1F:111:ILE:HD12	2.03	0.59
8:1H:91:MET:O	8:1H:93:TYR:N	2.35	0.59
9:1I:99:ARG:NH1	9:1I:101:ASP:OD2	2.35	0.59
12:1L:234:PRO:HA	12:1L:237:MET:HG2	1.84	0.59
35:1j:12:ARG:NH1	36:1k:47:ASN:O	2.36	0.59
8:1H:136:VAL:HG13	10:1J:65:LEU:HD21	1.85	0.59
13:1M:263:MET:HA	13:1M:266:MET:HB2	1.83	0.59
21:1V:76:ILE:O	21:1V:80:ILE:HD12	2.03	0.59
38:1m:45:GLU:OE1	38:1m:45:GLU:N	2.36	0.59
42:1q:143:PRO:O	42:1q:145:LYS:N	2.35	0.59
44:1s:60:LYS:HZ3	44:1s:61:PHE:HD1	1.51	0.59
1:1A:81:THR:HG23	1:1A:83:ASN:H	1.68	0.58
7:1G:644:GLN:NE2	19:1S:37:GLU:O	2.36	0.58
14:1N:100:MET:SD	14:1N:100:MET:N	2.64	0.58
16:1P:132:ILE:HD11	16:1P:214:ILE:HD11	1.84	0.58
34:1i:13:GLN:O	34:1i:17:LEU:HG	2.03	0.58
38:1m:111:LYS:O	38:1m:115:ILE:HD12	2.02	0.58
1:1A:7:LEU:O	1:1A:11:VAL:HG22	2.03	0.58
4:1D:19:MET:H	4:1D:19:MET:CE	2.16	0.58
6:1F:257:ASN:ND2	6:1F:267:THR:OG1	2.36	0.58
13:1M:76:MET:O	13:1M:80:SER:OG	2.15	0.58
13:1M:433:GLU:O	13:1M:437:MET:HE2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:68:ILE:HG22	32:1g:72:LEU:HD12	1.85	0.58
38:1m:2:PHE:C	38:1m:3:PRO:CG	2.72	0.58
10:1J:79:TYR:CE1	16:1P:325:ARG:HD2	2.38	0.58
12:1L:7:LEU:O	12:1L:11:THR:OG1	2.21	0.58
13:1M:60:SER:HB3	13:1M:457:PRO:HA	1.85	0.58
15:1O:214:MET:HE1	15:1O:218:CYS:HB2	1.85	0.58
18:1R:46:GLU:OE2	18:1R:46:GLU:N	2.28	0.58
21:1V:76:ILE:HG22	21:1V:80:ILE:HD11	1.85	0.58
25:1Z:98:MET:HG3	25:1Z:104:TRP:CG	2.38	0.58
29:1d:111:GLU:N	29:1d:111:GLU:OE2	2.36	0.58
33:1h:10:ILE:HG13	33:1h:12:LYS:CD	2.33	0.58
39:1n:158:LYS:HD2	39:1n:159:GLU:H	1.69	0.58
12:1L:246:LEU:O	12:1L:251:THR:OG1	2.13	0.58
12:1L:250:SER:HB3	12:1L:333:ALA:HA	1.85	0.58
12:1L:594:THR:O	12:1L:598:SER:OG	2.21	0.58
13:1M:118:PHE:O	13:1M:122:PHE:HB3	2.04	0.58
26:1a:9:ILE:H	26:1a:9:ILE:HD12	1.68	0.58
28:1c:21:LEU:O	28:1c:25:VAL:HG22	2.02	0.58
37:1l:131:LYS:HZ1	40:1o:56:ASP:HB2	1.67	0.58
40:1o:52:LEU:HA	40:1o:55:ARG:HD2	1.84	0.58
4:1D:155:THR:HB	4:1D:167:PHE:HA	1.83	0.58
5:1E:164:LEU:HD13	5:1E:169:ILE:HD12	1.84	0.58
7:1G:171:ASP:OD1	7:1G:189:LYS:NZ	2.35	0.58
9:1I:132:VAL:HG21	9:1I:165:ILE:HG21	1.84	0.58
10:1J:7:PHE:O	10:1J:11:THR:HG23	2.03	0.58
10:1J:47:PHE:CD2	11:1K:46:LEU:HD21	2.39	0.58
13:1M:280:THR:HG22	13:1M:341:THR:HG23	1.86	0.58
17:1Q:33:ARG:NH1	17:1Q:77:ASP:OD1	2.37	0.58
31:1f:54:VAL:HG21	31:1f:57:LYS:HE3	1.84	0.58
34:1i:11:LEU:HB3	34:1i:15:ARG:HH22	1.67	0.58
34:1i:30:ARG:HH21	39:1n:116:ASP:HB3	1.67	0.58
41:1p:34:LYS:O	41:1p:38:LEU:HD23	2.02	0.58
41:1p:112:CYS:O	41:1p:116:GLU:HG2	2.03	0.58
6:1F:9:LYS:HZ2	6:1F:11:SER:H	1.51	0.58
8:1H:311:THR:O	25:1Z:55:ARG:NH1	2.37	0.58
12:1L:50:PRO:HA	12:1L:53:MET:SD	2.43	0.58
12:1L:439:PRO:HB3	35:1j:12:ARG:HE	1.68	0.58
14:1N:290:LEU:O	14:1N:294:MET:HG2	2.04	0.58
18:1R:11:VAL:HG12	18:1R:17:ALA:HB2	1.86	0.58
30:1e:88:GLU:OE1	30:1e:88:GLU:N	2.34	0.58
12:1L:237:MET:HE1	12:1L:244:SER:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:133:ILE:HD11	13:1M:231:LEU:HD11	1.85	0.58
16:1P:20:VAL:HG22	16:1P:44:GLN:HB3	1.85	0.58
20:1T:22:TYR:HE2	20:1T:24:LYS:HE3	1.68	0.58
40:1o:45:MET:HE3	40:1o:55:ARG:HG2	1.86	0.58
4:1D:409:HIS:HB3	4:1D:413:ASP:CB	2.34	0.58
8:1H:161:THR:OG1	8:1H:164:THR:HG23	2.03	0.58
9:1I:150:ASN:ND2	42:1q:127:TYR:O	2.37	0.58
11:1K:4:VAL:O	11:1K:8:ILE:HG12	2.04	0.58
13:1M:2:LEU:HA	13:1M:5:ILE:HB	1.85	0.58
16:1P:96:GLY:HA3	55:1P:501:NDP:H3D	1.85	0.58
37:1l:116:PHE:O	37:1l:116:PHE:HD1	1.86	0.58
40:1o:73:PHE:CD1	40:1o:74:PRO:HA	2.38	0.58
5:1E:166:PRO:O	5:1E:170:GLU:HG2	2.04	0.58
7:1G:12:PHE:HB2	7:1G:78:ASN:HA	1.86	0.58
10:1J:79:TYR:CD1	16:1P:325:ARG:HD2	2.39	0.58
12:1L:160:GLY:H	39:1n:95:CYS:HB3	1.69	0.58
12:1L:434:LYS:HZ1	36:1k:57:ALA:HA	1.68	0.58
13:1M:92:LYS:O	13:1M:96:ILE:HG12	2.03	0.58
20:1U:15:VAL:O	20:1U:19:LEU:HG	2.04	0.58
21:1V:95:ARG:HB2	21:1V:95:ARG:NH1	2.19	0.58
22:1W:70:ASN:ND2	22:1W:82:LEU:HD22	2.13	0.58
24:1Y:13:GLU:OE2	24:1Y:83:PRO:HB2	2.03	0.58
26:1a:31:ASN:HD22	26:1a:36:LYS:HA	1.68	0.58
10:1J:168:ILE:O	10:1J:172:THR:OG1	2.18	0.58
12:1L:249:SER:HA	12:1L:340:PHE:HE1	1.69	0.58
12:1L:514:LYS:NZ	52:1L:701:3PE:O12	2.28	0.58
13:1M:378:GLU:O	13:1M:382:ILE:HG12	2.03	0.58
14:1N:310:ASN:HB2	15:1O:274:THR:HG22	1.86	0.58
16:1P:138:ASP:OD1	16:1P:140:LYS:NZ	2.36	0.58
39:1n:144:PRO:HG2	39:1n:149:ARG:H	1.69	0.58
2:1B:62:MET:SD	2:1B:69:MET:HG2	2.44	0.57
6:1F:150:GLN:HG2	44:1s:54:LEU:HG	1.86	0.57
12:1L:203:MET:HB2	41:1p:113:GLN:HG3	1.86	0.57
21:1V:29:LYS:HA	21:1V:32:ASP:OD1	2.02	0.57
37:1l:71:LEU:HD21	37:1l:77:ILE:HG22	1.86	0.57
42:1q:29:ARG:NH2	42:1q:64:TYR:O	2.37	0.57
10:1J:94:VAL:HG13	10:1J:98:MET:SD	2.44	0.57
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.37	0.57
36:1k:33:GLU:N	36:1k:33:GLU:OE2	2.37	0.57
4:1D:84:HIS:HA	4:1D:429:ASP:HB3	1.85	0.57
7:1G:460:ARG:NH1	7:1G:659:ASP:OD2	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:41:SER:O	12:1L:45:THR:HG23	2.04	0.57
13:1M:71:TRP:HH2	13:1M:439:LEU:HD12	1.69	0.57
13:1M:204:MET:HA	13:1M:207:MET:HG2	1.86	0.57
13:1M:431:THR:HG21	32:1g:58:MET:HE1	1.87	0.57
17:1Q:66:GLU:OE1	17:1Q:66:GLU:N	2.37	0.57
33:1h:94:LEU:HD13	41:1p:81:ILE:HG13	1.85	0.57
40:1o:7:ARG:HG2	40:1o:12:ALA:HA	1.86	0.57
2:1B:62:MET:HE2	2:1B:157:LEU:HG	1.85	0.57
2:1B:116:MET:HG3	2:1B:151:PRO:HG2	1.86	0.57
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.36	0.57
12:1L:116:ARG:HG2	12:1L:120:TYR:CZ	2.39	0.57
12:1L:300:LYS:NZ	39:1n:77:GLN:OE1	2.36	0.57
20:1T:35:HIS:CE1	20:1T:71:MET:HE2	2.39	0.57
32:1g:76:PHE:CZ	33:1h:75:ILE:HD11	2.39	0.57
37:1l:105:LEU:O	37:1l:109:VAL:HG22	2.04	0.57
40:1o:113:ARG:O	40:1o:117:ARG:HB3	2.05	0.57
4:1D:423:ILE:HD11	4:1D:428:VAL:HG21	1.86	0.57
7:1G:8:LEU:HD12	7:1G:19:MET:HB3	1.86	0.57
8:1H:234:MET:HA	8:1H:234:MET:HE3	1.87	0.57
13:1M:76:MET:HB3	13:1M:226:ALA:HB1	1.87	0.57
15:1O:312:VAL:HB	28:1c:2:PHE:HD2	1.69	0.57
20:1U:54:MET:HA	20:1U:57:GLU:OE2	2.03	0.57
34:1i:34:LEU:HD22	34:1i:35:PRO:HD2	1.87	0.57
36:1k:75:ALA:O	36:1k:79:VAL:HG13	2.04	0.57
2:1B:25:ARG:HE	2:1B:27:GLU:HB3	1.70	0.57
4:1D:109:VAL:HG11	4:1D:152:MET:HG2	1.86	0.57
6:1F:337:MET:HG2	6:1F:341:THR:HG21	1.87	0.57
14:1N:53:THR:O	14:1N:57:THR:OG1	2.21	0.57
37:1l:21:ALA:O	37:1l:25:LYS:HD3	2.04	0.57
7:1G:469:ALA:O	7:1G:473:ILE:HG12	2.05	0.57
12:1L:279:CYS:O	12:1L:283:ILE:HG12	2.04	0.57
12:1L:419:THR:O	12:1L:423:SER:OG	2.17	0.57
13:1M:241:TYR:O	13:1M:245:ARG:HG2	2.04	0.57
37:1l:66:HIS:HB2	37:1l:71:LEU:HB3	1.86	0.57
39:1n:111:LYS:HG2	39:1n:118:PHE:CE1	2.40	0.57
5:1E:34:ILE:HD11	44:1s:52:LEU:HD22	1.86	0.57
10:1J:70:TYR:HE1	11:1K:79:VAL:HG23	1.69	0.57
12:1L:160:GLY:HA3	39:1n:94:GLU:HB2	1.86	0.57
16:1P:293:THR:HG22	16:1P:295:PRO:HD3	1.86	0.57
34:1i:9:LEU:HA	34:1i:12:GLN:NE2	2.12	0.57
34:1i:94:TYR:OH	41:1p:10:PRO:O	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:315:VAL:HA	7:1G:521:VAL:HG12	1.86	0.57
7:1G:418:ARG:HD2	7:1G:418:ARG:C	2.30	0.57
12:1L:161:ARG:NH1	12:1L:238:GLU:OE2	2.37	0.57
12:1L:210:ASN:OD1	12:1L:270:ASN:ND2	2.34	0.57
12:1L:366:MET:HE2	12:1L:366:MET:HA	1.85	0.57
14:1N:144:GLN:OE1	30:1e:2:PHE:N	2.37	0.57
2:1B:116:MET:HE2	2:1B:156:LEU:HD13	1.85	0.57
10:1J:8:ILE:O	10:1J:12:ILE:HG12	2.05	0.57
12:1L:553:LEU:HD21	38:1m:93:GLY:HA3	1.87	0.57
13:1M:269:MET:HE1	13:1M:296:LEU:HD13	1.85	0.57
15:1O:281:GLU:HA	32:1g:27:GLN:HE22	1.68	0.57
16:1P:319:ARG:HA	16:1P:322:ARG:HD3	1.86	0.57
17:1Q:6:GLN:HB2	17:1Q:10:LEU:HD23	1.86	0.57
19:1S:12:LYS:HE2	19:1S:98:ALA:HB3	1.86	0.57
25:1Z:98:MET:HG3	25:1Z:104:TRP:CD1	2.40	0.57
26:1a:1:MET:HA	26:1a:1:MET:HE3	1.87	0.57
34:1i:43:GLU:HG2	34:1i:44:GLN:OE1	2.04	0.57
37:1l:14:PRO:HD3	37:1l:46:ASP:HA	1.87	0.57
8:1H:63:PRO:O	8:1H:66:SER:OG	2.20	0.56
12:1L:249:SER:HA	12:1L:340:PHE:CE1	2.40	0.56
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.39	0.56
17:1Q:104:ASP:N	17:1Q:104:ASP:OD1	2.38	0.56
37:1l:143:GLY:HA2	41:1p:121:ARG:HH11	1.70	0.56
58:1l:201:MYR:O1	40:1o:1:GLY:N	2.38	0.56
13:1M:203:PHE:HB2	13:1M:243:MET:HE2	1.88	0.56
13:1M:243:MET:HA	13:1M:246:ILE:HG22	1.87	0.56
22:1W:89:GLU:O	22:1W:93:THR:OG1	2.24	0.56
24:1Y:29:GLY:O	24:1Y:33:LEU:HD23	2.04	0.56
25:1Z:21:TYR:OH	43:1r:108:ASP:OD2	2.20	0.56
3:1C:81:VAL:HG22	4:1D:388:ARG:HG2	1.87	0.56
4:1D:40:LYS:HA	4:1D:40:LYS:HE3	1.87	0.56
6:1F:22:PHE:HE2	6:1F:110:ILE:HD13	1.71	0.56
6:1F:224:ASN:ND2	48:1F:501:FMN:O2	2.24	0.56
7:1G:175:THR:O	7:1G:181:MET:HA	2.05	0.56
8:1H:70:MET:HA	8:1H:73:ILE:HG22	1.86	0.56
8:1H:76:ILE:O	8:1H:80:SER:OG	2.16	0.56
9:1I:79:ALA:O	9:1I:104:ARG:NH2	2.33	0.56
9:1I:162:GLU:HG2	42:1q:108:TYR:HE2	1.70	0.56
12:1L:555:LEU:HB2	38:1m:75:ILE:HD13	1.86	0.56
14:1N:25:HIS:NE2	30:1e:17:MET:HG2	2.20	0.56
14:1N:36:ASN:OD1	14:1N:134:GLN:NE2	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:89:MET:HE2	14:1N:89:MET:HA	1.87	0.56
23:1X:81:PHE:HD2	26:1a:66:LEU:HD21	1.71	0.56
25:1Z:88:ARG:NH2	25:1Z:92:GLU:OE2	2.38	0.56
32:1g:107:LEU:HD23	32:1g:107:LEU:H	1.71	0.56
34:1i:37:ARG:HB3	34:1i:37:ARG:HH11	1.69	0.56
40:1o:34:LYS:HD2	40:1o:35:GLU:N	2.20	0.56
40:1o:108:LEU:O	40:1o:112:LYS:HG2	2.05	0.56
2:1B:108:PRO:HB2	8:1H:58:LYS:HZ3	1.70	0.56
4:1D:4:TRP:CE3	13:1M:140:THR:HA	2.39	0.56
8:1H:80:SER:O	8:1H:84:THR:OG1	2.21	0.56
10:1J:122:LEU:HD12	10:1J:126:VAL:HG21	1.87	0.56
12:1L:19:ILE:HD11	12:1L:122:VAL:HB	1.86	0.56
13:1M:1:FME:HE3	13:1M:111:THR:HG21	1.88	0.56
13:1M:16:TRP:NE1	13:1M:97:THR:HG1	2.02	0.56
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.86	0.56
16:1P:176:ASP:OD1	16:1P:180:ASN:ND2	2.39	0.56
19:1S:29:SER:OG	19:1S:33:ARG:NH1	2.39	0.56
7:1G:221:GLU:HG3	7:1G:243:ARG:HD3	1.87	0.56
12:1L:44:PHE:O	12:1L:48:LEU:HD22	2.06	0.56
12:1L:152:PHE:HB2	12:1L:172:ILE:HD11	1.86	0.56
13:1M:282:LEU:O	13:1M:286:ILE:HG13	2.05	0.56
14:1N:57:THR:O	14:1N:61:LEU:HD12	2.04	0.56
15:1O:233:LYS:HA	15:1O:236:GLU:HG3	1.88	0.56
20:1U:47:GLN:NE2	20:1U:67:ALA:O	2.38	0.56
23:1X:35:CYS:O	23:1X:39:ASN:ND2	2.38	0.56
20:1T:79:TYR:HA	20:1T:82:ASP:OD1	2.05	0.56
3:1C:114:LEU:HD12	17:1Q:17:LEU:HD11	1.87	0.56
16:1P:60:ARG:HE	16:1P:70:PHE:HE2	1.52	0.56
32:1g:120:LEU:HD12	41:1p:163:LEU:HD13	1.87	0.56
34:1i:58:ASN:OD1	34:1i:62:LYS:NZ	2.39	0.56
35:1j:8:GLU:HB2	35:1j:10:ARG:HH22	1.69	0.56
35:1j:36:ILE:HD12	35:1j:37:LEU:HD12	1.87	0.56
37:1l:125:TYR:OH	40:1o:7:ARG:NH1	2.39	0.56
39:1n:111:LYS:HA	39:1n:118:PHE:CE2	2.41	0.56
12:1L:2:ASN:HB2	12:1L:3:PRO:HD3	1.88	0.56
4:1D:94:LYS:NZ	9:1I:88:PRO:O	2.38	0.56
4:1D:259:MET:HE1	4:1D:421:GLN:HG3	1.88	0.56
7:1G:378:LEU:HD11	7:1G:409:ILE:HD11	1.88	0.56
7:1G:449:PRO:O	7:1G:487:TRP:NE1	2.38	0.56
12:1L:298:ILE:HG22	12:1L:426:ILE:HD11	1.87	0.56
16:1P:46:ILE:O	16:1P:46:ILE:HG22	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:46:ASP:HA	20:1U:49:GLU:HG3	1.87	0.56
32:1g:41:ASN:O	32:1g:44:SER:OG	2.23	0.56
37:1l:20:ARG:HH11	37:1l:36:PRO:HG3	1.71	0.56
41:1p:59:ARG:HD3	41:1p:59:ARG:H	1.70	0.56
1:1A:21:ALA:HB1	8:1H:218:GLY:HA3	1.88	0.56
7:1G:141:ASN:HD21	7:1G:698:VAL:HG23	1.70	0.56
8:1H:259:PHE:O	8:1H:263:THR:HG23	2.05	0.56
10:1J:126:VAL:HG13	25:1Z:122:GLY:HA3	1.87	0.56
12:1L:293:ILE:O	12:1L:425:ARG:NH1	2.39	0.56
13:1M:247:THR:HG1	41:1p:148:HIS:HE2	1.52	0.56
15:1O:162:GLU:N	15:1O:162:GLU:OE2	2.39	0.56
20:1U:12:LYS:O	20:1U:16:LEU:HG	2.06	0.56
20:1U:23:ASP:HB2	36:1k:43:PRO:HB3	1.87	0.56
23:1X:39:ASN:HB3	25:1Z:73:PRO:HG2	1.87	0.56
29:1d:120:ARG:NH2	38:1m:112:GLU:OE2	2.36	0.56
3:1C:147:ASP:OD2	3:1C:149:ARG:NH1	2.39	0.55
4:1D:287:ILE:HG12	9:1I:2:TYR:HB2	1.87	0.55
5:1E:153:MET:HB3	5:1E:162:GLU:HA	1.87	0.55
7:1G:522:LEU:HB3	7:1G:543:ILE:HD13	1.87	0.55
9:1I:8:ARG:CZ	9:1I:8:ARG:HA	2.36	0.55
12:1L:176:ARG:HG2	12:1L:176:ARG:NH1	2.18	0.55
13:1M:298:ILE:O	13:1M:302:MET:HG2	2.05	0.55
40:1o:38:MET:HE1	40:1o:57:TYR:HA	1.87	0.55
40:1o:70:ARG:NE	41:1p:19:PRO:HB3	2.21	0.55
5:1E:150:ASN:HB3	5:1E:162:GLU:HB3	1.88	0.55
8:1H:90:PRO:HD3	8:1H:162:LEU:HD13	1.88	0.55
9:1I:27:TRP:HB3	9:1I:30:LEU:HD22	1.87	0.55
11:1K:50:ASN:HD22	11:1K:50:ASN:C	2.14	0.55
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.42	0.55
13:1M:342:MET:O	13:1M:342:MET:HG3	2.06	0.55
14:1N:255:PRO:HG3	14:1N:260:PHE:CD1	2.41	0.55
20:1U:61:GLU:HB2	39:1n:84:SER:HB3	1.88	0.55
40:1o:74:PRO:HD3	41:1p:27:ASN:HA	1.89	0.55
41:1p:31:TYR:O	41:1p:35:ILE:HG13	2.05	0.55
42:1q:51:ASP:OD1	42:1q:54:GLN:NE2	2.39	0.55
1:1A:54:LYS:HB3	1:1A:114:ALA:HB3	1.88	0.55
8:1H:253:GLU:OE1	8:1H:253:GLU:N	2.35	0.55
12:1L:40:VAL:HG12	12:1L:98:TRP:HB2	1.88	0.55
15:1O:151:HIS:CD2	15:1O:277:VAL:HG21	2.40	0.55
23:1X:31:TYR:CE2	25:1Z:74:LEU:HD11	2.41	0.55
29:1d:113:LEU:HD23	32:1g:121:PRO:HG3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:90:ARG:HH12	41:1p:100:GLU:HB3	1.71	0.55
5:1E:27:ASN:OD1	5:1E:30:ARG:NH1	2.40	0.55
6:1F:262:VAL:HG11	6:1F:284:ALA:HB1	1.89	0.55
7:1G:559:VAL:C	7:1G:560:ILE:HD12	2.32	0.55
12:1L:277:THR:O	12:1L:314:MET:HE1	2.07	0.55
15:1O:159:THR:HG22	15:1O:272:TYR:HB2	1.88	0.55
20:1T:63:PRO:HB2	20:1T:65:ILE:HG22	1.88	0.55
34:1i:46:TRP:HA	34:1i:46:TRP:CE3	2.42	0.55
39:1n:116:ASP:OD1	39:1n:116:ASP:N	2.38	0.55
7:1G:273:GLY:O	7:1G:549:HIS:NE2	2.30	0.55
8:1H:31:MET:HE2	9:1I:41:LEU:HD13	1.88	0.55
9:1I:103:SER:HB3	9:1I:105:ARG:HE	1.72	0.55
13:1M:190:TRP:CD2	24:1Y:126:MET:HE1	2.41	0.55
23:1X:109:CYS:O	23:1X:113:LYS:HB2	2.06	0.55
35:1j:36:ILE:HD12	35:1j:37:LEU:N	2.22	0.55
6:1F:400:GLU:O	6:1F:402:HIS:ND1	2.38	0.55
9:1I:49:ASN:O	9:1I:53:GLU:N	2.39	0.55
12:1L:62:ILE:HD11	12:1L:81:LYS:HD3	1.88	0.55
12:1L:356:ILE:HG13	12:1L:357:ARG:HD3	1.89	0.55
13:1M:400:MET:O	13:1M:404:ALA:N	2.23	0.55
16:1P:141:SER:O	16:1P:147:ARG:NH1	2.39	0.55
23:1X:15:GLN:HG3	23:1X:67:LEU:HD12	1.88	0.55
23:1X:49:GLU:OE1	23:1X:54:ARG:NH1	2.39	0.55
24:1Y:51:GLY:O	24:1Y:55:THR:HG22	2.05	0.55
34:1i:1:SAC:H	34:1i:2:GLY:HA3	1.72	0.55
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.88	0.55
12:1L:221:ALA:HA	12:1L:226:GLN:HB2	1.88	0.55
13:1M:25:ILE:O	13:1M:29:VAL:HG12	2.05	0.55
13:1M:382:ILE:HD12	13:1M:396:MET:HB3	1.89	0.55
19:1S:24:GLN:HB3	19:1S:25:ARG:CZ	2.36	0.55
28:1c:31:LEU:HD11	29:1d:26:LEU:HD11	1.88	0.55
30:1e:4:ASP:OD1	30:1e:7:LYS:HD3	2.06	0.55
34:1i:97:VAL:HG13	41:1p:114:GLN:HG2	1.89	0.55
43:1r:90:GLU:OE2	43:1r:91:LYS:N	2.33	0.55
4:1D:228:MET:HE3	4:1D:228:MET:HA	1.89	0.55
7:1G:241:SER:OG	7:1G:249:ARG:HG2	2.07	0.55
12:1L:35:TYR:OH	34:1i:73:HIS:NE2	2.33	0.55
12:1L:401:MET:HE2	12:1L:479:ASN:HD21	1.72	0.55
12:1L:573:MET:HE1	14:1N:167:TRP:CE3	2.41	0.55
14:1N:154:MET:HE1	14:1N:191:THR:HB	1.87	0.55
20:1T:70:LEU:HD23	20:1T:76:ILE:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:119:LEU:O	24:1Y:123:LEU:HG	2.07	0.55
28:1c:12:PRO:HG2	28:1c:14:TRP:HZ3	1.72	0.55
1:1A:41:PHE:HB3	22:1W:99:GLN:HE21	1.72	0.55
4:1D:291:GLY:O	4:1D:296:ARG:NH1	2.39	0.55
12:1L:373:LEU:HD12	12:1L:427:ILE:HD13	1.88	0.55
12:1L:584:ILE:HG12	14:1N:58:LYS:HE3	1.88	0.55
23:1X:134:ARG:O	27:1b:57:ARG:NH2	2.40	0.55
2:1B:114:VAL:HG22	2:1B:144:ILE:HB	1.89	0.55
8:1H:139:THR:O	8:1H:143:GLU:HB2	2.07	0.55
13:1M:190:TRP:HH2	46:1M:501:PC1:H222	1.72	0.55
14:1N:236:LYS:HD3	14:1N:314:LYS:HG2	1.89	0.55
17:1Q:13:VAL:C	17:1Q:15:GLU:OE1	2.50	0.55
20:1T:22:TYR:CE2	20:1T:24:LYS:HE3	2.42	0.55
21:1V:81:LEU:HA	21:1V:84:GLU:OE1	2.07	0.55
24:1Y:65:ILE:HD12	24:1Y:96:GLY:HA2	1.89	0.55
33:1h:40:ILE:HD12	33:1h:41:THR:N	2.21	0.55
35:1j:12:ARG:NH2	36:1k:47:ASN:OD1	2.30	0.55
39:1n:60:THR:O	39:1n:64:ARG:HG3	2.07	0.55
4:1D:307:SER:O	4:1D:311:ILE:HG13	2.06	0.54
5:1E:27:ASN:ND2	5:1E:57:GLN:OE1	2.40	0.54
12:1L:289:ALA:O	12:1L:293:ILE:HD13	2.07	0.54
12:1L:548:SER:HA	12:1L:552:LEU:HB3	1.89	0.54
13:1M:65:LEU:O	13:1M:69:THR:HG23	2.06	0.54
13:1M:231:LEU:HD23	13:1M:235:LEU:HD12	1.88	0.54
15:1O:38:LEU:HD21	15:1O:234:VAL:HG21	1.88	0.54
34:1i:108:THR:HG23	41:1p:18:ALA:HB3	1.89	0.54
38:1m:32:GLN:NE2	39:1n:8:TYR:HA	2.22	0.54
3:1C:8:ARG:HE	3:1C:11:ILE:HD13	1.71	0.54
4:1D:83:LEU:O	4:1D:83:LEU:HD13	2.07	0.54
5:1E:56:ARG:HH11	44:1s:48:THR:HG23	1.72	0.54
6:1F:57:LEU:HD13	6:1F:80:SER:HA	1.89	0.54
6:1F:78:LYS:HG2	6:1F:79:TRP:HD1	1.71	0.54
7:1G:194:GLU:HG3	7:1G:389:PRO:HB3	1.90	0.54
7:1G:366:THR:O	7:1G:366:THR:OG1	2.21	0.54
9:1I:92:ILE:HD11	45:1I:201:SF4:S3	2.47	0.54
10:1J:20:PHE:CE1	11:1K:32:CYS:HA	2.41	0.54
15:1O:147:GLN:O	15:1O:150:GLU:HG3	2.06	0.54
15:1O:164:LEU:HD11	15:1O:248:TRP:CD1	2.43	0.54
20:1U:52:MET:HA	20:1U:55:GLU:HB2	1.89	0.54
37:1l:137:ASP:HB3	37:1l:153:VAL:HG11	1.90	0.54
1:1A:38:GLU:OE2	8:1H:126:LYS:NZ	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:444:LYS:NZ	7:1G:445:GLU:OE1	2.40	0.54
12:1L:311:GLY:O	12:1L:315:VAL:HG23	2.08	0.54
12:1L:539:TYR:HE2	38:1m:9:ARG:HH21	1.55	0.54
51:1N:402:CDL:OA3	15:1O:257:HIS:NE2	2.36	0.54
17:1Q:37:ILE:HD12	17:1Q:92:ALA:HB1	1.89	0.54
20:1T:76:ILE:O	20:1T:80:ILE:HG13	2.08	0.54
21:1V:8:THR:O	21:1V:75:GLN:NE2	2.26	0.54
4:1D:4:TRP:CD1	4:1D:4:TRP:C	2.84	0.54
6:1F:298:ILE:HB	6:1F:335:ILE:HB	1.89	0.54
8:1H:20:LEU:HD21	8:1H:267:THR:HG21	1.89	0.54
10:1J:159:TRP:HE1	14:1N:12:THR:HG22	1.72	0.54
12:1L:377:SER:O	12:1L:381:THR:OG1	2.19	0.54
12:1L:441:VAL:HG13	12:1L:443:ILE:HD12	1.89	0.54
15:1O:173:ASP:OD2	15:1O:222:GLN:NE2	2.40	0.54
16:1P:80:SER:O	16:1P:84:VAL:HG23	2.07	0.54
31:1f:39:ASN:ND2	31:1f:46:ARG:O	2.33	0.54
38:1m:94:ILE:O	38:1m:97:LEU:HB2	2.08	0.54
2:1B:176:TRP:HB2	46:1B:202:PC1:H2	1.89	0.54
11:1K:37:MET:HG2	11:1K:67:ALA:CB	2.38	0.54
14:1N:55:ALA:O	14:1N:118:VAL:HG12	2.07	0.54
25:1Z:78:GLU:OE1	26:1a:50:ARG:NH2	2.40	0.54
31:1f:53:GLU:CD	31:1f:53:GLU:H	2.15	0.54
7:1G:284:ILE:HG22	7:1G:559:VAL:HG12	1.89	0.54
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.89	0.54
10:1J:33:LEU:HD22	10:1J:64:MET:SD	2.47	0.54
13:1M:25:ILE:HG12	32:1g:57:ASN:HB2	1.88	0.54
15:1O:133:VAL:HG13	15:1O:205:ALA:HB3	1.89	0.54
19:1S:92:ASN:OD1	19:1S:92:ASN:N	2.40	0.54
25:1Z:120:MET:HG2	25:1Z:122:GLY:H	1.72	0.54
51:1a:101:CDL:H162	51:1a:101:CDL:H331	1.88	0.54
7:1G:584:LYS:HE2	17:1Q:36:ARG:HD2	1.89	0.54
11:1K:10:MET:C	11:1K:10:MET:HE3	2.33	0.54
14:1N:178:ILE:HD12	14:1N:179:MET:N	2.22	0.54
32:1g:85:MET:HE2	32:1g:85:MET:N	2.22	0.54
32:1g:92:GLU:HG2	41:1p:64:HIS:NE2	2.22	0.54
33:1h:9:PHE:CE2	39:1n:114:TYR:HD2	2.26	0.54
33:1h:32:THR:O	33:1h:36:VAL:HG12	2.07	0.54
35:1j:20:SER:O	35:1j:23:ILE:HG12	2.06	0.54
40:1o:112:LYS:HA	40:1o:115:GLU:OE1	2.07	0.54
1:1A:6:THR:HG21	8:1H:87:VAL:HG11	1.90	0.54
10:1J:51:PHE:N	10:1J:139:GLU:OE2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:190:TRP:CG	24:1Y:126:MET:HE1	2.42	0.54
13:1M:254:THR:O	13:1M:258:ALA:N	2.40	0.54
15:1O:316:TRP:HZ3	15:1O:318:TRP:CZ2	2.26	0.54
25:1Z:88:ARG:O	25:1Z:92:GLU:HG2	2.08	0.54
38:1m:21:GLU:O	39:1n:14:LYS:NZ	2.41	0.54
12:1L:122:VAL:HG12	12:1L:126:ILE:CD1	2.37	0.54
46:1M:501:PC1:H32	24:1Y:87:LEU:HD21	1.89	0.54
14:1N:213:LEU:O	14:1N:217:MET:HG3	2.08	0.54
30:1e:44:HIS:CG	33:1h:130:LYS:HG2	2.43	0.54
37:1l:72:ASN:ND2	38:1m:39:ARG:HD3	2.22	0.54
39:1n:178:MET:HE2	39:1n:178:MET:N	2.21	0.54
2:1B:47:PRO:HD3	2:1B:74:VAL:HG22	1.90	0.54
4:1D:63:ARG:HB3	4:1D:79:HIS:HB2	1.90	0.54
5:1E:153:MET:C	5:1E:153:MET:HE2	2.33	0.54
9:1I:112:ASP:OD2	9:1I:114:THR:HG22	2.09	0.54
12:1L:73:THR:HG21	38:1m:126:ILE:HD13	1.89	0.54
12:1L:100:ILE:HG22	12:1L:341:MET:HE3	1.90	0.54
14:1N:316:GLN:HE22	15:1O:60:ASP:HA	1.73	0.54
32:1g:57:ASN:HA	32:1g:60:VAL:HG22	1.89	0.54
34:1i:77:PRO:O	34:1i:81:ILE:HG13	2.08	0.54
36:1k:27:PRO:O	36:1k:30:THR:HG22	2.08	0.54
39:1n:131:SER:HB2	39:1n:162:LEU:HB2	1.90	0.54
3:1C:205:ALA:HA	7:1G:122:MET:HE2	1.89	0.53
10:1J:115:ILE:O	10:1J:117:PHE:N	2.41	0.53
12:1L:455:LYS:HZ3	12:1L:456:ARG:HH12	1.55	0.53
14:1N:44:LEU:HD11	14:1N:59:TYR:CD1	2.37	0.53
14:1N:211:MET:HE1	14:1N:251:MET:HG2	1.89	0.53
20:1T:58:PHE:HB3	20:1T:60:PHE:HE1	1.73	0.53
21:1V:22:ARG:HH11	21:1V:26:LEU:HG	1.73	0.53
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.38	0.53
4:1D:352:TYR:HD1	9:1I:86:VAL:HG21	1.73	0.53
5:1E:29:LYS:O	5:1E:32:GLU:HG3	2.08	0.53
10:1J:86:ASN:HB3	10:1J:89:VAL:HG22	1.90	0.53
12:1L:14:ILE:HG22	34:1i:77:PRO:HG2	1.90	0.53
12:1L:486:MET:HB3	58:1l:201:MYR:H71	1.89	0.53
13:1M:137:GLY:O	13:1M:142:ARG:NH1	2.42	0.53
15:1O:94:TYR:OH	15:1O:151:HIS:ND1	2.24	0.53
23:1X:120:ASP:OD1	23:1X:121:LEU:N	2.40	0.53
30:1e:37:LYS:NZ	30:1e:38:GLU:OE2	2.42	0.53
33:1h:32:THR:C	33:1h:35:PRO:HD2	2.34	0.53
38:1m:4:LYS:HD3	38:1m:17:LEU:HD22	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:1m:36:LEU:O	38:1m:40:SER:OG	2.27	0.53
1:1A:71:LEU:HD11	11:1K:65:VAL:HG22	1.90	0.53
4:1D:19:MET:H	4:1D:19:MET:HE3	1.72	0.53
4:1D:211:ILE:HG22	4:1D:315:LEU:HD11	1.90	0.53
7:1G:377:ILE:HG13	7:1G:404:LEU:HD11	1.90	0.53
12:1L:96:VAL:O	12:1L:100:ILE:HG13	2.08	0.53
13:1M:207:MET:HB3	13:1M:298:ILE:HD11	1.89	0.53
14:1N:218:LEU:HD12	14:1N:326:LEU:HD11	1.91	0.53
14:1N:281:LEU:O	14:1N:285:THR:HG22	2.08	0.53
20:1U:55:GLU:HG2	20:1U:62:ILE:H	1.74	0.53
24:1Y:116:TYR:O	24:1Y:120:THR:HG23	2.09	0.53
41:1p:51:ILE:HD12	41:1p:52:GLU:N	2.24	0.53
2:1B:81:ARG:HG3	8:1H:61:LEU:HD21	1.91	0.53
7:1G:475:GLN:OE1	7:1G:650:LYS:NZ	2.41	0.53
10:1J:100:GLU:HA	10:1J:103:MET:HG2	1.89	0.53
13:1M:341:THR:HG21	38:1m:64:LEU:HD11	1.89	0.53
13:1M:391:ILE:O	13:1M:394:ILE:HG22	2.09	0.53
24:1Y:32:GLY:O	24:1Y:36:SER:OG	2.26	0.53
31:1f:1:MET:HG2	31:1f:6:ILE:HD11	1.90	0.53
34:1i:10:ARG:NH2	39:1n:163:PRO:HB2	2.23	0.53
1:1A:73:LEU:HD23	8:1H:151:LEU:HD12	1.90	0.53
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	1.90	0.53
6:1F:372:MET:HE1	6:1F:412:ALA:HA	1.90	0.53
10:1J:103:MET:N	10:1J:103:MET:SD	2.81	0.53
13:1M:432:ARG:NE	32:1g:46:GLY:O	2.25	0.53
22:1W:57:LYS:O	22:1W:57:LYS:HD3	2.08	0.53
34:1i:3:TYR:HD2	34:1i:8:LYS:HE3	1.67	0.53
34:1i:22:LEU:HA	34:1i:25:GLN:HG2	1.89	0.53
37:1l:22:ALA:HA	37:1l:25:LYS:HZ3	1.74	0.53
37:1l:158:ILE:HB	40:1o:33:ARG:NH2	2.23	0.53
38:1m:101:TYR:OH	38:1m:105:LYS:NZ	2.42	0.53
4:1D:346:ILE:HG23	7:1G:117:GLN:HG2	1.90	0.53
8:1H:306:SER:O	8:1H:310:MET:HG2	2.08	0.53
12:1L:415:ALA:O	12:1L:419:THR:OG1	2.25	0.53
13:1M:36:LEU:HD11	46:1f:101:PC1:H371	1.89	0.53
15:1O:262:LEU:HD22	15:1O:268:GLU:HG3	1.89	0.53
19:1S:15:LEU:HB2	19:1S:97:LYS:HG2	1.90	0.53
20:1T:37:MET:HB2	20:1T:38:LYS:HD2	1.89	0.53
31:1f:28:ARG:NH2	46:1f:101:PC1:O14	2.42	0.53
32:1g:37:LEU:HD13	32:1g:40:LYS:NZ	2.24	0.53
1:1A:56:PHE:HB2	10:1J:70:TYR:OH	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:65:PHE:CD1	1:1A:98:LEU:HD11	2.44	0.53
1:1A:108:GLN:O	1:1A:110:GLY:N	2.42	0.53
5:1E:148:CYS:N	6:1F:105:CYS:SG	2.81	0.53
11:1K:25:HIS:ND1	11:1K:88:ASP:OD1	2.42	0.53
12:1L:342:CYS:O	12:1L:346:ILE:HG22	2.08	0.53
13:1M:290:SER:HB2	13:1M:319:HIS:HE2	1.73	0.53
13:1M:357:THR:O	13:1M:360:LEU:N	2.41	0.53
14:1N:274:GLU:OE2	14:1N:274:GLU:N	2.41	0.53
20:1T:37:MET:HE2	20:1T:37:MET:HA	1.90	0.53
32:1g:112:CYS:HG	41:1p:142:TYR:HH	1.56	0.53
1:1A:102:LEU:HD21	8:1H:295:PRO:HG3	1.91	0.53
2:1B:79:SER:OG	2:1B:79:SER:O	2.24	0.53
2:1B:152:THR:HG22	2:1B:154:GLU:H	1.72	0.53
4:1D:8:VAL:O	4:1D:12:GLU:HG2	2.08	0.53
6:1F:99:GLU:O	6:1F:139:ARG:NH1	2.41	0.53
8:1H:137:ALA:O	8:1H:140:ILE:HG13	2.08	0.53
8:1H:192:GLU:OE1	8:1H:192:GLU:HA	2.08	0.53
9:1I:175:TYR:CZ	43:1r:38:PRO:HG3	2.43	0.53
12:1L:294:THR:HB	12:1L:520:TYR:CD1	2.44	0.53
12:1L:331:MET:HB3	12:1L:335:PHE:CE2	2.44	0.53
12:1L:338:MET:HA	12:1L:341:MET:SD	2.48	0.53
12:1L:583:LEU:HB2	12:1L:586:LEU:HD23	1.90	0.53
13:1M:278:ARG:NH2	37:1l:82:ASP:OD1	2.41	0.53
15:1O:101:TYR:HA	15:1O:131:ASP:OD1	2.09	0.53
32:1g:71:VAL:O	32:1g:75:THR:HG23	2.09	0.53
42:1q:48:TYR:OH	42:1q:83:PRO:HD2	2.08	0.53
44:1s:45:GLU:OE1	44:1s:45:GLU:N	2.38	0.53
12:1L:85:PHE:HA	12:1L:326:PHE:CE2	2.44	0.53
16:1P:147:ARG:O	16:1P:151:VAL:HG12	2.08	0.53
29:1d:12:GLN:O	46:1d:201:PC1:H221	2.09	0.53
4:1D:116:GLN:NE2	4:1D:276:ASP:OD2	2.38	0.53
5:1E:63:ILE:HA	5:1E:66:MET:HG3	1.91	0.53
8:1H:85:MET:CE	8:1H:108:MET:HB2	2.34	0.53
12:1L:247:LEU:H	12:1L:247:LEU:HD12	1.74	0.53
15:1O:279:LEU:O	15:1O:283:THR:HG23	2.09	0.53
16:1P:270:PHE:HD2	16:1P:279:THR:HB	1.73	0.53
20:1T:17:TYR:O	20:1T:21:LEU:HD22	2.09	0.53
43:1r:101:LYS:HA	43:1r:101:LYS:HE3	1.90	0.53
2:1B:62:MET:HA	2:1B:67:TYR:HB2	1.91	0.52
4:1D:29:LYS:HD2	4:1D:29:LYS:C	2.34	0.52
4:1D:282:GLU:O	4:1D:313:GLN:NE2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:14:ILE:HD11	12:1L:43:ALA:HA	1.92	0.52
12:1L:361:GLY:HA2	36:1k:59:ASN:HD21	1.74	0.52
13:1M:391:ILE:H	13:1M:391:ILE:HD12	1.73	0.52
28:1c:29:ILE:HD12	28:1c:30:TYR:N	2.23	0.52
30:1e:19:ILE:HG21	33:1h:128:ILE:HG21	1.91	0.52
38:1m:116:GLN:HG2	38:1m:117:GLU:OE1	2.09	0.52
3:1C:175:ARG:NH2	3:1C:177:ASP:OD1	2.42	0.52
9:1I:99:ARG:HH21	9:1I:105:ARG:HG3	1.74	0.52
12:1L:573:MET:HA	12:1L:576:MET:HG2	1.91	0.52
34:1i:57:LYS:HG3	34:1i:58:ASN:N	2.25	0.52
35:1j:70:ASP:OD2	35:1j:70:ASP:N	2.42	0.52
4:1D:148:LEU:HG	4:1D:174:ARG:HE	1.75	0.52
4:1D:169:TRP:CE2	9:1I:40:TYR:CD2	2.98	0.52
9:1I:135:PRO:HG3	9:1I:164:GLU:HG2	1.92	0.52
12:1L:209:PRO:HG3	12:1L:266:LEU:HG	1.90	0.52
12:1L:257:VAL:O	12:1L:261:ILE:HG13	2.10	0.52
12:1L:554:ASP:OD2	13:1M:288:TYR:OH	2.17	0.52
27:1b:15:GLU:HB2	27:1b:18:LEU:HD23	1.91	0.52
32:1g:100:ARG:HD3	32:1g:107:LEU:HA	1.92	0.52
34:1i:97:VAL:HG23	41:1p:115:ARG:HD2	1.91	0.52
41:1p:28:PRO:O	41:1p:32:LEU:HD22	2.10	0.52
1:1A:20:ILE:H	1:1A:20:ILE:HD12	1.74	0.52
2:1B:71:ARG:HA	8:1H:37:PRO:HA	1.91	0.52
4:1D:83:LEU:O	4:1D:85:ARG:HD3	2.09	0.52
7:1G:36:GLN:HE22	17:1Q:48:GLY:HA2	1.74	0.52
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.26	0.52
12:1L:467:ILE:O	12:1L:471:ASN:ND2	2.33	0.52
12:1L:605:HIS:HB2	14:1N:96:THR:HG21	1.91	0.52
13:1M:299:VAL:O	13:1M:303:ILE:HG12	2.09	0.52
13:1M:354:LEU:HD22	33:1h:21:PHE:CD2	2.44	0.52
15:1O:136:GLU:N	15:1O:136:GLU:OE1	2.43	0.52
15:1O:221:LEU:HD11	15:1O:241:LEU:HD11	1.91	0.52
20:1T:29:LYS:O	20:1T:34:SER:OG	2.23	0.52
23:1X:106:PHE:O	23:1X:110:VAL:HG13	2.10	0.52
26:1a:21:MET:HG3	26:1a:22:ALA:N	2.23	0.52
34:1i:85:LEU:HA	34:1i:89:VAL:HB	1.92	0.52
40:1o:64:GLN:HE22	40:1o:82:GLU:HB3	1.74	0.52
41:1p:28:PRO:HA	41:1p:31:TYR:CD2	2.44	0.52
6:1F:108:ARG:HG2	6:1F:112:ARG:HD3	1.91	0.52
7:1G:303:VAL:HG22	7:1G:559:VAL:HG21	1.90	0.52
10:1J:70:TYR:CE1	11:1K:79:VAL:HG23	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:332:HIS:ND1	12:1L:336:LYS:HG3	2.25	0.52
16:1P:323:THR:OG1	16:1P:324:TYR:N	2.43	0.52
21:1V:68:GLU:HG3	21:1V:76:ILE:HG12	1.92	0.52
1:1A:32:GLU:H	1:1A:32:GLU:CD	2.18	0.52
11:1K:77:LEU:O	11:1K:81:VAL:HG13	2.10	0.52
12:1L:288:THR:HG21	12:1L:307:SER:HB2	1.92	0.52
12:1L:330:CYS:HB2	12:1L:331:MET:HE3	1.91	0.52
17:1Q:35:VAL:HA	17:1Q:58:GLU:O	2.09	0.52
28:1c:33:LYS:HZ1	28:1c:37:GLU:HB2	1.74	0.52
37:1l:10:PRO:C	38:1m:74:ASN:HD21	2.17	0.52
4:1D:75:LYS:HD2	4:1D:76:CYS:H	1.75	0.52
5:1E:166:PRO:HB2	5:1E:167:LYS:HE2	1.92	0.52
12:1L:353:GLU:OE1	39:1n:79:TYR:OH	2.26	0.52
13:1M:181:TYR:O	41:1p:152:ARG:NH1	2.43	0.52
13:1M:215:TRP:O	13:1M:219:ALA:CB	2.58	0.52
13:1M:403:THR:HA	13:1M:406:TYR:CZ	2.45	0.52
20:1T:58:PHE:HB3	20:1T:60:PHE:CE1	2.44	0.52
24:1Y:139:LYS:HD3	33:1h:112:ARG:HD3	1.91	0.52
36:1k:32:GLN:HE22	36:1k:41:ARG:HA	1.74	0.52
7:1G:40:PHE:HB2	7:1G:52:CYS:SG	2.49	0.52
7:1G:627:SER:HB3	7:1G:630:LEU:HG	1.91	0.52
12:1L:306:THR:O	12:1L:310:LEU:HD22	2.09	0.52
20:1U:50:ILE:HG22	36:1k:44:TRP:CZ2	2.42	0.52
32:1g:91:ARG:O	32:1g:95:ARG:NH2	2.43	0.52
34:1i:12:GLN:HA	34:1i:15:ARG:HB2	1.92	0.52
1:1A:46:SER:OG	1:1A:47:ALA:N	2.43	0.52
12:1L:172:ILE:O	12:1L:176:ARG:HG2	2.10	0.52
13:1M:196:TRP:HZ3	13:1M:261:PHE:HE1	1.58	0.52
13:1M:433:GLU:OE2	13:1M:433:GLU:N	2.36	0.52
15:1O:192:MET:HA	15:1O:192:MET:HE3	1.92	0.52
20:1T:22:TYR:HD2	20:1T:23:ASP:N	2.08	0.52
36:1k:87:LEU:HD12	36:1k:88:GLU:N	2.25	0.52
39:1n:23:LEU:HD21	39:1n:40:ALA:HB1	1.92	0.52
39:1n:25:HIS:HD2	39:1n:74:GLN:HB2	1.75	0.52
40:1o:52:LEU:HD23	40:1o:55:ARG:HD2	1.92	0.52
2:1B:37:VAL:HG21	46:1B:202:PC1:H382	1.91	0.52
4:1D:258:VAL:O	4:1D:262:GLY:N	2.32	0.52
6:1F:68:ARG:O	6:1F:106:LYS:NZ	2.40	0.52
12:1L:321:GLN:HB3	12:1L:324:LEU:HD13	1.92	0.52
13:1M:306:PRO:HB3	13:1M:458:LEU:HD12	1.91	0.52
13:1M:406:TYR:O	13:1M:410:MET:HE2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:280:THR:O	14:1N:284:MET:HG2	2.10	0.52
32:1g:95:ARG:HH22	41:1p:64:HIS:CG	2.28	0.52
37:1l:6:LYS:NZ	37:1l:9:PHE:O	2.42	0.52
39:1n:126:ARG:NH2	39:1n:130:GLU:OE1	2.42	0.52
42:1q:20:LEU:O	42:1q:24:LEU:HD22	2.10	0.52
4:1D:422:ASP:N	4:1D:422:ASP:OD1	2.41	0.51
7:1G:223:ARG:HH22	17:1Q:81:ASN:HD21	1.58	0.51
12:1L:482:MET:HB2	12:1L:486:MET:HE1	1.91	0.51
14:1N:269:GLU:OE1	14:1N:269:GLU:HA	2.09	0.51
16:1P:96:GLY:O	55:1P:501:NDP:H8A	2.10	0.51
20:1U:12:LYS:CE	20:1U:16:LEU:HD23	2.39	0.51
22:1W:113:PRO:O	22:1W:114:ARG:NH1	2.43	0.51
7:1G:46:LEU:HD12	7:1G:158:ARG:HG2	1.92	0.51
7:1G:324:ASP:HB2	7:1G:571:ALA:HB1	1.92	0.51
7:1G:646:ASN:OD1	7:1G:650:LYS:NZ	2.39	0.51
12:1L:123:LEU:O	12:1L:127:THR:HG22	2.09	0.51
12:1L:440:LEU:HG	12:1L:442:LEU:HD23	1.92	0.51
15:1O:221:LEU:HD21	15:1O:241:LEU:HD21	1.92	0.51
21:1V:36:GLN:HB3	21:1V:94:LEU:HD11	1.92	0.51
24:1Y:120:THR:O	24:1Y:124:VAL:HG12	2.11	0.51
29:1d:52:PRO:HD2	29:1d:56:ALA:HB2	1.92	0.51
30:1e:20:GLN:O	30:1e:24:GLN:NE2	2.42	0.51
32:1g:45:HIS:HB3	32:1g:58:MET:HE3	1.91	0.51
3:1C:90:PHE:HZ	3:1C:163:ARG:HE	1.59	0.51
7:1G:190:MET:HE3	7:1G:690:ALA:HB1	1.92	0.51
9:1I:13:ASP:OD1	9:1I:14:MET:N	2.43	0.51
9:1I:151:LYS:HE3	9:1I:155:LEU:HD11	1.93	0.51
12:1L:544:MET:O	12:1L:548:SER:OG	2.23	0.51
13:1M:24:TRP:O	13:1M:28:THR:OG1	2.25	0.51
20:1U:63:PRO:HB2	20:1U:65:ILE:HG22	1.93	0.51
23:1X:157:LEU:HD13	29:1d:88:HIS:HB2	1.93	0.51
32:1g:24:ILE:HD12	32:1g:26:LEU:H	1.75	0.51
33:1h:87:TYR:O	33:1h:91:MET:HE2	2.10	0.51
35:1j:14:PHE:HE1	35:1j:17:LEU:HD11	1.76	0.51
41:1p:29:VAL:HA	41:1p:32:LEU:HD23	1.92	0.51
11:1K:20:LEU:HB3	12:1L:592:LEU:HB2	1.93	0.51
12:1L:100:ILE:HD11	12:1L:246:LEU:HD22	1.93	0.51
13:1M:354:LEU:HD22	33:1h:21:PHE:HD2	1.76	0.51
15:1O:183:ILE:O	15:1O:192:MET:HE1	2.09	0.51
32:1g:88:TRP:CD1	41:1p:65:ARG:HB3	2.44	0.51
38:1m:124:PHE:HE1	41:1p:132:THR:HA	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:176:ARG:HA	39:1n:178:MET:HE3	1.91	0.51
4:1D:19:MET:HE1	14:1N:172:GLN:C	2.34	0.51
6:1F:118:LEU:HD23	6:1F:225:VAL:HG13	1.92	0.51
7:1G:415:LEU:O	7:1G:417:TYR:N	2.43	0.51
8:1H:207:LEU:O	8:1H:209:SER:N	2.43	0.51
12:1L:12:LEU:O	12:1L:16:THR:HG23	2.10	0.51
16:1P:173:GLY:H	16:1P:176:ASP:HB3	1.76	0.51
5:1E:172:ILE:HG23	5:1E:182:PRO:HG3	1.92	0.51
8:1H:97:ASN:OD1	26:1a:40:HIS:NE2	2.30	0.51
13:1M:133:ILE:HG12	13:1M:223:ALA:HB2	1.93	0.51
16:1P:9:GLY:HA3	16:1P:15:SER:HB3	1.93	0.51
29:1d:106:LYS:NZ	41:1p:78:GLU:O	2.44	0.51
38:1m:117:GLU:OE1	38:1m:117:GLU:N	2.44	0.51
40:1o:36:ARG:HB2	40:1o:57:TYR:CE2	2.45	0.51
1:1A:60:ILE:HD13	11:1K:75:LEU:HD11	1.93	0.51
1:1A:69:ILE:HA	1:1A:72:LEU:HB2	1.92	0.51
2:1B:47:PRO:HD3	2:1B:74:VAL:CG2	2.41	0.51
2:1B:66:ARG:HD2	4:1D:175:GLU:HG2	1.92	0.51
3:1C:96:LEU:HB2	3:1C:105:ILE:HG22	1.92	0.51
8:1H:90:PRO:HG2	8:1H:240:ILE:HD12	1.93	0.51
11:1K:5:TYR:HA	11:1K:43:MET:HE1	1.93	0.51
11:1K:8:ILE:HB	11:1K:43:MET:HE3	1.93	0.51
12:1L:293:ILE:HD11	12:1L:418:LEU:HB3	1.93	0.51
14:1N:72:MET:HE2	14:1N:72:MET:HA	1.92	0.51
14:1N:194:LEU:HD13	14:1N:201:THR:HG21	1.93	0.51
20:1U:17:TYR:O	20:1U:21:LEU:HB2	2.11	0.51
4:1D:233:ARG:HG2	9:1I:30:LEU:HD11	1.92	0.51
10:1J:165:VAL:O	10:1J:168:ILE:HG22	2.11	0.51
12:1L:419:THR:HA	12:1L:422:TYR:CE1	2.45	0.51
13:1M:116:ILE:O	13:1M:120:ILE:HG12	2.11	0.51
13:1M:352:LEU:HD22	13:1M:429:SER:HB3	1.93	0.51
13:1M:355:MET:HE2	13:1M:429:SER:HB2	1.93	0.51
14:1N:270:MET:HG3	14:1N:279:PRO:HG3	1.93	0.51
20:1U:45:LEU:O	20:1U:49:GLU:HG3	2.11	0.51
23:1X:101:LYS:O	23:1X:105:LYS:HG2	2.11	0.51
51:1a:101:CDL:OA4	51:1a:101:CDL:HA4	2.11	0.51
1:1A:68:GLU:CD	1:1A:98:LEU:HD13	2.35	0.51
2:1B:166:LYS:HD3	2:1B:166:LYS:O	2.10	0.51
7:1G:223:ARG:HH22	17:1Q:81:ASN:ND2	2.09	0.51
10:1J:132:ASP:OD1	10:1J:134:GLY:N	2.43	0.51
13:1M:294:MET:O	13:1M:298:ILE:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:20:VAL:HG11	14:1N:137:ALA:HB1	1.93	0.51
15:1O:80:GLU:HB3	15:1O:190:HIS:CE1	2.46	0.51
23:1X:21:SER:HB2	26:1a:47:LEU:HD13	1.93	0.51
29:1d:104:LYS:HD2	29:1d:106:LYS:HE2	1.91	0.51
38:1m:115:ILE:HD12	38:1m:115:ILE:H	1.76	0.51
2:1B:73:GLY:HA2	8:1H:47:GLN:NE2	2.26	0.51
10:1J:67:VAL:HG11	11:1K:31:LEU:HD21	1.92	0.51
10:1J:110:GLU:OE2	10:1J:110:GLU:N	2.36	0.51
12:1L:153:LEU:HA	13:1M:416:ARG:HH22	1.74	0.51
12:1L:545:SER:HA	12:1L:549:ALA:HB3	1.93	0.51
13:1M:69:THR:HG22	13:1M:234:VAL:HG11	1.93	0.51
14:1N:40:MET:HE1	14:1N:129:LEU:HG	1.92	0.51
15:1O:231:ALA:O	15:1O:235:VAL:HG13	2.11	0.51
12:1L:305:SER:HB3	12:1L:422:TYR:HE2	1.75	0.50
13:1M:135:ARG:HH12	52:1N:401:3PE:C34	2.16	0.50
13:1M:204:MET:HE1	13:1M:261:PHE:HB3	1.93	0.50
15:1O:169:VAL:HB	15:1O:214:MET:CE	2.40	0.50
15:1O:180:GLN:O	15:1O:183:ILE:HG13	2.11	0.50
15:1O:291:ARG:NH1	32:1g:29:ASP:OD2	2.44	0.50
20:1T:8:LEU:HD23	20:1T:86:VAL:HG11	1.93	0.50
23:1X:12:LEU:HD23	23:1X:12:LEU:H	1.76	0.50
39:1n:82:PRO:HA	39:1n:87:GLY:HA3	1.93	0.50
39:1n:125:LYS:O	39:1n:129:ARG:HG2	2.11	0.50
42:1q:48:TYR:HE1	42:1q:86:TRP:CG	2.28	0.50
1:1A:16:LEU:O	1:1A:20:ILE:HD12	2.11	0.50
1:1A:109:LYS:HZ2	10:1J:169:MET:HE1	1.75	0.50
10:1J:45:LEU:HD23	10:1J:50:SER:HA	1.93	0.50
15:1O:295:LYS:O	15:1O:298:GLU:HG2	2.12	0.50
21:1V:113:TRP:CG	21:1V:113:TRP:O	2.64	0.50
22:1W:69:LYS:HB2	22:1W:69:LYS:NZ	2.26	0.50
33:1h:45:VAL:HG23	33:1h:46:PHE:HD1	1.75	0.50
41:1p:4:TRP:HB2	41:1p:9:TYR:HD2	1.76	0.50
42:1q:53:LYS:NZ	42:1q:53:LYS:HB2	2.26	0.50
4:1D:151:ILE:HG21	4:1D:174:ARG:HG3	1.93	0.50
8:1H:111:LEU:HD12	10:1J:57:PHE:CE1	2.46	0.50
12:1L:313:MET:HE3	12:1L:329:ILE:CG2	2.41	0.50
12:1L:386:LEU:O	12:1L:389:PHE:HD1	1.94	0.50
14:1N:24:SER:HB3	30:1e:1:PRO:HG3	1.93	0.50
17:1Q:36:ARG:NE	17:1Q:106:GLU:OE2	2.29	0.50
20:1T:68:GLU:OE1	20:1T:68:GLU:N	2.44	0.50
20:1U:53:ALA:O	20:1U:57:GLU:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:52:LEU:HD21	22:1W:103:ILE:HG21	1.92	0.50
23:1X:10:GLU:HA	23:1X:13:LYS:HE2	1.94	0.50
29:1d:15:PRO:O	29:1d:17:GLU:N	2.38	0.50
33:1h:14:SER:HB2	39:1n:106:TRP:HA	1.92	0.50
33:1h:84:GLU:O	33:1h:88:GLU:HG2	2.11	0.50
36:1k:46:ARG:H	36:1k:46:ARG:NE	2.09	0.50
37:1l:18:GLU:H	37:1l:18:GLU:CD	2.17	0.50
3:1C:45:PHE:HD1	3:1C:47:GLU:HG3	1.76	0.50
4:1D:306:GLN:O	4:1D:310:ILE:HG13	2.12	0.50
12:1L:100:ILE:HD12	12:1L:101:MET:N	2.25	0.50
13:1M:76:MET:HG3	13:1M:229:MET:HE2	1.92	0.50
29:1d:104:LYS:NZ	29:1d:107:LYS:HG2	2.25	0.50
37:1l:30:ARG:HD2	37:1l:32:GLU:HB3	1.93	0.50
6:1F:200:GLN:HG3	6:1F:202:LYS:HE2	1.92	0.50
7:1G:215:PHE:CD1	9:1I:104:ARG:HD2	2.47	0.50
10:1J:64:MET:HE1	11:1K:31:LEU:HD22	1.93	0.50
11:1K:59:MET:HG3	14:1N:84:TRP:CH2	2.46	0.50
12:1L:227:PHE:HD1	12:1L:228:GLY:H	1.60	0.50
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.39	0.50
14:1N:322:GLN:HA	14:1N:322:GLN:OE1	2.11	0.50
16:1P:134:HIS:HB2	16:1P:149:LYS:HD3	1.92	0.50
23:1X:14:VAL:HG13	23:1X:16:GLU:H	1.74	0.50
24:1Y:25:THR:HG23	24:1Y:67:ALA:HB2	1.93	0.50
25:1Z:99:LYS:HE2	25:1Z:99:LYS:CA	2.39	0.50
37:1l:156:TYR:HB3	40:1o:33:ARG:HG3	1.94	0.50
2:1B:144:ILE:HG13	2:1B:163:LEU:HB2	1.93	0.50
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.11	0.50
5:1E:6:LEU:O	5:1E:92:ARG:NH2	2.40	0.50
5:1E:120:ILE:HG21	5:1E:139:LEU:HD13	1.93	0.50
6:1F:226:GLU:O	6:1F:230:VAL:HG13	2.12	0.50
7:1G:211:LYS:HD3	7:1G:700:GLU:OE1	2.11	0.50
10:1J:31:LEU:O	10:1J:35:VAL:HG12	2.12	0.50
12:1L:202:PHE:CD1	12:1L:265:PRO:HG2	2.46	0.50
12:1L:206:ASN:H	12:1L:206:ASN:ND2	2.10	0.50
12:1L:231:PRO:C	12:1L:234:PRO:HD2	2.37	0.50
17:1Q:97:GLU:N	17:1Q:97:GLU:OE2	2.44	0.50
22:1W:18:LYS:O	22:1W:77:ARG:HD3	2.11	0.50
22:1W:39:TRP:O	22:1W:43:VAL:HG23	2.12	0.50
32:1g:92:GLU:HG2	41:1p:64:HIS:HE2	1.76	0.50
34:1i:10:ARG:HD2	39:1n:155:PRO:HA	1.93	0.50
34:1i:70:ALA:HA	34:1i:74:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:125:GLN:O	34:1i:126:HIS:ND1	2.45	0.50
38:1m:34:GLU:N	38:1m:34:GLU:OE2	2.45	0.50
40:1o:38:MET:HA	40:1o:38:MET:HE3	1.93	0.50
6:1F:46:LYS:HZ2	6:1F:50:LEU:HD11	1.77	0.50
6:1F:61:LYS:HG2	6:1F:76:GLY:HA3	1.94	0.50
7:1G:19:MET:HA	7:1G:19:MET:HE3	1.93	0.50
11:1K:33:LEU:HD11	14:1N:64:ALA:HB1	1.93	0.50
12:1L:359:MET:N	12:1L:359:MET:SD	2.84	0.50
13:1M:127:VAL:O	13:1M:131:ILE:HG12	2.12	0.50
16:1P:271:GLU:OE2	16:1P:281:ARG:N	2.31	0.50
21:1V:47:THR:O	21:1V:51:THR:OG1	2.25	0.50
28:1c:17:VAL:O	28:1c:21:LEU:HD22	2.11	0.50
38:1m:55:ARG:HG3	38:1m:55:ARG:O	2.10	0.50
3:1C:90:PHE:HB2	3:1C:111:THR:O	2.12	0.50
4:1D:109:VAL:HG12	4:1D:152:MET:HE3	1.94	0.50
6:1F:389:ILE:HD11	6:1F:430:MET:HE1	1.94	0.50
8:1H:113:VAL:HG11	10:1J:65:LEU:HD12	1.93	0.50
12:1L:597:ILE:HA	12:1L:601:LEU:HB2	1.94	0.50
13:1M:25:ILE:HG23	32:1g:60:VAL:HG21	1.93	0.50
13:1M:286:ILE:HD13	13:1M:326:LEU:HB3	1.94	0.50
14:1N:338:PRO:O	23:1X:169:TRP:NE1	2.44	0.50
20:1T:83:LYS:NZ	20:1T:84:LYS:HB3	2.27	0.50
34:1i:26:GLU:OE1	34:1i:26:GLU:HA	2.10	0.50
34:1i:68:ILE:HD12	34:1i:69:PHE:N	2.27	0.50
39:1n:120:LYS:HA	39:1n:123:GLN:HG3	1.93	0.50
39:1n:128:ARG:HD2	39:1n:167:TRP:CD2	2.46	0.50
4:1D:207:LEU:N	25:1Z:9:ASP:OD2	2.34	0.50
7:1G:337:ARG:HD2	7:1G:609:MET:HB2	1.93	0.50
8:1H:91:MET:HG2	8:1H:259:PHE:CE1	2.47	0.50
13:1M:29:VAL:HG13	13:1M:30:HIS:ND1	2.27	0.50
13:1M:94:LEU:CD1	52:1N:401:3PE:H351	2.41	0.50
13:1M:104:LEU:O	13:1M:108:MET:HG2	2.12	0.50
13:1M:438:ALA:HA	13:1M:441:ILE:HG22	1.93	0.50
15:1O:235:VAL:HA	15:1O:238:ILE:HG22	1.94	0.50
16:1P:35:VAL:O	16:1P:39:GLY:N	2.36	0.50
18:1R:80:LYS:NZ	18:1R:81:THR:H	2.10	0.50
34:1i:10:ARG:NH1	39:1n:154:PRO:O	2.45	0.50
38:1m:110:LYS:HA	38:1m:113:LYS:HZ3	1.76	0.50
41:1p:109:LEU:HD13	41:1p:127:GLU:CB	2.35	0.50
7:1G:321:GLY:HA3	7:1G:496:ILE:HD12	1.92	0.49
9:1I:6:ASN:O	9:1I:7:MET:HE2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:1K:10:MET:O	11:1K:14:ILE:HG23	2.12	0.49
12:1L:371:THR:HA	12:1L:374:ILE:HD11	1.94	0.49
12:1L:502:LEU:HD13	36:1k:62:PHE:HD2	1.77	0.49
13:1M:423:ILE:HG22	38:1m:58:VAL:HG13	1.93	0.49
14:1N:17:THR:O	14:1N:21:MET:HG3	2.12	0.49
19:1S:36:ILE:HD12	19:1S:40:TYR:HB2	1.94	0.49
24:1Y:48:PHE:O	24:1Y:52:VAL:HG23	2.12	0.49
32:1g:76:PHE:O	32:1g:80:LEU:HD23	2.12	0.49
32:1g:100:ARG:HA	32:1g:103:ASN:ND2	2.27	0.49
34:1i:1:SAC:O	34:1i:2:GLY:N	2.45	0.49
34:1i:42:MET:HG3	34:1i:43:GLU:N	2.27	0.49
41:1p:35:ILE:HD12	41:1p:36:PHE:N	2.27	0.49
4:1D:259:MET:CE	4:1D:421:GLN:HG3	2.41	0.49
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.93	0.49
10:1J:105:TYR:O	10:1J:109:LYS:HG2	2.12	0.49
16:1P:157:ARG:NH1	16:1P:225:GLY:O	2.45	0.49
24:1Y:49:LEU:HD12	24:1Y:50:GLU:H	1.77	0.49
37:1l:114:PHE:C	37:1l:114:PHE:CD1	2.89	0.49
42:1q:86:TRP:CE3	42:1q:98:PRO:HD2	2.46	0.49
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.95	0.49
5:1E:89:MET:HG3	6:1F:181:ALA:C	2.37	0.49
6:1F:31:TRP:NE1	44:1s:42:GLN:OE1	2.34	0.49
9:1I:72:SER:HB2	18:1R:47:GLN:HG3	1.94	0.49
12:1L:101:MET:C	12:1L:101:MET:HE2	2.37	0.49
12:1L:233:LEU:HD11	12:1L:248:HIS:HB3	1.94	0.49
12:1L:458:LEU:O	12:1L:462:ILE:HG23	2.12	0.49
14:1N:245:MET:HE1	52:1N:401:3PE:H3A2	1.94	0.49
15:1O:182:ARG:HA	15:1O:185:LYS:HE2	1.94	0.49
25:1Z:104:TRP:CH2	30:1e:77:ALA:HB3	2.47	0.49
28:1c:5:ARG:HB3	28:1c:5:ARG:NH1	2.28	0.49
28:1c:12:PRO:HG2	28:1c:14:TRP:CZ3	2.48	0.49
31:1f:5:GLN:O	31:1f:5:GLN:NE2	2.39	0.49
32:1g:73:GLY:O	32:1g:77:VAL:HG12	2.12	0.49
4:1D:20:TYR:HB3	12:1L:575:ILE:HD11	1.94	0.49
12:1L:385:TYR:O	35:1j:36:ILE:HG22	2.12	0.49
12:1L:528:TYR:HE1	37:1l:96:VAL:HG21	1.77	0.49
14:1N:118:VAL:O	14:1N:122:ILE:HG12	2.12	0.49
14:1N:159:MET:HG2	14:1N:278:MET:HE1	1.94	0.49
16:1P:16:VAL:HG22	17:1Q:68:PRO:HG3	1.94	0.49
16:1P:144:ARG:O	16:1P:148:SER:OG	2.28	0.49
19:1S:39:ARG:HH21	19:1S:87:THR:HG21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:64:ASP:OD2	22:1W:30:ARG:HG3	2.12	0.49
23:1X:46:ARG:CZ	23:1X:52:PRO:HA	2.42	0.49
28:1c:25:VAL:O	28:1c:29:ILE:HG13	2.11	0.49
33:1h:40:ILE:HD12	33:1h:41:THR:H	1.75	0.49
37:1l:68:ASP:OD1	37:1l:68:ASP:N	2.45	0.49
2:1B:46:TRP:HH2	50:1H:701:U10:H353	1.77	0.49
3:1C:40:VAL:HG23	43:1r:68:VAL:HG23	1.94	0.49
3:1C:198:ASP:OD1	3:1C:198:ASP:N	2.44	0.49
8:1H:53:LEU:O	8:1H:57:THR:HG22	2.12	0.49
12:1L:174:TYR:HE2	12:1L:231:PRO:HD2	1.78	0.49
12:1L:439:PRO:HB3	35:1j:12:ARG:NE	2.27	0.49
12:1L:525:MET:HE2	37:1l:96:VAL:HG23	1.93	0.49
13:1M:287:ALA:O	13:1M:291:VAL:HG23	2.13	0.49
16:1P:285:GLU:C	16:1P:289:MET:HE2	2.37	0.49
34:1i:90:THR:HG22	34:1i:96:VAL:HG21	1.93	0.49
37:1l:30:ARG:HH21	38:1m:35:ARG:HB3	1.77	0.49
5:1E:126:ILE:HG23	5:1E:130:GLU:HB2	1.94	0.49
7:1G:256:GLU:O	7:1G:394:ARG:NH2	2.41	0.49
7:1G:543:ILE:HB	7:1G:557:ALA:HA	1.95	0.49
8:1H:194:ASN:ND2	8:1H:201:THR:HG21	2.27	0.49
9:1I:36:MET:HE2	9:1I:36:MET:HA	1.94	0.49
9:1I:153:LYS:O	9:1I:157:ASN:ND2	2.37	0.49
12:1L:556:ILE:HD11	38:1m:75:ILE:HG12	1.94	0.49
13:1M:233:ALA:HA	13:1M:320:GLY:HA2	1.93	0.49
14:1N:59:TYR:CE2	14:1N:63:GLN:HG3	2.48	0.49
20:1T:60:PHE:CZ	20:1T:80:ILE:HG23	2.47	0.49
20:1U:48:VAL:HG21	39:1n:16:LEU:HD22	1.94	0.49
30:1e:44:HIS:HD2	33:1h:129:ASP:HA	1.77	0.49
38:1m:44:ARG:O	38:1m:48:LEU:HD12	2.12	0.49
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.12	0.49
12:1L:241:THR:HA	12:1L:244:SER:HG	1.77	0.49
13:1M:45:LEU:HD13	13:1M:46:GLY:N	2.26	0.49
15:1O:25:ILE:HA	15:1O:168:VAL:O	2.13	0.49
19:1S:15:LEU:HD12	19:1S:50:LEU:HD21	1.95	0.49
21:1V:1:ALA:HA	21:1V:64:VAL:HG23	1.93	0.49
21:1V:13:LEU:HD22	21:1V:77:GLU:HB3	1.94	0.49
23:1X:47:TRP:O	23:1X:50:LYS:NZ	2.40	0.49
23:1X:150:ASN:ND2	33:1h:124:GLN:OE1	2.45	0.49
46:1f:101:PC1:H372	46:1f:101:PC1:H3B1	1.94	0.49
32:1g:90:ARG:NH1	41:1p:100:GLU:HB3	2.27	0.49
33:1h:9:PHE:CE2	39:1n:114:TYR:CD2	3.01	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:18:ASP:OD2	33:1h:18:ASP:N	2.45	0.49
40:1o:6:ARG:NE	40:1o:105:ARG:HH21	2.10	0.49
7:1G:283:MET:HE3	7:1G:293:TYR:CD1	2.48	0.49
13:1M:222:GLU:N	13:1M:222:GLU:CD	2.71	0.49
13:1M:235:LEU:HA	13:1M:238:LEU:HD23	1.95	0.49
14:1N:55:ALA:HB1	14:1N:118:VAL:HA	1.95	0.49
15:1O:260:ARG:HA	15:1O:263:VAL:HG22	1.93	0.49
22:1W:87:LYS:HB2	22:1W:87:LYS:NZ	2.27	0.49
32:1g:41:ASN:HB2	32:1g:43:ASP:OD1	2.12	0.49
33:1h:56:PRO:HD2	33:1h:59:TYR:HB3	1.95	0.49
37:1l:69:LEU:HG	37:1l:71:LEU:HB2	1.93	0.49
41:1p:43:PRO:O	41:1p:46:LEU:HD12	2.12	0.49
2:1B:149:CYS:SG	4:1D:105:ARG:NH1	2.86	0.49
4:1D:259:MET:SD	4:1D:405:MET:HE1	2.53	0.49
4:1D:414:VAL:O	4:1D:418:ILE:HG13	2.13	0.49
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	1.95	0.49
12:1L:573:MET:HE1	14:1N:167:TRP:CD2	2.48	0.49
13:1M:390:ASN:O	13:1M:393:ILE:HG22	2.13	0.49
25:1Z:133:ILE:O	25:1Z:137:THR:HG23	2.13	0.49
36:1k:77:PHE:HE1	36:1k:81:VAL:HG11	1.78	0.49
37:1l:29:MET:SD	37:1l:33:ASP:HB2	2.53	0.49
41:1p:98:ASP:HB3	41:1p:138:PHE:HE1	1.77	0.49
1:1A:48:ARG:HG3	1:1A:48:ARG:HH11	1.78	0.49
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.42	0.49
9:1I:4:PHE:HB3	9:1I:7:MET:HB2	1.95	0.49
11:1K:30:LEU:O	11:1K:34:GLU:HG3	2.13	0.49
11:1K:47:ILE:CD1	14:1N:79:LEU:HB2	2.42	0.49
12:1L:237:MET:SD	12:1L:303:ALA:HB2	2.53	0.49
12:1L:295:GLN:HB3	12:1L:301:ILE:HD11	1.95	0.49
12:1L:338:MET:HE3	12:1L:457:LEU:HD22	1.94	0.49
12:1L:396:ILE:HG21	12:1L:490:ALA:HB2	1.94	0.49
14:1N:154:MET:CE	14:1N:191:THR:HB	2.42	0.49
18:1R:78:GLU:OE1	18:1R:78:GLU:N	2.44	0.49
32:1g:71:VAL:HG11	33:1h:32:THR:HG23	1.95	0.49
32:1g:111:ASN:HB3	41:1p:161:ARG:HH22	1.76	0.49
37:1l:153:VAL:O	37:1l:153:VAL:HG12	2.13	0.49
1:1A:49:LEU:HD12	4:1D:45:SER:OG	2.12	0.48
1:1A:113:TRP:HH2	8:1H:282:TYR:CD1	2.31	0.48
6:1F:154:ARG:HA	44:1s:58:LEU:HD21	1.95	0.48
7:1G:94:MET:SD	7:1G:120:SER:HA	2.53	0.48
7:1G:560:ILE:O	7:1G:560:ILE:HG22	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:309:ILE:HG22	27:1b:38:THR:HG23	1.95	0.48
14:1N:44:LEU:HB3	14:1N:122:ILE:CG2	2.41	0.48
14:1N:165:GLY:HA2	14:1N:181:TYR:HD1	1.77	0.48
15:1O:23:LYS:HA	15:1O:167:HIS:ND1	2.28	0.48
15:1O:165:PRO:HB2	15:1O:218:CYS:SG	2.53	0.48
16:1P:38:LEU:O	16:1P:43:SER:OG	2.31	0.48
16:1P:133:SER:HA	16:1P:149:LYS:HE3	1.94	0.48
24:1Y:24:SER:OG	24:1Y:66:GLY:O	2.29	0.48
32:1g:76:PHE:CE1	33:1h:75:ILE:HD11	2.48	0.48
34:1i:11:LEU:O	34:1i:15:ARG:NH1	2.46	0.48
34:1i:44:GLN:HA	34:1i:47:ASN:HD21	1.78	0.48
34:1i:60:ILE:HD12	34:1i:61:TYR:N	2.28	0.48
37:1l:10:PRO:HB2	38:1m:74:ASN:ND2	2.28	0.48
39:1n:19:TYR:HE2	39:1n:23:LEU:HD22	1.78	0.48
40:1o:34:LYS:HD2	40:1o:34:LYS:C	2.37	0.48
7:1G:201:ASP:OD2	7:1G:268:ARG:NH2	2.33	0.48
9:1I:99:ARG:HE	9:1I:105:ARG:HG3	1.77	0.48
12:1L:137:LEU:HD12	12:1L:196:TRP:O	2.13	0.48
12:1L:452:ASN:O	12:1L:456:ARG:HD2	2.13	0.48
14:1N:61:LEU:HD12	14:1N:61:LEU:H	1.78	0.48
15:1O:134:PHE:O	15:1O:138:MET:HG3	2.12	0.48
16:1P:29:PHE:CE2	16:1P:176:ASP:HA	2.48	0.48
16:1P:97:ARG:NH1	55:1P:501:NDP:O3X	2.41	0.48
19:1S:66:ALA:O	19:1S:74:LYS:NZ	2.42	0.48
20:1T:31:SER:OG	20:1T:33:ASN:OD1	2.30	0.48
22:1W:17:VAL:HG22	22:1W:18:LYS:H	1.78	0.48
34:1i:44:GLN:HA	34:1i:47:ASN:ND2	2.29	0.48
38:1m:47:LEU:HB3	39:1n:165:LEU:HD22	1.94	0.48
39:1n:13:GLN:O	39:1n:17:ARG:HG2	2.13	0.48
6:1F:45:THR:HA	6:1F:48:ILE:HD12	1.95	0.48
12:1L:227:PHE:CE2	12:1L:283:ILE:HG22	2.48	0.48
12:1L:295:GLN:HG3	12:1L:304:PHE:HE2	1.78	0.48
13:1M:252:PRO:HG3	29:1d:117:HIS:NE2	2.28	0.48
14:1N:211:MET:HE1	14:1N:251:MET:CG	2.43	0.48
20:1U:24:LYS:HB3	20:1U:42:LEU:HD11	1.95	0.48
30:1e:69:GLN:HA	30:1e:72:MET:H	1.78	0.48
31:1f:49:ARG:HB3	31:1f:52:GLU:HB3	1.94	0.48
41:1p:14:ARG:HH11	41:1p:115:ARG:NH2	2.11	0.48
2:1B:101:ARG:NH1	2:1B:105:ASP:OD1	2.44	0.48
4:1D:6:PRO:HB3	4:1D:10:TRP:CD1	2.49	0.48
5:1E:183:LYS:O	5:1E:187:ARG:NH1	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:364:PRO:HB2	6:1F:403:THR:HG22	1.95	0.48
7:1G:146:VAL:HG21	7:1G:199:ILE:HD11	1.96	0.48
12:1L:599:MET:HE2	12:1L:599:MET:HA	1.95	0.48
13:1M:17:MET:SD	13:1M:17:MET:C	2.97	0.48
15:1O:283:THR:O	15:1O:283:THR:OG1	2.29	0.48
20:1U:36:PHE:CD2	20:1U:50:ILE:HD11	2.48	0.48
32:1g:109:GLU:O	41:1p:141:ARG:NE	2.41	0.48
34:1i:10:ARG:HH21	39:1n:163:PRO:HB2	1.78	0.48
36:1k:63:VAL:O	36:1k:67:LEU:HB2	2.13	0.48
39:1n:135:GLU:HB2	39:1n:164:PRO:HA	1.94	0.48
43:1r:20:GLN:HE21	43:1r:23:LEU:HD11	1.78	0.48
1:1A:71:LEU:HD11	11:1K:65:VAL:CG2	2.42	0.48
4:1D:117:ALA:HB2	4:1D:367:ILE:HG12	1.94	0.48
10:1J:157:THR:HG21	11:1K:62:ILE:HD12	1.96	0.48
12:1L:455:LYS:HA	12:1L:458:LEU:HB2	1.95	0.48
20:1U:13:ASP:HA	20:1U:16:LEU:HG	1.94	0.48
21:1V:26:LEU:HD11	21:1V:84:GLU:HG3	1.95	0.48
34:1i:93:PRO:HB3	41:1p:4:TRP:CG	2.48	0.48
36:1k:77:PHE:CE1	36:1k:81:VAL:HG11	2.49	0.48
37:1l:126:GLN:HB2	37:1l:128:VAL:HG23	1.95	0.48
37:1l:158:ILE:HG23	40:1o:96:LYS:HB3	1.95	0.48
38:1m:123:THR:HA	41:1p:136:LYS:HE2	1.95	0.48
42:1q:9:ARG:HG2	42:1q:10:GLY:N	2.29	0.48
5:1E:100:ILE:HD11	5:1E:137:PHE:HD2	1.79	0.48
7:1G:489:VAL:O	7:1G:491:ASN:ND2	2.47	0.48
8:1H:52:ALA:HB2	50:1H:701:U10:H421	1.95	0.48
12:1L:172:ILE:HG23	12:1L:176:ARG:NH1	2.29	0.48
12:1L:462:ILE:HD12	12:1L:463:PHE:HB3	1.96	0.48
13:1M:186:LEU:HD11	13:1M:192:ASN:HB3	1.95	0.48
13:1M:359:TRP:O	13:1M:363:SER:OG	2.30	0.48
14:1N:22:ILE:HB	30:1e:5:VAL:HG12	1.95	0.48
14:1N:30:TRP:O	14:1N:34:GLU:HG2	2.13	0.48
21:1V:76:ILE:O	21:1V:79:VAL:N	2.46	0.48
23:1X:122:GLY:HA3	27:1b:77:LEU:HD21	1.95	0.48
32:1g:34:ASP:OD1	32:1g:34:ASP:N	2.41	0.48
34:1i:122:PHE:O	34:1i:124:ASP:N	2.46	0.48
39:1n:106:TRP:HE3	39:1n:110:GLU:HB3	1.77	0.48
44:1s:38:TYR:CZ	44:1s:40:ASN:HB3	2.49	0.48
4:1D:410:MET:N	4:1D:413:ASP:OD1	2.43	0.48
7:1G:54:MET:HE1	7:1G:94:MET:HE3	1.96	0.48
10:1J:19:GLY:O	10:1J:83:TRP:NE1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:233:LEU:HB3	12:1L:234:PRO:HD3	1.96	0.48
12:1L:291:CYS:O	12:1L:295:GLN:HG2	2.13	0.48
12:1L:414:ILE:HG13	52:1L:701:3PE:H3B2	1.95	0.48
13:1M:158:LEU:HB3	14:1N:283:ALA:HB1	1.94	0.48
13:1M:182:TRP:CD1	41:1p:79:LYS:HG2	2.49	0.48
14:1N:153:LEU:O	14:1N:157:MET:HG2	2.13	0.48
15:1O:163:TYR:CE1	15:1O:262:LEU:HD12	2.48	0.48
17:1Q:16:LYS:HD2	17:1Q:16:LYS:C	2.38	0.48
19:1S:82:SER:H	19:1S:85:GLN:HB2	1.77	0.48
52:1Y:202:3PE:H242	52:1Y:202:3PE:H2	1.96	0.48
38:1m:24:ILE:HD13	38:1m:29:ARG:HE	1.79	0.48
40:1o:105:ARG:O	40:1o:109:GLN:HG2	2.13	0.48
42:1q:8:ARG:HG2	42:1q:12:GLN:OE1	2.14	0.48
1:1A:72:LEU:HD11	1:1A:95:LEU:HD21	1.95	0.48
4:1D:68:LEU:HB2	4:1D:73:VAL:HA	1.96	0.48
4:1D:75:LYS:HD2	4:1D:403:ASP:OD2	2.12	0.48
8:1H:40:VAL:HG23	8:1H:44:GLY:HA2	1.96	0.48
10:1J:139:GLU:O	10:1J:143:ILE:HG13	2.14	0.48
11:1K:41:PHE:C	11:1K:41:PHE:CD2	2.92	0.48
12:1L:106:TRP:CZ3	12:1L:450:LEU:HD13	2.49	0.48
12:1L:182:PHE:O	12:1L:185:SER:OG	2.31	0.48
12:1L:297:ASP:OD2	12:1L:354:GLN:NE2	2.45	0.48
12:1L:434:LYS:NZ	36:1k:57:ALA:HA	2.27	0.48
12:1L:454:ILE:HG22	12:1L:458:LEU:HD23	1.95	0.48
12:1L:504:LEU:HA	12:1L:507:THR:HG23	1.95	0.48
12:1L:525:MET:N	12:1L:525:MET:SD	2.87	0.48
12:1L:532:ILE:HG13	12:1L:533:MET:N	2.28	0.48
16:1P:3:HIS:HD2	16:1P:4:ALA:N	2.11	0.48
16:1P:131:HIS:HB3	16:1P:165:ILE:HD13	1.94	0.48
34:1i:8:LYS:O	34:1i:11:LEU:N	2.46	0.48
36:1k:19:LYS:N	36:1k:19:LYS:HD2	2.29	0.48
2:1B:89:ALA:HB2	2:1B:116:MET:HE3	1.96	0.48
3:1C:171:TYR:HE1	17:1Q:79:LEU:HD11	1.77	0.48
12:1L:295:GLN:NE2	12:1L:524:ASN:HA	2.24	0.48
13:1M:135:ARG:HG2	13:1M:135:ARG:HH11	1.79	0.48
19:1S:23:CYS:SG	19:1S:26:SER:OG	2.60	0.48
19:1S:32:VAL:HG22	19:1S:86:VAL:HG21	1.96	0.48
34:1i:71:VAL:HG23	34:1i:75:LEU:HD23	1.96	0.48
35:1j:63:GLU:OE1	40:1o:99:LYS:NZ	2.46	0.48
37:1l:108:PHE:CE1	37:1l:112:MET:HE1	2.48	0.48
37:1l:130:PRO:HD3	40:1o:21:MET:SD	2.54	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:30:THR:HG22	41:1p:34:LYS:HZ3	1.78	0.48
8:1H:277:TYR:HE2	9:1I:30:LEU:HG	1.79	0.48
12:1L:407:TRP:O	12:1L:411:MET:HG2	2.14	0.48
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.78	0.48
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.13	0.48
14:1N:187:MET:HE2	14:1N:187:MET:HA	1.95	0.48
15:1O:37:ARG:O	15:1O:41:GLU:HG2	2.13	0.48
20:1U:32:VAL:O	20:1U:73:PRO:HG2	2.14	0.48
20:1U:63:PRO:HG2	20:1U:66:ASP:HB2	1.95	0.48
21:1V:80:ILE:HD12	21:1V:80:ILE:H	1.79	0.48
34:1i:86:LYS:HD2	34:1i:87:TYR:CE1	2.49	0.48
39:1n:11:HIS:O	39:1n:15:VAL:HG13	2.14	0.48
41:1p:50:PHE:O	41:1p:53:GLN:HG3	2.14	0.48
7:1G:441:GLN:HG2	7:1G:444:LYS:HZ2	1.78	0.47
12:1L:435:PRO:HB3	12:1L:437:PHE:CE1	2.49	0.47
13:1M:33:LEU:O	13:1M:37:ILE:HG12	2.13	0.47
13:1M:261:PHE:HB2	13:1M:302:MET:HE2	1.96	0.47
14:1N:149:ILE:HG21	14:1N:154:MET:HG2	1.96	0.47
15:1O:188:ASN:OD1	15:1O:191:GLU:HG3	2.14	0.47
15:1O:285:GLY:O	15:1O:289:SER:OG	2.23	0.47
23:1X:16:GLU:O	23:1X:18:LYS:HG3	2.14	0.47
23:1X:52:PRO:HB3	25:1Z:80:ASP:HB2	1.96	0.47
23:1X:81:PHE:CD2	26:1a:66:LEU:HD21	2.49	0.47
25:1Z:138:TYR:HD1	25:1Z:142:TRP:CH2	2.32	0.47
36:1k:16:PRO:HD2	36:1k:21:TRP:HH2	1.79	0.47
36:1k:32:GLN:HB3	36:1k:33:GLU:OE2	2.14	0.47
5:1E:111:ARG:HB2	5:1E:152:PRO:CD	2.44	0.47
5:1E:163:ASP:OD2	5:1E:190:ARG:NH1	2.47	0.47
7:1G:141:ASN:ND2	7:1G:698:VAL:O	2.47	0.47
9:1I:120:GLY:O	9:1I:124:GLU:HG3	2.14	0.47
12:1L:31:LEU:H	12:1L:31:LEU:HD13	1.79	0.47
13:1M:252:PRO:HG3	29:1d:117:HIS:CD2	2.49	0.47
19:1S:64:LEU:HB2	19:1S:78:LEU:HD11	1.96	0.47
20:1T:51:ILE:O	20:1T:55:GLU:HG3	2.14	0.47
25:1Z:73:PRO:HD3	27:1b:52:TYR:HE2	1.79	0.47
27:1b:43:ARG:HG2	27:1b:79:TRP:CZ2	2.48	0.47
29:1d:78:ARG:NH1	46:1d:201:PC1:H222	2.27	0.47
33:1h:23:LYS:HD2	33:1h:23:LYS:C	2.39	0.47
41:1p:32:LEU:O	41:1p:35:ILE:HD12	2.13	0.47
6:1F:19:ASP:OD2	6:1F:241:TRP:NE1	2.41	0.47
6:1F:215:VAL:HG13	6:1F:220:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:313:SER:HB2	25:1Z:51:MET:HA	1.95	0.47
12:1L:97:THR:HA	12:1L:100:ILE:HD11	1.96	0.47
12:1L:368:PHE:HE2	12:1L:454:ILE:HD12	1.78	0.47
12:1L:596:MET:SD	12:1L:596:MET:N	2.86	0.47
13:1M:293:HIS:HD2	13:1M:319:HIS:HD2	1.62	0.47
13:1M:369:LEU:HD22	13:1M:370:PRO:HD2	1.95	0.47
17:1Q:69:LEU:HD11	42:1q:126:PRO:HG2	1.97	0.47
25:1Z:104:TRP:HH2	30:1e:77:ALA:HB3	1.79	0.47
29:1d:34:MET:HE3	29:1d:72:GLY:CA	2.42	0.47
39:1n:133:GLU:HA	39:1n:136:VAL:HG22	1.95	0.47
1:1A:95:LEU:HB3	8:1H:302:MET:SD	2.55	0.47
6:1F:428:GLU:O	6:1F:432:GLN:HG2	2.14	0.47
7:1G:283:MET:HE3	7:1G:293:TYR:CE1	2.48	0.47
12:1L:69:MET:HE1	13:1M:451:PRO:HD2	1.95	0.47
12:1L:511:LEU:HA	39:1n:35:LYS:HE3	1.95	0.47
14:1N:162:ILE:CD1	14:1N:282:MET:HG2	2.41	0.47
51:1a:101:CDL:HA62	42:1q:6:VAL:HG13	1.94	0.47
36:1k:38:ARG:HD3	36:1k:38:ARG:N	2.29	0.47
37:1l:30:ARG:HG3	37:1l:32:GLU:N	2.29	0.47
37:1l:108:PHE:CZ	37:1l:112:MET:HE1	2.49	0.47
39:1n:99:PRO:HG2	39:1n:102:CYS:SG	2.54	0.47
40:1o:19:LEU:H	40:1o:19:LEU:HD22	1.78	0.47
1:1A:10:ASN:ND2	8:1H:83:LEU:HB3	2.26	0.47
3:1C:189:GLU:HG3	17:1Q:76:ALA:HB2	1.96	0.47
7:1G:337:ARG:HB2	7:1G:337:ARG:HH11	1.79	0.47
12:1L:203:MET:HE3	41:1p:109:LEU:CG	2.40	0.47
12:1L:481:THR:CG2	35:1j:51:PHE:HB2	2.45	0.47
12:1L:510:TYR:O	39:1n:35:LYS:HE3	2.14	0.47
13:1M:329:LEU:HD22	13:1M:359:TRP:CD1	2.49	0.47
14:1N:89:MET:CG	14:1N:95:MET:HB2	2.42	0.47
15:1O:317:ILE:HG22	15:1O:320:LYS:HZ2	1.79	0.47
16:1P:82:ARG:HH11	16:1P:82:ARG:HG3	1.79	0.47
20:1T:45:LEU:HD23	57:1W:201:EHZ:C18	2.45	0.47
20:1T:60:PHE:CE2	20:1T:83:LYS:HG3	2.50	0.47
21:1V:63:ASP:OD1	21:1V:65:LYS:N	2.47	0.47
23:1X:52:PRO:HD2	25:1Z:116:TRP:HE3	1.79	0.47
28:1c:48:LEU:H	28:1c:48:LEU:HD22	1.79	0.47
29:1d:106:LYS:HE2	29:1d:106:LYS:HA	1.95	0.47
34:1i:6:ASP:OD1	39:1n:155:PRO:HG3	2.15	0.47
36:1k:35:LEU:HA	36:1k:38:ARG:HG2	1.95	0.47
38:1m:27:GLU:OE1	38:1m:27:GLU:N	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:80:LYS:O	40:1o:83:GLN:HG3	2.14	0.47
42:1q:44:TYR:HE2	42:1q:83:PRO:HB3	1.78	0.47
2:1B:48:MET:HE1	2:1B:103:VAL:CG1	2.44	0.47
6:1F:22:PHE:CE1	6:1F:255:LEU:HD11	2.48	0.47
7:1G:654:GLN:OE1	7:1G:655:GLN:N	2.48	0.47
9:1I:68:ARG:NH1	9:1I:129:ASP:O	2.47	0.47
12:1L:295:GLN:HE22	12:1L:524:ASN:CA	2.22	0.47
13:1M:154:LEU:O	13:1M:158:LEU:HD22	2.14	0.47
14:1N:231:SER:O	14:1N:234:TRP:HD1	1.98	0.47
14:1N:279:PRO:HA	14:1N:282:MET:HE3	1.97	0.47
14:1N:346:LEU:HD21	46:1d:201:PC1:H372	1.96	0.47
20:1T:12:LYS:HE3	20:1T:77:VAL:HG21	1.96	0.47
20:1T:52:MET:HA	20:1T:55:GLU:OE2	2.15	0.47
23:1X:137:PRO:HB2	23:1X:140:PRO:HG3	1.97	0.47
32:1g:96:LEU:CD1	32:1g:100:ARG:HD2	2.43	0.47
34:1i:34:LEU:HD13	34:1i:35:PRO:O	2.15	0.47
39:1n:161:ASP:N	39:1n:161:ASP:OD1	2.46	0.47
1:1A:33:LYS:HG2	8:1H:61:LEU:HD12	1.96	0.47
3:1C:51:PHE:HB3	21:1V:111:TRP:CZ2	2.50	0.47
3:1C:137:MET:HA	3:1C:137:MET:HE2	1.95	0.47
4:1D:55:HIS:HD2	4:1D:57:ALA:H	1.62	0.47
4:1D:183:ARG:NH1	4:1D:210:ASP:OD2	2.48	0.47
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.42	0.47
4:1D:417:ILE:O	4:1D:420:THR:HG22	2.15	0.47
6:1F:242:PHE:O	6:1F:251:SER:OG	2.33	0.47
7:1G:258:ILE:HD11	7:1G:579:ARG:NE	2.29	0.47
7:1G:412:PRO:HG3	7:1G:421:HIS:CE1	2.49	0.47
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.49	0.47
9:1I:172:ASP:OD2	9:1I:176:ARG:NE	2.45	0.47
12:1L:2:ASN:HB2	12:1L:3:PRO:CD	2.44	0.47
12:1L:315:VAL:O	12:1L:319:ILE:HD12	2.15	0.47
12:1L:370:THR:O	12:1L:374:ILE:HG13	2.15	0.47
12:1L:387:THR:HA	12:1L:465:GLY:HA3	1.96	0.47
12:1L:457:LEU:O	12:1L:457:LEU:HD23	2.15	0.47
12:1L:569:ILE:O	12:1L:573:MET:HG3	2.15	0.47
13:1M:388:TRP:CE3	13:1M:389:SER:HB3	2.50	0.47
15:1O:53:GLU:OE2	15:1O:104:ARG:NH2	2.48	0.47
16:1P:59:LEU:HA	16:1P:62:MET:CE	2.44	0.47
18:1R:52:VAL:HG11	18:1R:57:ILE:HB	1.96	0.47
21:1V:71:LEU:HD13	21:1V:79:VAL:HG11	1.97	0.47
22:1W:40:TYR:HE1	22:1W:60:ARG:HD3	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:67:LEU:HD23	23:1X:67:LEU:HA	1.78	0.47
32:1g:55:LEU:O	32:1g:59:ARG:HG2	2.14	0.47
34:1i:71:VAL:HG13	34:1i:72:THR:HG23	1.96	0.47
36:1k:23:ILE:O	36:1k:26:THR:OG1	2.22	0.47
38:1m:68:THR:O	38:1m:72:SER:OG	2.22	0.47
40:1o:111:LYS:O	40:1o:115:GLU:HG3	2.14	0.47
41:1p:9:TYR:HD1	41:1p:108:ARG:HG3	1.80	0.47
41:1p:35:ILE:HD12	41:1p:36:PHE:H	1.79	0.47
42:1q:96:ASP:HB3	42:1q:101:LYS:HB3	1.96	0.47
2:1B:25:ARG:HD2	2:1B:27:GLU:H	1.79	0.47
2:1B:108:PRO:HG3	8:1H:61:LEU:HD22	1.97	0.47
6:1F:57:LEU:O	6:1F:61:LYS:HG3	2.15	0.47
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.48	0.47
6:1F:224:ASN:O	6:1F:228:VAL:HG22	2.15	0.47
7:1G:41:CYS:O	7:1G:161:ARG:NH2	2.42	0.47
11:1K:37:MET:HG2	11:1K:67:ALA:HB2	1.97	0.47
15:1O:82:PHE:C	15:1O:82:PHE:CD1	2.91	0.47
15:1O:230:ASP:OD1	15:1O:233:LYS:HG2	2.15	0.47
16:1P:23:VAL:HG12	16:1P:92:ILE:HB	1.95	0.47
16:1P:106:PHE:HD2	16:1P:144:ARG:HB2	1.80	0.47
23:1X:52:PRO:HD2	25:1Z:116:TRP:CE3	2.49	0.47
4:1D:15:GLY:HA3	14:1N:228:LEU:HD11	1.97	0.47
4:1D:141:PHE:HZ	4:1D:184:VAL:HG21	1.80	0.47
5:1E:119:ALA:HA	5:1E:122:LYS:HE3	1.96	0.47
6:1F:437:HIS:O	6:1F:437:HIS:ND1	2.42	0.47
7:1G:287:GLU:OE2	7:1G:288:LYS:HG3	2.15	0.47
12:1L:295:GLN:OE1	39:1n:77:GLN:NE2	2.42	0.47
12:1L:296:ASN:HD22	12:1L:357:ARG:NH1	2.13	0.47
22:1W:62:LYS:HG3	22:1W:107:PHE:CD1	2.50	0.47
23:1X:8:THR:HG23	23:1X:10:GLU:H	1.79	0.47
23:1X:25:LYS:HE2	23:1X:25:LYS:HB2	1.69	0.47
34:1i:46:TRP:HA	34:1i:46:TRP:HE3	1.80	0.47
42:1q:9:ARG:O	42:1q:13:GLN:HG2	2.14	0.47
2:1B:81:ARG:NE	8:1H:61:LEU:HD11	2.19	0.47
4:1D:6:PRO:HB3	4:1D:10:TRP:HD1	1.79	0.47
8:1H:24:GLU:OE1	8:1H:228:TYR:OH	2.21	0.47
8:1H:179:TRP:HH2	9:1I:26:LEU:HD11	1.80	0.47
8:1H:272:TRP:CZ2	9:1I:38:LEU:HB2	2.50	0.47
10:1J:120:ASN:HB3	11:1K:1:FME:O1	2.15	0.47
11:1K:20:LEU:HB2	12:1L:592:LEU:HD23	1.97	0.47
11:1K:80:MET:O	11:1K:84:THR:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:305:SER:HB3	12:1L:422:TYR:CE2	2.49	0.47
12:1L:593:ILE:O	12:1L:597:ILE:HG13	2.15	0.47
13:1M:196:TRP:CD1	13:1M:250:LEU:HB3	2.50	0.47
13:1M:373:ILE:HA	13:1M:376:ILE:HG12	1.96	0.47
18:1R:52:VAL:O	18:1R:94:PRO:HD3	2.15	0.47
33:1h:21:PHE:CD1	33:1h:21:PHE:C	2.93	0.47
37:1l:129:GLY:CA	40:1o:21:MET:HE1	2.38	0.47
38:1m:114:LEU:HB3	38:1m:120:LEU:HG	1.96	0.47
2:1B:137:ASP:OD1	2:1B:137:ASP:N	2.46	0.46
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.97	0.46
6:1F:256:PHE:CE1	6:1F:317:MET:HG2	2.51	0.46
9:1I:108:ARG:NH1	9:1I:110:ASP:OD1	2.48	0.46
10:1J:39:VAL:O	10:1J:43:ILE:HG13	2.15	0.46
12:1L:127:THR:O	12:1L:130:ILE:HD12	2.15	0.46
12:1L:335:PHE:CD1	12:1L:336:LYS:HG2	2.50	0.46
13:1M:400:MET:HA	13:1M:403:THR:HB	1.97	0.46
14:1N:159:MET:HE3	14:1N:278:MET:SD	2.55	0.46
16:1P:87:HIS:HB2	18:1R:26:VAL:HG23	1.97	0.46
25:1Z:50:MET:HA	25:1Z:50:MET:HE3	1.97	0.46
26:1a:2:TRP:O	26:1a:5:ILE:HB	2.15	0.46
28:1c:26:PHE:C	28:1c:26:PHE:CD1	2.93	0.46
29:1d:104:LYS:C	29:1d:104:LYS:HD3	2.40	0.46
33:1h:61:PRO:HG3	33:1h:66:TYR:OH	2.15	0.46
2:1B:106:GLN:OE1	2:1B:106:GLN:N	2.48	0.46
6:1F:273:SER:HB3	6:1F:318:ASP:HB3	1.98	0.46
6:1F:370:ASP:O	6:1F:374:LYS:HG3	2.14	0.46
13:1M:160:LEU:HD13	13:1M:199:CYS:HA	1.97	0.46
13:1M:253:LEU:HB3	13:1M:257:MET:HE1	1.97	0.46
13:1M:282:LEU:HG	13:1M:342:MET:HE2	1.97	0.46
15:1O:84:ASP:HA	15:1O:193:LYS:HD3	1.98	0.46
15:1O:208:LYS:HE3	15:1O:208:LYS:HB3	1.69	0.46
22:1W:65:GLU:OE1	22:1W:69:LYS:NZ	2.48	0.46
23:1X:74:LYS:HD2	26:1a:66:LEU:HB3	1.95	0.46
25:1Z:34:SER:O	25:1Z:38:VAL:HG23	2.16	0.46
36:1k:14:GLU:CD	36:1k:14:GLU:H	2.23	0.46
39:1n:114:TYR:O	39:1n:118:PHE:HD2	1.98	0.46
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.44	0.46
6:1F:317:MET:HE1	6:1F:334:VAL:HG22	1.98	0.46
7:1G:624:GLU:HB2	7:1G:631:VAL:HG21	1.96	0.46
11:1K:63:LEU:HA	11:1K:63:LEU:HD22	1.56	0.46
12:1L:341:MET:HE1	12:1L:457:LEU:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:94:LEU:HD13	52:1N:401:3PE:C35	2.45	0.46
13:1M:94:LEU:HD23	13:1M:94:LEU:O	2.15	0.46
14:1N:108:LEU:HD13	14:1N:191:THR:HG21	1.97	0.46
32:1g:40:LYS:HD3	32:1g:41:ASN:H	1.79	0.46
2:1B:162:GLN:OE1	9:1I:140:SER:OG	2.28	0.46
3:1C:119:SER:OG	3:1C:144:ASN:O	2.32	0.46
5:1E:103:CYS:SG	5:1E:144:CYS:HA	2.55	0.46
5:1E:147:ALA:HB3	5:1E:153:MET:HG2	1.98	0.46
9:1I:60:ARG:HG2	9:1I:172:ASP:OD1	2.15	0.46
12:1L:359:MET:HB2	12:1L:362:LEU:HD11	1.97	0.46
12:1L:437:PHE:HE2	12:1L:441:VAL:HG22	1.80	0.46
12:1L:582:GLY:O	14:1N:58:LYS:NZ	2.43	0.46
13:1M:216:LEU:HB2	13:1M:217:PRO:HD3	1.96	0.46
15:1O:171:TYR:HE2	15:1O:206:TYR:CD1	2.34	0.46
16:1P:166:ILE:HG22	16:1P:168:PRO:HD3	1.97	0.46
22:1W:91:GLU:OE1	22:1W:91:GLU:HA	2.15	0.46
29:1d:109:TYR:CE1	41:1p:78:GLU:HA	2.51	0.46
35:1j:67:LEU:HD23	35:1j:68:PRO:HD2	1.97	0.46
36:1k:44:TRP:HB2	39:1n:37:ARG:CZ	2.45	0.46
38:1m:37:ALA:HB2	39:1n:149:ARG:CZ	2.46	0.46
43:1r:8:GLN:O	43:1r:12:ASN:ND2	2.48	0.46
2:1B:79:SER:O	2:1B:81:ARG:N	2.49	0.46
8:1H:277:TYR:CE2	9:1I:30:LEU:HG	2.51	0.46
9:1I:106:THR:HG21	9:1I:109:TYR:HD2	1.79	0.46
13:1M:141:GLU:OE2	13:1M:222:GLU:HG3	2.15	0.46
14:1N:63:GLN:NE2	14:1N:105:LYS:HD2	2.31	0.46
14:1N:236:LYS:HA	14:1N:315:TRP:CD1	2.50	0.46
18:1R:3:ARG:HB3	18:1R:3:ARG:HH11	1.81	0.46
37:1l:112:MET:HA	37:1l:115:MET:SD	2.56	0.46
38:1m:48:LEU:HD21	39:1n:139:LEU:HD11	1.97	0.46
39:1n:156:ALA:HB2	39:1n:163:PRO:HA	1.97	0.46
42:1q:65:THR:O	42:1q:73:THR:OG1	2.30	0.46
7:1G:475:GLN:HB2	7:1G:646:ASN:ND2	2.31	0.46
8:1H:72:ILE:O	8:1H:75:PRO:HD2	2.15	0.46
8:1H:245:ALA:HB3	8:1H:255:TYR:CE1	2.51	0.46
12:1L:13:ILE:O	12:1L:17:ILE:HG12	2.16	0.46
15:1O:64:GLY:HA3	15:1O:302:ARG:HH21	1.80	0.46
16:1P:133:SER:O	16:1P:168:PRO:HD2	2.16	0.46
20:1U:23:ASP:HB2	36:1k:43:PRO:CB	2.45	0.46
24:1Y:21:ALA:O	24:1Y:25:THR:OG1	2.31	0.46
33:1h:62:GLU:HG3	33:1h:64:TRP:NE1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:72:SER:HA	33:1h:75:ILE:HG22	1.98	0.46
41:1p:61:TYR:HD1	41:1p:62:TYR:H	1.62	0.46
2:1B:92:LEU:HD22	2:1B:100:LEU:HD13	1.96	0.46
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.40	0.46
10:1J:98:MET:N	10:1J:98:MET:HE3	2.31	0.46
10:1J:159:TRP:NE1	14:1N:12:THR:HG22	2.30	0.46
12:1L:163:ASP:N	12:1L:163:ASP:OD1	2.48	0.46
12:1L:455:LYS:NZ	12:1L:456:ARG:HH12	2.12	0.46
15:1O:25:ILE:HD12	15:1O:25:ILE:N	2.31	0.46
15:1O:245:LYS:HA	15:1O:245:LYS:HD2	1.78	0.46
18:1R:93:GLN:OE1	18:1R:94:PRO:HD2	2.16	0.46
22:1W:33:ARG:O	22:1W:37:ARG:HG3	2.16	0.46
27:1b:61:ASN:OD1	27:1b:61:ASN:N	2.46	0.46
33:1h:62:GLU:HG3	33:1h:64:TRP:CE2	2.51	0.46
1:1A:111:LEU:HD22	8:1H:290:TRP:HB3	1.97	0.46
4:1D:111:MET:HE3	4:1D:189:MET:O	2.15	0.46
9:1I:8:ARG:HA	9:1I:8:ARG:NE	2.31	0.46
12:1L:15:LEU:O	12:1L:18:PRO:HD2	2.16	0.46
12:1L:127:THR:HA	12:1L:130:ILE:HD11	1.98	0.46
12:1L:205:ASN:HB3	12:1L:207:GLU:OE1	2.16	0.46
12:1L:596:MET:HA	12:1L:599:MET:HB3	1.98	0.46
18:1R:1:GLY:N	18:1R:42:ASP:OD2	2.39	0.46
29:1d:94:VAL:HG22	29:1d:101:PHE:CE1	2.51	0.46
34:1i:1:SAC:N	34:1i:2:GLY:HA3	2.31	0.46
42:1q:137:TRP:CZ3	42:1q:139:PRO:HB3	2.51	0.46
1:1A:67:LEU:HG	11:1K:68:ALA:HB3	1.97	0.46
3:1C:25:PHE:CD2	43:1r:96:PRO:HG3	2.51	0.46
7:1G:249:ARG:C	7:1G:250:ILE:HD13	2.41	0.46
7:1G:458:LEU:HD11	7:1G:492:ILE:HD12	1.98	0.46
12:1L:297:ASP:C	12:1L:301:ILE:HD13	2.41	0.46
12:1L:368:PHE:HE1	35:1j:28:PHE:HE2	1.64	0.46
12:1L:399:VAL:HG22	12:1L:409:LEU:HB3	1.98	0.46
13:1M:403:THR:O	13:1M:407:SER:N	2.37	0.46
24:1Y:19:ARG:H	24:1Y:19:ARG:HG2	1.57	0.46
29:1d:104:LYS:NZ	29:1d:106:LYS:HA	2.31	0.46
38:1m:49:GLN:O	38:1m:49:GLN:NE2	2.41	0.46
40:1o:2:ALA:O	40:1o:6:ARG:HG3	2.16	0.46
40:1o:110:ARG:HG2	40:1o:114:ARG:HE	1.81	0.46
3:1C:133:GLU:OE2	4:1D:390:LYS:NZ	2.49	0.46
4:1D:141:PHE:CZ	4:1D:184:VAL:HG21	2.51	0.46
4:1D:366:ALA:HB1	4:1D:373:GLU:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:79:ARG:O	5:1E:83:VAL:HG13	2.15	0.46
8:1H:272:TRP:CH2	9:1I:38:LEU:HD22	2.50	0.46
9:1I:148:LEU:HB3	17:1Q:70:MET:SD	2.55	0.46
12:1L:115:ASN:O	12:1L:119:LYS:HG3	2.16	0.46
12:1L:496:MET:SD	12:1L:497:GLY:N	2.89	0.46
13:1M:252:PRO:HG3	29:1d:117:HIS:CE1	2.51	0.46
13:1M:354:LEU:HD11	33:1h:18:ASP:HB3	1.98	0.46
22:1W:99:GLN:H	22:1W:102:HIS:HB2	1.81	0.46
24:1Y:89:TYR:CD2	24:1Y:125:LYS:HB2	2.51	0.46
28:1c:26:PHE:C	28:1c:26:PHE:HD1	2.23	0.46
33:1h:39:GLY:O	33:1h:43:VAL:HG13	2.16	0.46
37:1l:79:TRP:O	38:1m:71:ARG:NH1	2.46	0.46
37:1l:86:ARG:H	37:1l:86:ARG:HG2	1.47	0.46
43:1r:8:GLN:NE2	43:1r:20:GLN:OE1	2.49	0.46
2:1B:32:LYS:HA	2:1B:35:ASP:OD2	2.17	0.45
3:1C:69:ASN:ND2	43:1r:94:VAL:O	2.49	0.45
7:1G:299:ALA:O	7:1G:303:VAL:HG23	2.15	0.45
8:1H:46:LEU:HD21	46:1q:201:PC1:H271	1.98	0.45
9:1I:101:ASP:OD1	9:1I:102:GLY:N	2.49	0.45
12:1L:268:GLU:HA	12:1L:274:GLN:NE2	2.30	0.45
12:1L:330:CYS:HB2	12:1L:331:MET:CE	2.45	0.45
12:1L:405:ASN:OD1	12:1L:407:TRP:N	2.49	0.45
12:1L:527:GLY:O	37:1l:105:LEU:HD13	2.16	0.45
13:1M:135:ARG:NH1	52:1N:401:3PE:H342	2.16	0.45
13:1M:306:PRO:HA	13:1M:458:LEU:HG	1.98	0.45
16:1P:90:VAL:HG21	16:1P:218:ILE:HD12	1.96	0.45
16:1P:203:GLN:NE2	16:1P:232:GLY:O	2.48	0.45
16:1P:235:ARG:NH2	16:1P:291:ASP:O	2.41	0.45
16:1P:315:ILE:O	16:1P:319:ARG:HB2	2.16	0.45
20:1T:35:HIS:CE1	20:1T:37:MET:HB2	2.51	0.45
29:1d:70:PHE:HE1	29:1d:74:TYR:CE2	2.34	0.45
33:1h:7:ARG:HE	34:1i:27:LEU:HB2	1.80	0.45
39:1n:42:LEU:HD23	39:1n:43:MET:HE2	1.97	0.45
1:1A:16:LEU:O	1:1A:19:LEU:N	2.49	0.45
1:1A:21:ALA:O	8:1H:60:PRO:HG3	2.16	0.45
1:1A:112:GLU:OE2	1:1A:113:TRP:N	2.47	0.45
46:1B:202:PC1:H321	46:1B:202:PC1:H31	1.45	0.45
4:1D:144:ILE:HG12	4:1D:311:ILE:HD13	1.98	0.45
5:1E:123:LYS:HD3	5:1E:173:ILE:HB	1.97	0.45
5:1E:127:LYS:N	5:1E:130:GLU:OE1	2.48	0.45
7:1G:55:CYS:SG	7:1G:69:CYS:N	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.56	0.45
7:1G:545:TYR:CE2	7:1G:553:GLY:HA3	2.51	0.45
12:1L:204:LEU:HD21	38:1m:124:PHE:CD2	2.50	0.45
12:1L:573:MET:O	12:1L:576:MET:HG3	2.16	0.45
14:1N:329:MET:O	14:1N:333:SER:HB2	2.17	0.45
15:1O:278:TYR:HA	15:1O:283:THR:HG22	1.97	0.45
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.51	0.45
16:1P:133:SER:OG	16:1P:134:HIS:N	2.48	0.45
17:1Q:16:LYS:NZ	17:1Q:18:ASP:OD1	2.50	0.45
23:1X:24:LEU:HB3	25:1Z:71:LEU:CD2	2.45	0.45
29:1d:29:PRO:HA	29:1d:32:VAL:HG12	1.98	0.45
36:1k:40:LEU:HG	39:1n:45:ALA:HB2	1.98	0.45
37:1l:85:ILE:HG23	37:1l:88:ARG:H	1.80	0.45
38:1m:54:ASN:OD1	39:1n:129:ARG:NH2	2.49	0.45
39:1n:174:ARG:O	39:1n:177:PRO:HD3	2.16	0.45
2:1B:102:LYS:HD3	2:1B:106:GLN:OE1	2.16	0.45
4:1D:177:MET:HE2	4:1D:214:PHE:CZ	2.51	0.45
5:1E:123:LYS:NZ	5:1E:174:ASP:HB3	2.32	0.45
7:1G:102:PRO:HG3	7:1G:151:THR:HG23	1.98	0.45
7:1G:228:ILE:HG13	7:1G:581:GLN:HB2	1.98	0.45
8:1H:105:MET:SD	8:1H:162:LEU:HD11	2.56	0.45
8:1H:181:LEU:HA	8:1H:184:MET:HE3	1.97	0.45
12:1L:44:PHE:CE1	12:1L:95:PHE:HB2	2.51	0.45
12:1L:122:VAL:HG12	12:1L:126:ILE:HD11	1.98	0.45
12:1L:602:PHE:CD1	12:1L:604:TYR:CE1	3.04	0.45
13:1M:1:FME:HE1	13:1M:4:ILE:HD12	1.98	0.45
13:1M:7:PRO:HB2	13:1M:34:ILE:HD11	1.97	0.45
15:1O:123:VAL:O	15:1O:124:LEU:HD23	2.16	0.45
15:1O:198:TYR:CZ	15:1O:202:ILE:HD11	2.51	0.45
22:1W:22:SER:HB2	22:1W:27:GLU:HB2	1.97	0.45
25:1Z:74:LEU:H	25:1Z:74:LEU:HD12	1.82	0.45
51:1a:101:CDL:H131	51:1a:101:CDL:H311	1.98	0.45
31:1f:4:LEU:O	31:1f:7:VAL:HG12	2.16	0.45
32:1g:114:ASP:HB3	32:1g:117:LYS:HD3	1.97	0.45
35:1j:10:ARG:HG2	35:1j:13:GLN:CD	2.41	0.45
2:1B:49:THR:HB	50:1H:701:U10:H103	1.97	0.45
2:1B:73:GLY:HA2	8:1H:47:GLN:HE22	1.81	0.45
3:1C:40:VAL:HG22	43:1r:69:MET:HE3	1.98	0.45
3:1C:77:ASP:OD1	3:1C:78:LEU:N	2.50	0.45
4:1D:237:ASN:HB3	8:1H:284:GLN:NE2	2.31	0.45
5:1E:162:GLU:HB2	5:1E:186:PRO:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:68:ILE:HG12	8:1H:69:SER:N	2.31	0.45
8:1H:286:MET:HE3	8:1H:286:MET:HB3	1.84	0.45
12:1L:293:ILE:HG22	12:1L:294:THR:CG2	2.46	0.45
14:1N:321:LYS:NZ	51:1N:402:CDL:OB5	2.47	0.45
15:1O:58:TYR:O	15:1O:62:THR:HG23	2.17	0.45
16:1P:59:LEU:HB3	16:1P:70:PHE:CZ	2.52	0.45
20:1T:18:VAL:HA	20:1T:21:LEU:CD2	2.46	0.45
23:1X:43:MET:HE1	27:1b:52:TYR:CG	2.52	0.45
25:1Z:88:ARG:HH21	25:1Z:91:LEU:HD22	1.80	0.45
35:1j:12:ARG:HD3	36:1k:50:TRP:CD1	2.51	0.45
38:1m:76:TYR:HB3	38:1m:77:PRO:HD3	1.98	0.45
40:1o:109:GLN:O	40:1o:113:ARG:HG3	2.17	0.45
44:1s:39:ARG:O	44:1s:42:GLN:NE2	2.45	0.45
2:1B:175:ILE:HA	2:1B:178:ARG:HG2	1.98	0.45
5:1E:202:LEU:HD11	6:1F:25:LEU:HD23	1.97	0.45
6:1F:363:THR:HG21	7:1G:97:LEU:HG	1.99	0.45
8:1H:260:VAL:HG22	26:1a:16:LEU:HB3	1.98	0.45
10:1J:1:FME:HG2	10:1J:2:THR:H	1.81	0.45
10:1J:63:GLY:O	10:1J:66:VAL:HG12	2.16	0.45
10:1J:125:TRP:CZ3	25:1Z:122:GLY:HA2	2.52	0.45
11:1K:62:ILE:HG21	14:1N:31:ILE:HD11	1.98	0.45
12:1L:293:ILE:HG22	12:1L:294:THR:HG22	1.99	0.45
16:1P:71:MET:HE1	18:1R:29:SER:OG	2.16	0.45
20:1U:8:LEU:N	20:1U:88:GLU:OE2	2.27	0.45
21:1V:26:LEU:HD23	21:1V:26:LEU:HA	1.79	0.45
26:1a:9:ILE:HD12	26:1a:9:ILE:N	2.31	0.45
31:1f:46:ARG:HD2	31:1f:47:GLU:O	2.16	0.45
33:1h:64:TRP:CE2	33:1h:77:ARG:HD3	2.52	0.45
34:1i:94:TYR:CE2	41:1p:108:ARG:HA	2.51	0.45
40:1o:51:MET:HA	41:1p:118:GLU:CD	2.42	0.45
41:1p:28:PRO:HA	41:1p:31:TYR:HD2	1.81	0.45
4:1D:201:GLN:HA	4:1D:323:ILE:HD12	1.98	0.45
6:1F:425:GLU:O	6:1F:428:GLU:HG3	2.16	0.45
7:1G:504:ASP:HA	19:1S:55:ARG:HE	1.82	0.45
10:1J:129:ASP:HB2	30:1e:31:ARG:HE	1.81	0.45
12:1L:424:THR:HA	12:1L:427:ILE:HG22	1.98	0.45
12:1L:493:VAL:HA	12:1L:496:MET:HG3	1.97	0.45
13:1M:141:GLU:O	13:1M:145:ALA:N	2.47	0.45
13:1M:207:MET:HG2	13:1M:243:MET:HE1	1.98	0.45
15:1O:41:GLU:O	15:1O:45:LYS:HB2	2.15	0.45
15:1O:152:TYR:O	15:1O:155:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:36:ILE:HD12	19:1S:36:ILE:HA	1.82	0.45
20:1T:43:ASP:OD2	22:1W:64:ARG:NH2	2.50	0.45
24:1Y:101:GLY:O	24:1Y:105:ARG:N	2.50	0.45
29:1d:-1:MET:SD	33:1h:111:ARG:HD2	2.57	0.45
37:1l:30:ARG:NH2	38:1m:35:ARG:HB3	2.31	0.45
39:1n:158:LYS:HD2	39:1n:159:GLU:N	2.30	0.45
2:1B:92:LEU:HD11	2:1B:97:ALA:HA	1.98	0.45
5:1E:156:ILE:O	5:1E:158:ASP:N	2.50	0.45
7:1G:263:ILE:HD11	7:1G:268:ARG:HG3	1.98	0.45
11:1K:16:LEU:HA	11:1K:36:MET:SD	2.56	0.45
13:1M:250:LEU:O	13:1M:254:THR:OG1	2.29	0.45
13:1M:260:PRO:HG3	46:1M:501:PC1:H251	1.99	0.45
14:1N:3:PRO:HB3	51:1N:402:CDL:HA61	1.98	0.45
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.97	0.45
14:1N:95:MET:CE	14:1N:149:ILE:HG12	2.47	0.45
15:1O:107:GLN:NE2	15:1O:124:LEU:HD22	2.31	0.45
15:1O:233:LYS:HD2	15:1O:233:LYS:N	2.31	0.45
16:1P:78:LYS:HA	16:1P:81:ILE:HD12	1.98	0.45
17:1Q:12:ALA:HA	22:1W:16:SER:HA	1.97	0.45
20:1U:9:GLU:HA	20:1U:12:LYS:HB3	1.97	0.45
23:1X:146:ARG:HD2	30:1e:41:GLU:CD	2.42	0.45
24:1Y:105:ARG:N	24:1Y:105:ARG:HD3	2.32	0.45
28:1c:26:PHE:HD1	28:1c:26:PHE:O	1.99	0.45
38:1m:111:LYS:HG3	38:1m:115:ILE:HD11	1.99	0.45
43:1r:47:LYS:H	43:1r:51:ASN:ND2	2.14	0.45
4:1D:265:ILE:HG13	21:1V:10:LEU:HD23	1.98	0.45
4:1D:342:MET:HE1	7:1G:103:LEU:HA	1.98	0.45
5:1E:53:LEU:HD23	5:1E:53:LEU:HA	1.78	0.45
5:1E:53:LEU:HG	44:1s:52:LEU:HD13	1.99	0.45
12:1L:434:LYS:HD3	36:1k:52:TYR:HD1	1.82	0.45
13:1M:135:ARG:NH1	52:1N:401:3PE:H362	2.32	0.45
13:1M:349:GLN:HB2	13:1M:415:GLN:HB3	1.99	0.45
15:1O:168:VAL:HG11	15:1O:238:ILE:HG13	1.99	0.45
16:1P:280:THR:O	16:1P:284:VAL:HG12	2.17	0.45
16:1P:335:LYS:HD2	16:1P:335:LYS:C	2.42	0.45
19:1S:91:GLU:HA	19:1S:94:LEU:HD23	1.99	0.45
23:1X:141:TYR:HA	25:1Z:115:ARG:HD3	1.99	0.45
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.35	0.45
32:1g:120:LEU:HD11	41:1p:162:MET:HB2	1.99	0.45
33:1h:7:ARG:NH2	34:1i:28:SER:O	2.50	0.45
35:1j:35:TRP:CE3	35:1j:39:ARG:HG3	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:6:ASP:OD1	3:1C:7:THR:N	2.48	0.45
8:1H:20:LEU:HA	26:1a:12:MET:HE1	1.99	0.45
9:1I:42:PHE:HB3	43:1r:11:ARG:HG2	1.98	0.45
10:1J:20:PHE:CZ	11:1K:35:GLY:HA3	2.52	0.45
12:1L:298:ILE:HD13	12:1L:343:SER:HB2	1.99	0.45
13:1M:176:PHE:HE1	13:1M:248:THR:HG21	1.82	0.45
13:1M:329:LEU:HB3	13:1M:359:TRP:CE2	2.51	0.45
14:1N:240:ILE:HD13	14:1N:240:ILE:HA	1.80	0.45
15:1O:116:LEU:CD2	15:1O:259:LEU:HD23	2.47	0.45
18:1R:80:LYS:NZ	18:1R:81:THR:OG1	2.49	0.45
20:1T:66:ASP:HA	20:1T:69:LYS:HG3	1.98	0.45
20:1U:21:LEU:O	36:1k:46:ARG:HD3	2.17	0.45
20:1U:22:TYR:CE1	36:1k:43:PRO:HB2	2.52	0.45
25:1Z:71:LEU:HB3	25:1Z:75:PHE:CE2	2.52	0.45
31:1f:3:VAL:HA	31:1f:6:ILE:HD12	1.98	0.45
34:1i:62:LYS:HA	34:1i:65:ARG:HG2	1.98	0.45
37:1l:18:GLU:N	37:1l:18:GLU:CD	2.74	0.45
37:1l:116:PHE:HE1	37:1l:120:GLU:HB3	1.81	0.45
40:1o:74:PRO:HD2	41:1p:25:LEU:HB3	1.99	0.45
42:1q:2:GLU:OE1	42:1q:2:GLU:HA	2.17	0.45
2:1B:118:SER:N	45:1B:201:SF4:S1	2.90	0.45
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.18	0.45
7:1G:38:PRO:HB2	7:1G:54:MET:HG2	1.98	0.45
9:1I:43:ARG:NH1	43:1r:19:LEU:HD22	2.26	0.45
12:1L:49:VAL:O	12:1L:52:LEU:N	2.50	0.45
12:1L:174:TYR:HD2	12:1L:232:TRP:HD1	1.65	0.45
13:1M:116:ILE:HG12	13:1M:174:LEU:HD13	1.99	0.45
13:1M:430:PHE:CE1	32:1g:37:LEU:HB2	2.52	0.45
17:1Q:60:ASP:OD1	17:1Q:60:ASP:N	2.48	0.45
32:1g:77:VAL:HA	32:1g:80:LEU:HD21	1.98	0.45
37:1l:22:ALA:HA	37:1l:25:LYS:NZ	2.31	0.45
41:1p:5:ASP:OD1	41:1p:6:LYS:N	2.50	0.45
2:1B:39:TRP:HA	2:1B:42:ARG:NE	2.32	0.44
2:1B:69:MET:HE1	2:1B:76:PHE:CD2	2.52	0.44
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.45	0.44
4:1D:245:VAL:HG11	4:1D:405:MET:HE2	2.00	0.44
6:1F:215:VAL:HG22	6:1F:220:THR:OG1	2.17	0.44
12:1L:481:THR:HG22	35:1j:51:PHE:HB2	1.99	0.44
13:1M:243:MET:HB3	13:1M:301:ILE:HG21	1.99	0.44
13:1M:400:MET:N	13:1M:400:MET:SD	2.88	0.44
13:1M:449:LEU:HD23	13:1M:450:ASN:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:86:MET:HE3	25:1Z:86:MET:HB2	1.79	0.44
30:1e:57:ILE:HD12	30:1e:58:GLU:N	2.32	0.44
32:1g:87:GLU:H	32:1g:87:GLU:CD	2.25	0.44
32:1g:112:CYS:N	41:1p:158:GLN:OE1	2.50	0.44
34:1i:18:ARG:HH22	39:1n:174:ARG:HA	1.82	0.44
35:1j:59:TRP:O	40:1o:106:ARG:NH2	2.48	0.44
39:1n:92:ARG:HD2	39:1n:93:TYR:CE1	2.53	0.44
39:1n:92:ARG:HD2	39:1n:93:TYR:CZ	2.52	0.44
1:1A:73:LEU:O	1:1A:76:PRO:HD2	2.17	0.44
2:1B:42:ARG:HB2	2:1B:164:GLN:HG3	1.98	0.44
7:1G:363:LEU:HD23	7:1G:363:LEU:HA	1.80	0.44
7:1G:416:THR:OG1	7:1G:417:TYR:N	2.49	0.44
8:1H:55:LEU:HD13	8:1H:221:ALA:HB2	1.99	0.44
12:1L:293:ILE:CD1	12:1L:418:LEU:HB3	2.48	0.44
13:1M:94:LEU:HD23	13:1M:98:MET:HG2	1.99	0.44
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	1.98	0.44
16:1P:202:LYS:HD2	16:1P:202:LYS:HA	1.73	0.44
23:1X:60:LYS:O	23:1X:64:GLN:HG2	2.18	0.44
25:1Z:124:LEU:HD12	25:1Z:124:LEU:HA	1.86	0.44
26:1a:12:MET:HE3	26:1a:12:MET:HB2	1.86	0.44
30:1e:88:GLU:HG2	30:1e:90:LYS:NZ	2.32	0.44
34:1i:69:PHE:O	34:1i:73:HIS:HB2	2.16	0.44
42:1q:95:ASP:OD2	42:1q:95:ASP:N	2.49	0.44
43:1r:92:LYS:HA	43:1r:92:LYS:HE3	1.99	0.44
1:1A:73:LEU:N	1:1A:74:PRO:HD2	2.32	0.44
2:1B:172:ARG:HB3	46:1B:202:PC1:H222	1.99	0.44
6:1F:15:LEU:HD13	6:1F:271:GLU:HB3	1.98	0.44
7:1G:672:TYR:CE2	7:1G:687:CYS:HB3	2.52	0.44
9:1I:150:ASN:N	42:1q:124:TYR:OH	2.51	0.44
10:1J:57:PHE:HD1	10:1J:61:LEU:HD13	1.82	0.44
12:1L:6:SER:O	12:1L:10:THR:HG23	2.17	0.44
12:1L:190:LEU:HD22	12:1L:196:TRP:CE2	2.52	0.44
13:1M:114:GLU:OE2	23:1X:168:PHE:N	2.50	0.44
13:1M:152:TYR:O	13:1M:205:VAL:HG11	2.17	0.44
14:1N:234:TRP:CE2	14:1N:304:MET:HB3	2.52	0.44
16:1P:48:PRO:HB3	16:1P:84:VAL:HG11	1.99	0.44
20:1T:78:ASP:O	20:1T:82:ASP:OD1	2.35	0.44
20:1U:15:VAL:HA	20:1U:18:VAL:HG22	1.99	0.44
24:1Y:69:PHE:CD1	24:1Y:69:PHE:C	2.94	0.44
29:1d:10:PRO:HB2	29:1d:11:LEU:HD12	1.99	0.44
29:1d:85:LEU:HD23	29:1d:85:LEU:HA	1.85	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:78:ASP:OD1	42:1q:80:SER:N	2.46	0.44
3:1C:199:LEU:HD12	4:1D:385:ARG:HH11	1.82	0.44
5:1E:69:VAL:HG13	5:1E:73:LEU:HD12	1.99	0.44
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.17	0.44
7:1G:84:GLU:O	7:1G:88:LYS:HG3	2.17	0.44
8:1H:258:ASN:O	8:1H:262:LYS:HG3	2.17	0.44
8:1H:264:LEU:HD22	26:1a:9:ILE:HG23	1.98	0.44
11:1K:37:MET:HE3	11:1K:63:LEU:HD13	1.99	0.44
12:1L:54:PHE:CZ	12:1L:84:TYR:HB2	2.53	0.44
12:1L:503:GLU:O	12:1L:507:THR:HG23	2.18	0.44
13:1M:43:ASN:HB2	33:1h:80:TYR:CE2	2.53	0.44
13:1M:82:SER:O	13:1M:86:LYS:NZ	2.51	0.44
13:1M:115:LEU:HB3	13:1M:164:LEU:HD22	1.98	0.44
13:1M:175:ASN:HD22	13:1M:178:ILE:HG13	1.83	0.44
15:1O:221:LEU:HD13	15:1O:223:TYR:OH	2.18	0.44
20:1T:52:MET:SD	22:1W:40:TYR:HD2	2.41	0.44
20:1U:52:MET:CE	39:1n:23:LEU:HB3	2.46	0.44
23:1X:34:GLN:HE21	23:1X:116:TRP:CD1	2.35	0.44
33:1h:99:GLU:HA	33:1h:102:GLU:OE2	2.18	0.44
38:1m:110:LYS:O	38:1m:114:LEU:HG	2.17	0.44
39:1n:23:LEU:HD11	39:1n:40:ALA:HA	1.97	0.44
42:1q:47:LYS:C	42:1q:48:TYR:HD2	2.25	0.44
43:1r:4:THR:O	43:1r:8:GLN:HG3	2.18	0.44
4:1D:241:ASP:OD1	4:1D:290:ARG:NH1	2.48	0.44
6:1F:371:TRP:CE2	7:1G:130:PHE:HD1	2.35	0.44
7:1G:609:MET:HE3	7:1G:609:MET:HB3	1.80	0.44
10:1J:153:LEU:O	10:1J:157:THR:OG1	2.28	0.44
12:1L:149:ILE:HD12	12:1L:150:MET:N	2.33	0.44
13:1M:95:TYR:HD2	13:1M:136:TRP:CD2	2.35	0.44
13:1M:168:GLN:HB2	13:1M:174:LEU:HD11	2.00	0.44
19:1S:49:ASP:OD1	19:1S:49:ASP:C	2.60	0.44
29:1d:15:PRO:C	29:1d:17:GLU:H	2.25	0.44
29:1d:36:PHE:CD1	29:1d:36:PHE:C	2.95	0.44
34:1i:76:ILE:HA	34:1i:79:TRP:HD1	1.82	0.44
34:1i:99:ARG:NH1	41:1p:117:GLY:HA3	2.33	0.44
38:1m:53:PRO:HA	39:1n:128:ARG:HH21	1.83	0.44
40:1o:26:PRO:O	40:1o:33:ARG:HD3	2.18	0.44
40:1o:32:GLU:H	40:1o:32:GLU:HG2	1.57	0.44
4:1D:51:PHE:O	4:1D:64:LEU:HB3	2.17	0.44
4:1D:417:ILE:O	4:1D:421:GLN:NE2	2.51	0.44
12:1L:331:MET:HE3	12:1L:331:MET:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:234:ASN:HB2	16:1P:236:TYR:CE1	2.52	0.44
19:1S:12:LYS:HZ1	19:1S:14:GLY:HA2	1.83	0.44
20:1T:11:ILE:HG22	20:1T:77:VAL:HG13	1.99	0.44
20:1U:12:LYS:HB2	20:1U:77:VAL:HG21	2.00	0.44
22:1W:17:VAL:HG22	22:1W:18:LYS:N	2.33	0.44
23:1X:131:LYS:HD3	23:1X:131:LYS:HA	1.71	0.44
31:1f:39:ASN:HB2	31:1f:55:THR:OG1	2.18	0.44
33:1h:87:TYR:HB3	33:1h:88:GLU:OE2	2.17	0.44
34:1i:32:PRO:HB3	39:1n:114:TYR:HE1	1.83	0.44
34:1i:67:SER:O	34:1i:71:VAL:HG12	2.18	0.44
34:1i:83:TYR:OH	41:1p:51:ILE:HG12	2.18	0.44
37:1l:23:ALA:HA	37:1l:26:LYS:HE2	1.99	0.44
39:1n:19:TYR:HB2	39:1n:47:PHE:CE2	2.52	0.44
41:1p:120:TYR:O	41:1p:124:CYS:HB2	2.17	0.44
1:1A:70:ALA:HB2	10:1J:59:ILE:HD11	1.99	0.44
2:1B:108:PRO:HB2	8:1H:58:LYS:NZ	2.33	0.44
4:1D:165:THR:OG1	4:1D:166:PRO:HD3	2.18	0.44
4:1D:285:VAL:HG21	43:1r:103:TRP:CZ3	2.53	0.44
5:1E:142:VAL:HG21	5:1E:145:LEU:HD11	1.98	0.44
6:1F:105:CYS:O	6:1F:109:GLU:HG2	2.17	0.44
7:1G:580:ALA:O	7:1G:633:TYR:HA	2.18	0.44
7:1G:615:THR:O	7:1G:619:VAL:HG23	2.18	0.44
10:1J:126:VAL:HG12	25:1Z:120:MET:SD	2.58	0.44
12:1L:413:LEU:HD13	12:1L:489:THR:HG21	2.00	0.44
13:1M:255:ASN:OD1	13:1M:256:TYR:N	2.51	0.44
13:1M:410:MET:HG2	13:1M:411:LEU:N	2.32	0.44
14:1N:95:MET:O	14:1N:99:THR:OG1	2.36	0.44
14:1N:210:THR:HG22	51:1N:402:CDL:H801	2.00	0.44
15:1O:308:TYR:OH	15:1O:320:LYS:O	2.33	0.44
17:1Q:9:GLN:HB2	22:1W:23:ARG:HD2	1.99	0.44
32:1g:56:TRP:HA	32:1g:59:ARG:HG2	1.99	0.44
33:1h:63:HIS:CE1	33:1h:64:TRP:HD1	2.35	0.44
34:1i:68:ILE:HA	34:1i:71:VAL:HG12	1.99	0.44
36:1k:12:LYS:HB3	36:1k:14:GLU:OE1	2.16	0.44
37:1l:133:TYR:HB3	37:1l:138:LEU:HD13	2.00	0.44
38:1m:43:LYS:HA	38:1m:43:LYS:HD3	1.89	0.44
2:1B:46:TRP:CH2	50:1H:701:U10:H353	2.53	0.44
4:1D:227:GLU:OE1	43:1r:17:ARG:NH2	2.50	0.44
5:1E:43:LYS:HB3	5:1E:43:LYS:HE3	1.84	0.44
6:1F:205:LEU:HB2	17:1Q:118:TYR:CE2	2.53	0.44
7:1G:560:ILE:HD12	7:1G:560:ILE:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:407:TRP:CG	37:1l:115:MET:HE1	2.53	0.44
12:1L:435:PRO:O	36:1k:51:ARG:HD3	2.17	0.44
12:1L:459:ILE:O	12:1L:462:ILE:HG13	2.18	0.44
13:1M:215:TRP:O	13:1M:219:ALA:HB3	2.17	0.44
13:1M:300:ALA:HB2	13:1M:381:ILE:HG12	1.98	0.44
14:1N:124:LEU:HB3	14:1N:220:ILE:CD1	2.45	0.44
14:1N:304:MET:H	14:1N:304:MET:HG3	1.67	0.44
15:1O:179:ILE:O	15:1O:183:ILE:HG23	2.18	0.44
15:1O:308:TYR:CZ	29:1d:51:ARG:HD3	2.52	0.44
17:1Q:16:LYS:NZ	17:1Q:18:ASP:HB2	2.32	0.44
20:1U:16:LEU:O	20:1U:20:LYS:HB3	2.17	0.44
25:1Z:98:MET:O	25:1Z:99:LYS:HE2	2.17	0.44
35:1j:29:SER:HA	35:1j:32:MET:HE3	2.00	0.44
38:1m:126:ILE:HG21	41:1p:138:PHE:HB3	1.98	0.44
39:1n:120:LYS:HB2	39:1n:123:GLN:HE21	1.83	0.44
40:1o:106:ARG:HA	40:1o:109:GLN:HG2	2.00	0.44
44:1s:57:GLU:O	44:1s:60:LYS:NZ	2.27	0.44
4:1D:289:SER:HB2	9:1I:7:MET:CE	2.47	0.44
5:1E:116:ILE:HD12	5:1E:152:PRO:HB2	1.99	0.44
7:1G:27:LEU:HD21	7:1G:39:ARG:NH2	2.33	0.44
8:1H:24:GLU:O	8:1H:28:LEU:HB2	2.18	0.44
9:1I:120:GLY:O	9:1I:123:GLN:HG2	2.18	0.44
12:1L:434:LYS:NZ	36:1k:52:TYR:HA	2.33	0.44
12:1L:566:THR:O	12:1L:570:GLN:HG2	2.18	0.44
13:1M:124:ALA:HB1	14:1N:256:PRO:HD3	2.00	0.44
13:1M:370:PRO:HB3	13:1M:375:LEU:HD12	2.00	0.44
13:1M:373:ILE:HG23	13:1M:448:THR:HA	2.00	0.44
15:1O:52:PRO:O	15:1O:107:GLN:NE2	2.51	0.44
15:1O:307:GLY:O	15:1O:320:LYS:NZ	2.33	0.44
15:1O:318:TRP:CE3	15:1O:319:LEU:HG	2.53	0.44
18:1R:53:GLY:HA2	18:1R:94:PRO:HD3	1.98	0.44
19:1S:24:GLN:HB3	19:1S:25:ARG:NH2	2.33	0.44
24:1Y:84:ASP:N	24:1Y:84:ASP:OD1	2.49	0.44
36:1k:58:ASN:ND2	36:1k:58:ASN:O	2.51	0.44
37:1l:125:TYR:CZ	40:1o:18:PRO:HD3	2.53	0.44
37:1l:157:GLU:HA	40:1o:36:ARG:HG2	1.99	0.44
41:1p:97:VAL:O	41:1p:101:ILE:HG12	2.18	0.44
41:1p:98:ASP:O	41:1p:102:VAL:HG12	2.18	0.44
41:1p:110:LYS:HE2	41:1p:110:LYS:HB2	1.76	0.44
6:1F:97:ALA:HB3	6:1F:138:ILE:HA	1.99	0.43
10:1J:65:LEU:HD23	10:1J:65:LEU:C	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:362:LEU:HA	12:1L:365:ALA:HB3	2.00	0.43
12:1L:447:ASN:OD1	12:1L:450:LEU:N	2.39	0.43
14:1N:159:MET:HE1	14:1N:282:MET:CG	2.43	0.43
28:1c:42:TYR:CZ	29:1d:22:PRO:HG3	2.52	0.43
29:1d:104:LYS:HZ3	29:1d:106:LYS:HA	1.82	0.43
38:1m:5:TYR:OH	38:1m:11:ALA:HB3	2.18	0.43
2:1B:56:ALA:O	2:1B:59:MET:HB3	2.18	0.43
2:1B:133:VAL:HG11	2:1B:139:ILE:HD13	2.00	0.43
4:1D:151:ILE:HD11	4:1D:218:PHE:CZ	2.52	0.43
5:1E:55:GLN:O	5:1E:59:GLY:N	2.51	0.43
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.99	0.43
6:1F:92:TYR:HE1	6:1F:133:ALA:HB3	1.83	0.43
12:1L:264:TYR:HA	12:1L:267:MET:HB3	2.00	0.43
12:1L:366:MET:HG3	12:1L:369:THR:OG1	2.18	0.43
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.18	0.43
13:1M:275:ILE:O	13:1M:279:GLN:HG2	2.18	0.43
13:1M:278:ARG:CZ	37:1l:83:MET:HB2	2.48	0.43
13:1M:355:MET:CE	13:1M:429:SER:HB2	2.48	0.43
13:1M:365:THR:HG21	13:1M:444:LEU:HD13	2.00	0.43
15:1O:81:LYS:HE3	15:1O:85:ASP:HB3	1.99	0.43
19:1S:74:LYS:HB2	19:1S:74:LYS:HE2	1.73	0.43
20:1T:49:GLU:HA	20:1T:52:MET:HB2	2.00	0.43
20:1U:78:ASP:OD2	34:1i:15:ARG:NH2	2.51	0.43
29:1d:30:ARG:HH21	29:1d:76:LEU:HD13	1.83	0.43
32:1g:64:PHE:HD1	32:1g:68:ILE:HD11	1.82	0.43
34:1i:122:PHE:CE1	40:1o:60:HIS:HB2	2.53	0.43
36:1k:21:TRP:CD1	36:1k:50:TRP:HB3	2.53	0.43
39:1n:103:LEU:HD23	39:1n:121:ARG:CD	2.45	0.43
6:1F:89:ARG:HD2	6:1F:218:CYS:HA	2.00	0.43
6:1F:215:VAL:N	6:1F:220:THR:OG1	2.45	0.43
6:1F:388:GLU:HA	6:1F:391:SER:HB2	2.00	0.43
9:1I:8:ARG:HG2	9:1I:8:ARG:HH11	1.84	0.43
12:1L:61:MET:HE2	12:1L:61:MET:HB3	1.79	0.43
12:1L:338:MET:HE2	12:1L:458:LEU:HA	2.00	0.43
13:1M:114:GLU:HG3	13:1M:174:LEU:HB2	2.01	0.43
14:1N:193:VAL:HB	14:1N:266:ILE:HD13	2.00	0.43
16:1P:193:LEU:H	16:1P:193:LEU:HD22	1.83	0.43
19:1S:50:LEU:HD22	19:1S:50:LEU:HA	1.81	0.43
20:1T:51:ILE:O	20:1T:54:MET:HB2	2.18	0.43
20:1T:60:PHE:HZ	20:1T:80:ILE:HG23	1.84	0.43
21:1V:106:PRO:HA	21:1V:107:PRO:HD3	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:56:LEU:O	23:1X:60:LYS:HG2	2.18	0.43
25:1Z:120:MET:HG2	25:1Z:121:MET:N	2.33	0.43
28:1c:8:PRO:HB2	28:1c:9:HIS:ND1	2.33	0.43
28:1c:20:THR:HG21	29:1d:59:HIS:HB2	2.00	0.43
52:1f:102:3PE:H2A2	52:1f:102:3PE:H271	1.86	0.43
33:1h:66:TYR:CE2	41:1p:65:ARG:HA	2.53	0.43
34:1i:9:LEU:HD22	39:1n:155:PRO:HB2	1.99	0.43
36:1k:67:LEU:HD13	36:1k:70:PHE:HB3	1.99	0.43
39:1n:138:GLN:OE1	39:1n:164:PRO:HD3	2.18	0.43
43:1r:7:ILE:HD13	43:1r:7:ILE:HA	1.90	0.43
2:1B:46:TRP:HZ3	8:1H:220:PHE:HE2	1.66	0.43
3:1C:82:ASP:CG	3:1C:89:ARG:HH21	2.25	0.43
4:1D:19:MET:HE3	4:1D:19:MET:N	2.33	0.43
6:1F:233:THR:HG23	6:1F:237:ARG:HG3	2.01	0.43
9:1I:12:MET:HE2	27:1b:9:LYS:HE2	1.98	0.43
12:1L:49:VAL:O	12:1L:52:LEU:HB2	2.17	0.43
12:1L:361:GLY:HA2	36:1k:59:ASN:ND2	2.33	0.43
20:1T:22:TYR:CE2	20:1T:24:LYS:HB2	2.52	0.43
33:1h:95:GLN:O	33:1h:99:GLU:HG3	2.17	0.43
34:1i:10:ARG:HD2	39:1n:154:PRO:C	2.43	0.43
34:1i:39:VAL:HG12	34:1i:44:GLN:OE1	2.18	0.43
35:1j:19:ARG:HA	35:1j:22:LEU:HD13	2.01	0.43
37:1l:98:TRP:O	37:1l:101:MET:HG2	2.17	0.43
37:1l:99:ASN:N	37:1l:99:ASN:OD1	2.51	0.43
38:1m:22:TYR:OH	39:1n:67:GLU:OE1	2.37	0.43
39:1n:70:PHE:O	39:1n:74:GLN:N	2.52	0.43
1:1A:30:TYR:CE2	1:1A:33:LYS:HB2	2.53	0.43
4:1D:110:SER:HA	4:1D:145:THR:HG22	2.00	0.43
6:1F:256:PHE:HE1	6:1F:317:MET:HG2	1.83	0.43
7:1G:372:GLU:HA	7:1G:398:SER:HB2	1.99	0.43
8:1H:270:PHE:O	8:1H:273:ILE:HG13	2.18	0.43
12:1L:432:LEU:HD13	36:1k:62:PHE:HD1	1.83	0.43
13:1M:392:THR:O	13:1M:396:MET:HG2	2.17	0.43
13:1M:398:MET:O	13:1M:401:MET:HB3	2.18	0.43
16:1P:173:GLY:N	16:1P:176:ASP:HB3	2.33	0.43
16:1P:206:TYR:O	16:1P:210:VAL:HG23	2.18	0.43
16:1P:322:ARG:NH2	16:1P:329:SER:HB2	2.33	0.43
19:1S:21:HIS:O	19:1S:62:PRO:HA	2.17	0.43
20:1U:55:GLU:CG	20:1U:62:ILE:H	2.30	0.43
23:1X:76:HIS:HB3	23:1X:113:LYS:HG2	2.00	0.43
25:1Z:51:MET:SD	25:1Z:55:ARG:NH2	2.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:1d:78:ARG:NH1	29:1d:82:MET:HE1	2.33	0.43
33:1h:40:ILE:HG22	33:1h:71:ILE:CD1	2.49	0.43
37:1l:114:PHE:O	37:1l:117:TRP:HB3	2.18	0.43
37:1l:156:TYR:HA	40:1o:35:GLU:HA	1.99	0.43
1:1A:84:LEU:HD13	1:1A:84:LEU:HA	1.85	0.43
4:1D:73:VAL:C	4:1D:74:ARG:HD2	2.44	0.43
4:1D:141:PHE:O	4:1D:145:THR:OG1	2.33	0.43
7:1G:218:ARG:O	7:1G:221:GLU:HG2	2.19	0.43
7:1G:555:PRO:HG3	42:1q:137:TRP:HZ2	1.83	0.43
8:1H:264:LEU:O	8:1H:268:ILE:HG12	2.19	0.43
9:1I:174:LEU:HD23	9:1I:174:LEU:HA	1.86	0.43
12:1L:202:PHE:CE1	12:1L:265:PRO:HG2	2.53	0.43
12:1L:404:THR:OG1	12:1L:405:ASN:N	2.52	0.43
12:1L:434:LYS:HE2	12:1L:434:LYS:HA	2.00	0.43
12:1L:590:SER:O	12:1L:593:ILE:HG22	2.18	0.43
13:1M:452:LYS:HG3	32:1g:83:TYR:CE2	2.53	0.43
14:1N:59:TYR:OH	14:1N:134:GLN:NE2	2.51	0.43
14:1N:93:VAL:HA	14:1N:96:THR:HG22	2.00	0.43
14:1N:211:MET:HE1	14:1N:251:MET:SD	2.59	0.43
14:1N:214:ALA:HB1	14:1N:330:ILE:HD13	2.01	0.43
15:1O:231:ALA:O	15:1O:234:VAL:HG22	2.18	0.43
18:1R:52:VAL:HG12	18:1R:54:SER:H	1.83	0.43
18:1R:74:ASN:OD1	18:1R:76:ASP:HB2	2.18	0.43
20:1U:42:LEU:HD12	20:1U:46:ASP:HB3	2.00	0.43
22:1W:70:ASN:OD1	22:1W:70:ASN:N	2.26	0.43
23:1X:15:GLN:H	23:1X:15:GLN:CD	2.27	0.43
26:1a:50:ARG:O	26:1a:54:ILE:HG22	2.19	0.43
51:1a:101:CDL:CB3	42:1q:6:VAL:HG11	2.45	0.43
41:1p:32:LEU:HA	41:1p:35:ILE:HD11	2.00	0.43
41:1p:91:TRP:CH2	41:1p:149:TYR:HD2	2.36	0.43
42:1q:67:GLU:OE2	42:1q:68:MET:N	2.51	0.43
43:1r:42:VAL:HB	43:1r:46:HIS:CG	2.54	0.43
1:1A:1:FME:O1	1:1A:2:ASN:N	2.49	0.43
2:1B:150:PRO:HG3	4:1D:189:MET:SD	2.58	0.43
4:1D:23:LYS:HA	4:1D:23:LYS:HD3	1.74	0.43
11:1K:37:MET:HE3	11:1K:63:LEU:CD1	2.48	0.43
11:1K:96:LEU:HD23	14:1N:51:ARG:HH11	1.83	0.43
12:1L:95:PHE:O	12:1L:99:SER:OG	2.36	0.43
12:1L:394:LEU:H	12:1L:394:LEU:HD12	1.84	0.43
13:1M:431:THR:H	13:1M:431:THR:HG22	1.55	0.43
15:1O:280:PRO:HG3	32:1g:25:ARG:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:46:THR:HG22	22:1W:52:LEU:HD22	2.00	0.43
32:1g:48:ASP:C	32:1g:48:ASP:OD1	2.62	0.43
34:1i:97:VAL:HG23	41:1p:115:ARG:HH11	1.84	0.43
38:1m:39:ARG:O	38:1m:43:LYS:HG2	2.19	0.43
1:1A:60:ILE:O	1:1A:63:LEU:HB3	2.19	0.43
4:1D:11:ALA:HA	14:1N:305:PHE:HE2	1.84	0.43
4:1D:266:GLN:HG2	4:1D:287:ILE:HG13	2.01	0.43
7:1G:55:CYS:SG	7:1G:68:ALA:N	2.92	0.43
7:1G:158:ARG:NH2	7:1G:202:ILE:O	2.50	0.43
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.54	0.43
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.19	0.43
12:1L:190:LEU:HD12	12:1L:190:LEU:HA	1.84	0.43
12:1L:338:MET:HE2	12:1L:458:LEU:HD22	2.01	0.43
12:1L:371:THR:O	12:1L:374:ILE:HD12	2.18	0.43
13:1M:281:ASP:OD1	13:1M:282:LEU:N	2.52	0.43
18:1R:80:LYS:HZ3	18:1R:81:THR:H	1.65	0.43
25:1Z:83:VAL:HG23	25:1Z:124:LEU:HD11	2.00	0.43
30:1e:69:GLN:OE1	30:1e:69:GLN:N	2.52	0.43
46:1f:101:PC1:H3C2	32:1g:72:LEU:HD22	2.01	0.43
33:1h:12:LYS:HE2	33:1h:12:LYS:HA	2.01	0.43
33:1h:34:ILE:CG1	33:1h:35:PRO:HD3	2.47	0.43
37:1l:32:GLU:C	37:1l:32:GLU:CD	2.87	0.43
37:1l:130:PRO:HG2	37:1l:132:GLN:HE22	1.83	0.43
2:1B:62:MET:HB3	2:1B:153:ALA:HB1	2.00	0.43
3:1C:32:ILE:HG21	3:1C:63:PHE:CE1	2.54	0.43
4:1D:74:ARG:HD2	4:1D:74:ARG:N	2.34	0.43
6:1F:12:PHE:O	6:1F:274:VAL:HA	2.18	0.43
6:1F:307:ILE:HG13	6:1F:311:VAL:HB	2.01	0.43
8:1H:27:VAL:O	8:1H:31:MET:HG2	2.19	0.43
11:1K:37:MET:HG2	11:1K:67:ALA:HB1	2.00	0.43
11:1K:66:PHE:CE1	14:1N:31:ILE:HG12	2.54	0.43
12:1L:285:THR:HG22	12:1L:308:SER:O	2.19	0.43
12:1L:496:MET:HE2	12:1L:496:MET:C	2.44	0.43
13:1M:109:THR:HG21	13:1M:238:LEU:HD11	1.99	0.43
13:1M:196:TRP:CZ2	13:1M:200:ILE:HG13	2.53	0.43
14:1N:30:TRP:CG	14:1N:71:MET:HE1	2.53	0.43
15:1O:89:ASN:HD21	32:1g:23:THR:N	2.16	0.43
15:1O:155:VAL:O	15:1O:159:THR:HG23	2.19	0.43
21:1V:97:LYS:HD2	21:1V:97:LYS:HA	1.78	0.43
25:1Z:80:ASP:HA	25:1Z:83:VAL:HG12	2.00	0.43
28:1c:37:GLU:O	28:1c:41:GLU:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1c:39:VAL:HG13	28:1c:40:LEU:HD12	2.01	0.43
31:1f:26:LEU:O	31:1f:29:ARG:C	2.62	0.43
37:1l:27:TYR:CE2	37:1l:48:PRO:HD3	2.53	0.43
37:1l:129:GLY:H	40:1o:97:ARG:HB3	1.84	0.43
42:1q:60:ARG:HH22	42:1q:95:ASP:HA	1.83	0.43
43:1r:33:ARG:HA	43:1r:33:ARG:HD2	1.70	0.43
1:1A:63:LEU:HD11	11:1K:68:ALA:HB1	2.01	0.43
2:1B:145:TYR:CZ	9:1I:144:HIS:HB2	2.54	0.43
6:1F:15:LEU:O	6:1F:20:ARG:NH2	2.52	0.43
6:1F:207:PRO:HB3	7:1G:72:PRO:HD3	2.01	0.43
7:1G:344:CYS:HB3	7:1G:510:GLY:O	2.19	0.43
7:1G:367:THR:HG22	7:1G:636:VAL:HG11	2.01	0.43
7:1G:544:ILE:HG23	7:1G:559:VAL:HG23	2.01	0.43
9:1I:173:TYR:HA	9:1I:176:ARG:HD2	2.01	0.43
10:1J:14:VAL:O	10:1J:18:VAL:HG23	2.19	0.43
12:1L:9:LEU:HD21	12:1L:63:ILE:HD11	2.00	0.43
12:1L:553:LEU:HD22	12:1L:553:LEU:HA	1.84	0.43
13:1M:45:LEU:HD13	13:1M:46:GLY:H	1.84	0.43
14:1N:86:ILE:HG23	14:1N:86:ILE:O	2.19	0.43
15:1O:233:LYS:HE2	21:1V:29:LYS:HG2	2.01	0.43
16:1P:154:LYS:HA	16:1P:154:LYS:HE3	2.00	0.43
17:1Q:59:PHE:CE2	17:1Q:79:LEU:HD22	2.54	0.43
21:1V:33:VAL:HG11	21:1V:91:ARG:HD3	2.01	0.43
25:1Z:28:ARG:NH2	43:1r:13:TRP:O	2.51	0.43
29:1d:30:ARG:HE	29:1d:30:ARG:HB2	1.65	0.43
34:1i:25:GLN:HA	39:1n:117:TYR:HE2	1.84	0.43
37:1l:73:TRP:CG	38:1m:46:TYR:HB2	2.53	0.43
37:1l:78:HIS:CD2	37:1l:80:ASP:HB2	2.54	0.43
37:1l:115:MET:HA	37:1l:118:VAL:HG22	2.01	0.43
38:1m:41:ARG:O	38:1m:45:GLU:OE1	2.37	0.43
39:1n:63:LEU:HG	39:1n:67:GLU:OE1	2.18	0.43
42:1q:51:ASP:CG	42:1q:54:GLN:HE21	2.27	0.43
2:1B:84:ASP:N	2:1B:84:ASP:OD1	2.52	0.42
4:1D:29:LYS:HD2	4:1D:29:LYS:O	2.19	0.42
4:1D:87:THR:HG21	4:1D:106:LEU:HD21	2.01	0.42
7:1G:328:LEU:O	7:1G:507:TYR:OH	2.30	0.42
7:1G:632:ARG:HG2	7:1G:632:ARG:NH1	2.33	0.42
51:1H:702:CDL:H512	51:1H:702:CDL:HB4	1.75	0.42
12:1L:146:GLY:O	12:1L:150:MET:HB2	2.19	0.42
12:1L:594:THR:HG21	14:1N:110:PRO:HG2	2.01	0.42
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:204:MET:HE1	13:1M:261:PHE:CG	2.53	0.42
16:1P:59:LEU:HA	16:1P:62:MET:HE2	2.01	0.42
18:1R:18:TYR:CE2	18:1R:24:ARG:HB3	2.54	0.42
20:1T:38:LYS:HE3	20:1T:38:LYS:CA	2.43	0.42
26:1a:3:PHE:HE2	51:1a:101:CDL:CA2	2.32	0.42
30:1e:16:TRP:CE3	30:1e:17:MET:HB2	2.54	0.42
32:1g:70:LEU:O	32:1g:74:SER:OG	2.37	0.42
34:1i:56:TRP:O	34:1i:60:ILE:HG13	2.19	0.42
35:1j:63:GLU:H	35:1j:63:GLU:HG3	1.50	0.42
39:1n:158:LYS:HE3	39:1n:158:LYS:HB3	1.72	0.42
3:1C:89:ARG:HD3	3:1C:113:GLU:OE2	2.19	0.42
3:1C:148:LEU:HD12	3:1C:148:LEU:HA	1.86	0.42
5:1E:82:GLU:OE1	6:1F:200:GLN:HB3	2.19	0.42
6:1F:307:ILE:HG23	6:1F:312:CYS:SG	2.59	0.42
7:1G:688:VAL:HA	7:1G:691:VAL:HG12	2.00	0.42
10:1J:3:MET:HE3	10:1J:3:MET:O	2.19	0.42
12:1L:336:LYS:O	12:1L:339:LEU:HD12	2.18	0.42
12:1L:507:THR:HA	12:1L:510:TYR:CE2	2.54	0.42
12:1L:605:HIS:CE1	14:1N:92:PRO:HB2	2.54	0.42
13:1M:295:ALA:HA	13:1M:298:ILE:HD12	2.01	0.42
13:1M:358:TRP:HA	13:1M:361:MET:SD	2.59	0.42
20:1U:19:LEU:HD12	20:1U:20:LYS:N	2.32	0.42
22:1W:75:ASP:O	22:1W:79:VAL:HG23	2.19	0.42
29:1d:45:ASP:O	29:1d:48:ILE:HG22	2.18	0.42
32:1g:96:LEU:HD13	32:1g:100:ARG:HD2	2.01	0.42
37:1l:95:PRO:HA	39:1n:71:TRP:CH2	2.53	0.42
39:1n:52:ASN:OD1	39:1n:52:ASN:N	2.51	0.42
39:1n:134:ARG:NH1	39:1n:138:GLN:HB2	2.34	0.42
40:1o:24:PHE:CE2	40:1o:107:LEU:HD22	2.54	0.42
40:1o:94:TYR:CE2	40:1o:98:MET:HE2	2.54	0.42
41:1p:4:TRP:HD1	41:1p:9:TYR:HB2	1.84	0.42
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.39	0.42
3:1C:45:PHE:CD1	3:1C:47:GLU:HG3	2.54	0.42
3:1C:113:GLU:OE2	17:1Q:98:LYS:HD2	2.19	0.42
4:1D:121:ALA:HA	4:1D:365:THR:HG21	1.99	0.42
5:1E:7:PHE:HB3	7:1G:175:THR:HB	2.01	0.42
12:1L:12:LEU:O	12:1L:15:LEU:HG	2.18	0.42
13:1M:271:MET:O	13:1M:275:ILE:HG13	2.19	0.42
14:1N:45:MET:HE2	14:1N:45:MET:HB2	1.89	0.42
15:1O:278:TYR:O	32:1g:25:ARG:NH1	2.52	0.42
18:1R:80:LYS:HD2	18:1R:80:LYS:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:79:TYR:CD2	20:1U:80:ILE:HD13	2.54	0.42
21:1V:27:TYR:HB3	21:1V:55:LEU:HD22	2.02	0.42
21:1V:29:LYS:O	21:1V:33:VAL:HG23	2.18	0.42
24:1Y:124:VAL:HA	52:1Y:202:3PE:H252	2.01	0.42
25:1Z:101:VAL:HG21	25:1Z:104:TRP:HB2	2.02	0.42
34:1i:81:ILE:C	34:1i:81:ILE:HD12	2.43	0.42
35:1j:64:LEU:HD13	35:1j:66:ILE:HG12	2.01	0.42
39:1n:106:TRP:CE3	39:1n:110:GLU:HB3	2.55	0.42
42:1q:61:TRP:HE1	42:1q:63:ILE:HD11	1.85	0.42
4:1D:4:TRP:HE1	4:1D:6:PRO:HA	1.83	0.42
5:1E:165:THR:HB	5:1E:168:ASP:OD1	2.19	0.42
6:1F:302:SER:O	6:1F:414:PRO:HG3	2.19	0.42
7:1G:623:LEU:HD22	7:1G:630:LEU:HD12	2.01	0.42
8:1H:121:TRP:CE2	10:1J:27:ILE:HD12	2.54	0.42
8:1H:125:SER:HB2	8:1H:214:GLU:OE2	2.20	0.42
9:1I:7:MET:O	9:1I:8:ARG:NH1	2.53	0.42
10:1J:57:PHE:O	10:1J:61:LEU:HD13	2.20	0.42
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.20	0.42
12:1L:314:MET:HA	12:1L:317:ILE:HG13	2.01	0.42
12:1L:379:ALA:O	12:1L:388:GLY:HA3	2.19	0.42
12:1L:414:ILE:O	12:1L:418:LEU:HG	2.18	0.42
19:1S:19:ARG:HG2	19:1S:21:HIS:NE2	2.34	0.42
22:1W:50:PHE:HB3	22:1W:52:LEU:HD13	2.00	0.42
52:1Y:202:3PE:C1	52:1Y:202:3PE:H221	2.48	0.42
25:1Z:58:ARG:HA	25:1Z:58:ARG:HD2	1.77	0.42
25:1Z:77:ALA:HA	25:1Z:80:ASP:OD2	2.19	0.42
40:1o:98:MET:HE3	40:1o:98:MET:HB2	1.60	0.42
1:1A:115:GLU:HA	4:1D:72:MET:SD	2.58	0.42
4:1D:115:GLU:HB2	4:1D:194:ILE:HB	2.02	0.42
8:1H:310:MET:O	27:1b:37:TYR:HB2	2.18	0.42
9:1I:160:LYS:HD3	42:1q:110:TRP:CZ3	2.54	0.42
10:1J:50:SER:H	10:1J:139:GLU:CD	2.27	0.42
12:1L:15:LEU:C	12:1L:18:PRO:HD2	2.44	0.42
12:1L:22:SER:HA	12:1L:27:TYR:CD1	2.55	0.42
12:1L:175:ASN:HD22	12:1L:223:LYS:NZ	2.18	0.42
13:1M:12:LEU:HB2	13:1M:13:PRO:HD3	2.00	0.42
13:1M:135:ARG:HG2	13:1M:135:ARG:NH1	2.34	0.42
13:1M:190:TRP:NE1	46:1M:501:PC1:H121	2.35	0.42
13:1M:422:HIS:HB2	38:1m:59:ILE:HD12	2.01	0.42
15:1O:280:PRO:HA	32:1g:25:ARG:HA	2.02	0.42
15:1O:291:ARG:O	15:1O:295:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:136:ASN:ND2	16:1P:290:SER:O	2.53	0.42
24:1Y:56:GLY:HA2	24:1Y:59:THR:HG22	2.01	0.42
34:1i:83:TYR:HD1	34:1i:87:TYR:CD2	2.37	0.42
37:1l:104:HIS:O	37:1l:108:PHE:HB2	2.19	0.42
38:1m:94:ILE:HD11	38:1m:98:PHE:CE2	2.54	0.42
40:1o:105:ARG:HD2	40:1o:109:GLN:OE1	2.20	0.42
41:1p:141:ARG:HD3	41:1p:142:TYR:CE2	2.54	0.42
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.45	0.42
4:1D:151:ILE:HG12	4:1D:170:MET:CE	2.47	0.42
8:1H:116:ILE:HG23	8:1H:211:PHE:CD2	2.55	0.42
10:1J:117:PHE:HZ	14:1N:76:ILE:HD13	1.84	0.42
12:1L:346:ILE:HD11	12:1L:359:MET:HG3	2.01	0.42
12:1L:379:ALA:HA	12:1L:386:LEU:HD13	2.02	0.42
13:1M:115:LEU:HB2	13:1M:174:LEU:HB3	2.01	0.42
13:1M:190:TRP:CE2	24:1Y:126:MET:HE1	2.55	0.42
15:1O:73:LEU:HD11	15:1O:295:LYS:HB2	2.01	0.42
16:1P:29:PHE:HB3	16:1P:30:LEU:H	1.63	0.42
16:1P:282:ASP:CG	16:1P:286:ARG:HE	2.27	0.42
20:1T:40:LEU:HD13	20:1T:40:LEU:HA	1.87	0.42
22:1W:46:THR:O	22:1W:50:PHE:HB2	2.19	0.42
22:1W:70:ASN:HD21	57:1W:201:EHZ:C8	2.33	0.42
23:1X:19:VAL:HG23	23:1X:24:LEU:HG	2.02	0.42
30:1e:21:SER:OG	30:1e:36:GLU:OE1	2.29	0.42
37:1l:115:MET:C	37:1l:115:MET:HE2	2.44	0.42
38:1m:120:LEU:HD23	38:1m:120:LEU:HA	1.79	0.42
43:1r:7:ILE:O	43:1r:11:ARG:HG3	2.19	0.42
43:1r:91:LYS:HE2	43:1r:91:LYS:H	1.82	0.42
1:1A:98:LEU:HD23	8:1H:298:LEU:HD21	2.02	0.42
2:1B:102:LYS:O	2:1B:105:ASP:HB2	2.19	0.42
4:1D:339:LYS:HE2	18:1R:67:GLY:O	2.20	0.42
7:1G:650:LYS:HB2	7:1G:650:LYS:HE2	1.89	0.42
8:1H:114:TYR:HE2	10:1J:34:ILE:CD1	2.32	0.42
10:1J:46:ASN:O	10:1J:128:TYR:OH	2.36	0.42
10:1J:153:LEU:HA	10:1J:156:VAL:HG22	2.01	0.42
12:1L:103:PHE:CD1	12:1L:341:MET:HB2	2.54	0.42
13:1M:44:GLN:OE1	13:1M:60:SER:HA	2.19	0.42
13:1M:71:TRP:CZ2	13:1M:439:LEU:HB3	2.54	0.42
13:1M:96:ILE:HG22	13:1M:100:ILE:CD1	2.49	0.42
13:1M:123:GLU:C	13:1M:123:GLU:OE1	2.63	0.42
13:1M:215:TRP:CD1	13:1M:215:TRP:H	2.37	0.42
14:1N:114:TRP:CE2	14:1N:115:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:116:LYS:HD2	17:1Q:116:LYS:HA	1.79	0.42
20:1U:83:LYS:HE3	20:1U:84:LYS:HG3	2.01	0.42
22:1W:51:GLN:HB3	22:1W:100:ARG:NH2	2.35	0.42
33:1h:23:LYS:HD2	33:1h:23:LYS:O	2.19	0.42
36:1k:19:LYS:HA	36:1k:22:LYS:NZ	2.34	0.42
42:1q:48:TYR:HE1	42:1q:86:TRP:CB	2.32	0.42
1:1A:93:PHE:C	1:1A:93:PHE:CD1	2.98	0.42
2:1B:102:LYS:HD3	2:1B:102:LYS:C	2.44	0.42
5:1E:140:ILE:C	5:1E:140:ILE:HD12	2.45	0.42
8:1H:20:LEU:HD12	8:1H:228:TYR:CD2	2.55	0.42
9:1I:111:ILE:HG22	9:1I:113:MET:HE3	2.01	0.42
11:1K:27:MET:O	11:1K:31:LEU:HG	2.19	0.42
12:1L:428:PHE:HA	12:1L:432:LEU:HB2	2.02	0.42
12:1L:522:PHE:HD1	12:1L:528:TYR:CE2	2.38	0.42
12:1L:586:LEU:H	12:1L:586:LEU:HD22	1.84	0.42
15:1O:46:LEU:HB2	15:1O:48:LEU:HD13	2.02	0.42
20:1T:49:GLU:HB3	22:1W:40:TYR:CE2	2.55	0.42
20:1U:69:LYS:HE2	20:1U:69:LYS:HB2	1.44	0.42
22:1W:98:LYS:C	22:1W:99:GLN:OE1	2.62	0.42
23:1X:162:HIS:NE2	33:1h:99:GLU:OE1	2.48	0.42
24:1Y:49:LEU:HD12	24:1Y:50:GLU:N	2.35	0.42
25:1Z:97:ILE:O	25:1Z:98:MET:HE2	2.19	0.42
34:1i:71:VAL:HA	34:1i:75:LEU:HB3	2.02	0.42
36:1k:30:THR:O	36:1k:34:LYS:HB2	2.19	0.42
36:1k:46:ARG:HA	36:1k:49:ALA:HB2	2.01	0.42
36:1k:81:VAL:HA	36:1k:84:GLU:HG3	2.02	0.42
40:1o:6:ARG:HE	40:1o:105:ARG:HH21	1.68	0.42
41:1p:6:LYS:O	41:1p:10:PRO:HD3	2.20	0.42
41:1p:82:LEU:O	41:1p:86:GLU:HG2	2.20	0.42
1:1A:38:GLU:HG2	1:1A:43:PRO:HA	2.01	0.42
7:1G:256:GLU:C	7:1G:394:ARG:HH22	2.28	0.42
10:1J:60:TYR:CE1	11:1K:38:LEU:HB2	2.49	0.42
11:1K:61:ILE:O	11:1K:65:VAL:HG23	2.20	0.42
12:1L:298:ILE:HG12	12:1L:347:ILE:HD11	2.01	0.42
12:1L:450:LEU:O	12:1L:454:ILE:HG13	2.19	0.42
13:1M:216:LEU:HD12	13:1M:216:LEU:H	1.84	0.42
14:1N:245:MET:HE2	14:1N:302:LEU:HD21	2.02	0.42
20:1T:6:LEU:HB2	20:1T:10:ALA:HB3	2.01	0.42
52:1Y:202:3PE:O12	52:1Y:202:3PE:H122	2.20	0.42
30:1e:29:PRO:HG3	33:1h:140:THR:HB	2.01	0.42
52:1f:102:3PE:O22	52:1f:102:3PE:H242	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:10:ILE:HD12	33:1h:10:ILE:HA	1.95	0.42
40:1o:112:LYS:HA	40:1o:115:GLU:CD	2.45	0.42
42:1q:78:ASP:OD1	42:1q:78:ASP:C	2.63	0.42
43:1r:57:ASP:CG	43:1r:60:ARG:HB2	2.45	0.42
2:1B:46:TRP:CZ3	8:1H:55:LEU:HD21	2.55	0.42
3:1C:164:LYS:NZ	4:1D:92:GLU:HG3	2.35	0.42
3:1C:184:VAL:HG21	22:1W:110:THR:HG21	2.01	0.42
6:1F:263:ASN:ND2	6:1F:286:GLY:O	2.52	0.42
7:1G:20:VAL:HG21	7:1G:73:VAL:HG21	2.01	0.42
8:1H:98:MET:HE1	8:1H:104:PHE:CD2	2.55	0.42
8:1H:303:TRP:HE3	27:1b:28:ALA:HB2	1.84	0.42
9:1I:17:VAL:CG2	27:1b:13:ALA:HA	2.50	0.42
10:1J:37:GLY:HA2	11:1K:38:LEU:HD21	2.01	0.42
13:1M:11:LEU:HD22	13:1M:100:ILE:HG12	2.02	0.42
13:1M:76:MET:HB3	13:1M:226:ALA:CB	2.49	0.42
13:1M:114:GLU:HG2	13:1M:116:ILE:H	1.85	0.42
14:1N:91:ASN:OD1	14:1N:94:ALA:N	2.49	0.42
15:1O:35:LYS:HE2	15:1O:126:ARG:NH2	2.35	0.42
15:1O:56:ILE:HD13	15:1O:99:TRP:CD1	2.55	0.42
15:1O:60:ASP:OD1	15:1O:60:ASP:N	2.53	0.42
15:1O:116:LEU:HD21	15:1O:259:LEU:HD23	2.02	0.42
20:1U:34:SER:HB2	20:1U:40:LEU:CD2	2.50	0.42
20:1U:34:SER:HB2	20:1U:40:LEU:HD21	2.01	0.42
24:1Y:139:LYS:HE2	24:1Y:140:VAL:HG13	2.02	0.42
31:1f:39:ASN:C	31:1f:40:LYS:HD3	2.45	0.42
33:1h:11:ILE:O	39:1n:98:VAL:HB	2.20	0.42
33:1h:55:ILE:HG23	33:1h:57:GLU:H	1.85	0.42
35:1j:10:ARG:HG2	35:1j:13:GLN:HB2	2.02	0.42
35:1j:64:LEU:CD1	35:1j:66:ILE:HG12	2.49	0.42
39:1n:117:TYR:HA	39:1n:120:LYS:CD	2.49	0.42
2:1B:67:TYR:CE1	2:1B:154:GLU:HG3	2.54	0.41
4:1D:302:GLU:O	4:1D:306:GLN:HG2	2.19	0.41
7:1G:254:MET:HE3	7:1G:254:MET:HB3	1.84	0.41
7:1G:324:ASP:O	7:1G:328:LEU:HG	2.18	0.41
7:1G:441:GLN:HG2	7:1G:444:LYS:NZ	2.35	0.41
8:1H:5:ASN:HD21	26:1a:23:THR:HG1	1.63	0.41
8:1H:98:MET:HE1	8:1H:104:PHE:CG	2.55	0.41
10:1J:79:TYR:OH	16:1P:325:ARG:O	2.32	0.41
12:1L:194:ASN:ND2	38:1m:127:SER:HB3	2.35	0.41
12:1L:504:LEU:HD13	52:1L:701:3PE:H321	2.02	0.41
12:1L:590:SER:HA	12:1L:593:ILE:HG22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:78:MET:SD	32:1g:61:VAL:HG21	2.60	0.41
14:1N:289:ASN:HA	14:1N:292:PHE:CZ	2.55	0.41
15:1O:50:HIS:HE2	15:1O:125:GLU:CD	2.27	0.41
15:1O:138:MET:O	15:1O:143:PHE:HB2	2.19	0.41
16:1P:3:HIS:C	16:1P:3:HIS:CD2	2.97	0.41
18:1R:9:GLU:HG3	18:1R:33:LYS:HD2	2.01	0.41
20:1U:49:GLU:O	20:1U:52:MET:HG2	2.20	0.41
29:1d:108:THR:OG1	41:1p:74:THR:O	2.38	0.41
35:1j:33:TRP:O	35:1j:36:ILE:HD12	2.20	0.41
37:1l:91:THR:HA	38:1m:10:LEU:O	2.20	0.41
37:1l:153:VAL:O	37:1l:153:VAL:CG1	2.67	0.41
42:1q:98:PRO:HA	42:1q:101:LYS:O	2.20	0.41
1:1A:60:ILE:HD11	11:1K:72:ALA:HA	2.02	0.41
8:1H:199:ASP:OD1	8:1H:279:ARG:NH1	2.53	0.41
9:1I:45:PRO:HG2	43:1r:0:ACE:H3	2.02	0.41
9:1I:70:TYR:CE2	9:1I:76:ARG:HA	2.54	0.41
12:1L:295:GLN:HG3	12:1L:304:PHE:CE2	2.55	0.41
12:1L:389:PHE:HB2	12:1L:393:ASP:OD1	2.19	0.41
12:1L:409:LEU:O	12:1L:412:THR:OG1	2.27	0.41
13:1M:329:LEU:O	13:1M:332:THR:OG1	2.33	0.41
13:1M:335:GLU:C	13:1M:335:GLU:OE1	2.63	0.41
13:1M:349:GLN:HA	13:1M:356:ALA:HB2	2.02	0.41
13:1M:459:TYR:C	32:1g:84:ARG:HH21	2.27	0.41
14:1N:59:TYR:HB2	14:1N:118:VAL:HG11	2.03	0.41
16:1P:211:SER:O	16:1P:215:ILE:HG12	2.20	0.41
20:1T:35:HIS:HE1	20:1T:71:MET:HE2	1.83	0.41
20:1T:48:VAL:HG12	20:1T:52:MET:HE3	2.03	0.41
20:1T:79:TYR:CD2	20:1T:79:TYR:C	2.98	0.41
22:1W:54:ILE:HG23	22:1W:104:MET:HE1	2.02	0.41
28:1c:29:ILE:HD12	28:1c:30:TYR:H	1.85	0.41
28:1c:32:ILE:O	28:1c:36:LYS:HG3	2.20	0.41
30:1e:35:PHE:CE1	30:1e:61:ASP:HB3	2.56	0.41
36:1k:85:TYR:O	36:1k:88:GLU:HG3	2.20	0.41
37:1l:125:TYR:H	40:1o:4:LEU:HD21	1.85	0.41
39:1n:25:HIS:CD2	39:1n:74:GLN:HB2	2.54	0.41
41:1p:145:LEU:HD11	41:1p:154:CYS:HB2	2.02	0.41
1:1A:19:LEU:HD23	1:1A:19:LEU:HA	1.89	0.41
2:1B:76:PHE:HD2	50:1H:701:U10:H171	1.85	0.41
2:1B:80:PRO:HA	2:1B:83:SER:OG	2.21	0.41
2:1B:125:TYR:HE2	4:1D:101:PRO:HB2	1.84	0.41
5:1E:30:ARG:NE	44:1s:53:ASP:OD1	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:102:VAL:HG22	5:1E:154:VAL:HG22	2.02	0.41
5:1E:183:LYS:HB3	5:1E:187:ARG:HH12	1.85	0.41
7:1G:94:MET:HB2	7:1G:94:MET:HE3	1.93	0.41
7:1G:190:MET:SD	7:1G:695:ILE:HG22	2.61	0.41
12:1L:154:LEU:HA	12:1L:154:LEU:HD23	1.84	0.41
12:1L:392:LYS:O	12:1L:395:ILE:HB	2.20	0.41
12:1L:396:ILE:O	12:1L:399:VAL:HG12	2.20	0.41
12:1L:481:THR:O	40:1o:94:TYR:CE2	2.73	0.41
13:1M:130:LEU:HD12	13:1M:130:LEU:HA	1.74	0.41
14:1N:30:TRP:CD2	14:1N:71:MET:HE1	2.55	0.41
14:1N:109:SER:C	14:1N:111:PHE:N	2.78	0.41
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.44	0.41
22:1W:88:MET:O	22:1W:92:GLU:HG3	2.20	0.41
29:1d:70:PHE:CD1	29:1d:70:PHE:C	2.98	0.41
34:1i:103:ILE:H	34:1i:103:ILE:HG12	1.74	0.41
35:1j:21:GLN:H	35:1j:21:GLN:HG3	1.70	0.41
36:1k:41:ARG:O	36:1k:43:PRO:HD3	2.19	0.41
41:1p:143:SER:O	41:1p:157:LYS:NZ	2.42	0.41
2:1B:117:GLY:HA2	2:1B:148:GLY:O	2.21	0.41
4:1D:19:MET:N	4:1D:19:MET:SD	2.87	0.41
4:1D:125:LEU:HD12	4:1D:378:LEU:HD23	2.01	0.41
4:1D:200:HIS:NE2	9:1I:124:GLU:OE2	2.53	0.41
4:1D:266:GLN:HB3	43:1r:103:TRP:CE3	2.55	0.41
7:1G:337:ARG:CD	7:1G:609:MET:HB2	2.49	0.41
12:1L:51:LEU:HD23	12:1L:51:LEU:HA	1.93	0.41
12:1L:137:LEU:HD11	12:1L:201:ILE:HD11	2.03	0.41
12:1L:241:THR:HG21	12:1L:344:GLY:HA3	2.02	0.41
12:1L:360:GLY:O	12:1L:435:PRO:HA	2.19	0.41
12:1L:386:LEU:O	12:1L:387:THR:C	2.63	0.41
16:1P:56:THR:O	16:1P:59:LEU:HB2	2.20	0.41
16:1P:335:LYS:HD2	16:1P:336:PRO:O	2.21	0.41
23:1X:88:ILE:HD12	23:1X:88:ILE:HA	1.86	0.41
30:1e:21:SER:N	30:1e:36:GLU:OE1	2.53	0.41
35:1j:12:ARG:HB3	36:1k:50:TRP:CG	2.55	0.41
36:1k:22:LYS:HB3	36:1k:24:GLU:OE1	2.20	0.41
39:1n:120:LYS:HE3	39:1n:120:LYS:HB3	1.80	0.41
41:1p:88:GLU:CD	41:1p:151:ALA:H	2.28	0.41
44:1s:43:HIS:HA	44:1s:46:TYR:CE2	2.54	0.41
1:1A:113:TRP:HH2	8:1H:282:TYR:CE1	2.39	0.41
2:1B:90:GLY:HA2	45:1B:201:SF4:S2	2.60	0.41
4:1D:407:LYS:HA	4:1D:407:LYS:HD3	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:93:LEU:HD12	6:1F:129:MET:HE2	2.03	0.41
6:1F:183:ALA:HA	7:1G:177:ARG:HH22	1.84	0.41
6:1F:406:ALA:HB3	48:1F:501:FMN:HM81	2.03	0.41
8:1H:39:VAL:HA	42:1q:31:ASN:ND2	2.35	0.41
8:1H:284:GLN:O	8:1H:288:LEU:N	2.44	0.41
12:1L:227:PHE:HE2	12:1L:283:ILE:HG22	1.85	0.41
12:1L:262:ARG:HD3	12:1L:262:ARG:HA	1.91	0.41
12:1L:326:PHE:O	12:1L:329:ILE:HG13	2.21	0.41
12:1L:486:MET:HA	12:1L:489:THR:OG1	2.21	0.41
13:1M:121:LEU:O	13:1M:125:THR:HG23	2.21	0.41
13:1M:204:MET:HG2	13:1M:243:MET:CE	2.51	0.41
13:1M:290:SER:CB	13:1M:319:HIS:HE2	2.33	0.41
13:1M:354:LEU:HD11	33:1h:18:ASP:CB	2.50	0.41
14:1N:324:LYS:HB3	14:1N:324:LYS:HE3	1.85	0.41
15:1O:65:ASP:N	15:1O:65:ASP:OD1	2.52	0.41
16:1P:311:GLU:HG2	16:1P:336:PRO:HB3	2.02	0.41
16:1P:338:LYS:HE3	16:1P:338:LYS:HB3	1.74	0.41
20:1T:62:ILE:HA	20:1T:63:PRO:HD3	1.95	0.41
21:1V:99:TRP:CE3	21:1V:100:GLU:HG3	2.56	0.41
24:1Y:117:MET:HE2	24:1Y:117:MET:HB3	1.78	0.41
30:1e:16:TRP:CZ3	30:1e:17:MET:HB2	2.55	0.41
33:1h:76:ALA:HA	33:1h:80:TYR:HB2	2.02	0.41
34:1i:108:THR:O	41:1p:18:ALA:N	2.53	0.41
37:1l:25:LYS:HD3	37:1l:25:LYS:H	1.85	0.41
40:1o:20:ARG:O	40:1o:20:ARG:NE	2.54	0.41
2:1B:165:ARG:O	2:1B:169:ARG:HG3	2.20	0.41
4:1D:8:VAL:HG22	32:1g:26:LEU:HD22	2.01	0.41
4:1D:182:GLU:OE1	9:1I:58:SER:N	2.52	0.41
4:1D:202:ASP:OD1	4:1D:203:LEU:N	2.53	0.41
5:1E:163:ASP:CG	5:1E:186:PRO:HB3	2.46	0.41
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	2.02	0.41
7:1G:141:ASN:ND2	7:1G:698:VAL:HG23	2.34	0.41
7:1G:281:GLN:HB2	7:1G:293:TYR:CD1	2.55	0.41
12:1L:352:ASP:O	39:1n:82:PRO:HG2	2.21	0.41
13:1M:20:HIS:ND1	13:1M:20:HIS:N	2.67	0.41
16:1P:82:ARG:HG3	16:1P:82:ARG:NH1	2.35	0.41
17:1Q:32:THR:HB	22:1W:128:PRO:HB2	2.01	0.41
21:1V:10:LEU:HD12	21:1V:10:LEU:H	1.85	0.41
22:1W:127:ASP:C	22:1W:127:ASP:OD1	2.63	0.41
28:1c:36:LYS:HB3	28:1c:36:LYS:HE2	1.88	0.41
30:1e:40:ILE:HD13	33:1h:128:ILE:HG21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:54:PRO:HG2	40:1o:98:MET:HE1	2.02	0.41
35:1j:66:ILE:HD11	40:1o:103:ARG:HG2	2.02	0.41
37:1l:7:ASP:O	37:1l:26:LYS:HD3	2.20	0.41
37:1l:37:TYR:CE1	37:1l:49:LYS:HE3	2.56	0.41
38:1m:80:ARG:HD2	38:1m:81:PRO:HD2	2.03	0.41
39:1n:23:LEU:HA	39:1n:23:LEU:HD12	1.80	0.41
39:1n:142:GLU:OE1	39:1n:155:PRO:HD2	2.21	0.41
40:1o:24:PHE:CD2	40:1o:107:LEU:HD22	2.56	0.41
40:1o:110:ARG:O	40:1o:114:ARG:HG2	2.21	0.41
7:1G:56:LEU:HD23	7:1G:56:LEU:HA	1.95	0.41
11:1K:78:LEU:HA	11:1K:81:VAL:HG22	2.02	0.41
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.56	0.41
12:1L:241:THR:HG21	12:1L:344:GLY:CA	2.51	0.41
13:1M:196:TRP:NE1	13:1M:250:LEU:HB3	2.35	0.41
14:1N:41:ILE:H	14:1N:41:ILE:HG12	1.69	0.41
15:1O:30:ASN:OD1	15:1O:199:LEU:HD12	2.20	0.41
24:1Y:85:ASP:HB3	24:1Y:88:ASN:ND2	2.36	0.41
24:1Y:121:ALA:HA	24:1Y:124:VAL:HG12	2.02	0.41
25:1Z:10:MET:HA	25:1Z:10:MET:HE2	2.02	0.41
25:1Z:104:TRP:CZ2	30:1e:74:ARG:HG3	2.50	0.41
28:1c:8:PRO:HB2	28:1c:9:HIS:CE1	2.55	0.41
30:1e:37:LYS:HA	33:1h:133:ILE:HD13	2.03	0.41
33:1h:10:ILE:HG23	33:1h:12:LYS:HG2	2.03	0.41
34:1i:31:GLU:OE2	39:1n:114:TYR:HA	2.19	0.41
34:1i:75:LEU:HG	34:1i:79:TRP:NE1	2.36	0.41
37:1l:53:ARG:HH22	37:1l:58:ARG:CD	2.34	0.41
40:1o:1:GLY:HA2	40:1o:4:LEU:HD12	2.02	0.41
42:1q:38:LEU:HD23	42:1q:49:TYR:CE2	2.56	0.41
2:1B:73:GLY:CA	8:1H:47:GLN:HE22	2.33	0.41
3:1C:76:ALA:O	4:1D:392:LYS:HD3	2.21	0.41
4:1D:285:VAL:HA	4:1D:286:PRO:HD3	1.92	0.41
6:1F:275:PRO:HB2	6:1F:278:GLU:HB3	2.03	0.41
7:1G:681:SER:OG	7:1G:684:MET:HG2	2.21	0.41
8:1H:77:LEU:HD12	8:1H:115:SER:HB3	2.03	0.41
8:1H:162:LEU:HD23	8:1H:162:LEU:HA	1.90	0.41
8:1H:310:MET:HE3	27:1b:32:PRO:HG3	2.03	0.41
11:1K:15:ALA:HB1	11:1K:36:MET:HG3	2.03	0.41
12:1L:188:TRP:CG	12:1L:212:PRO:HG3	2.56	0.41
13:1M:232:ALA:HA	13:1M:236:LEU:HD23	2.02	0.41
15:1O:116:LEU:HB3	15:1O:260:ARG:HD3	2.02	0.41
15:1O:239:GLU:OE2	15:1O:240:TYR:CG	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:171:ILE:HG12	55:1P:501:NDP:H42N	2.03	0.41
17:1Q:58:GLU:C	17:1Q:58:GLU:OE1	2.63	0.41
21:1V:27:TYR:OH	21:1V:54:LYS:HE2	2.21	0.41
22:1W:42:GLU:OE1	22:1W:46:THR:N	2.53	0.41
29:1d:38:GLY:HA3	29:1d:65:VAL:HA	2.03	0.41
46:1d:201:PC1:H222	46:1d:201:PC1:H252	1.88	0.41
34:1i:47:ASN:O	34:1i:51:GLN:HG2	2.20	0.41
41:1p:6:LYS:HA	41:1p:6:LYS:HD3	1.72	0.41
41:1p:58:ASN:N	41:1p:58:ASN:OD1	2.52	0.41
41:1p:73:ILE:HA	41:1p:76:CYS:HB2	2.02	0.41
1:1A:64:LEU:HD12	10:1J:165:VAL:HG23	2.02	0.41
2:1B:61:HIS:ND1	4:1D:175:GLU:OE1	2.25	0.41
4:1D:101:PRO:HB3	4:1D:105:ARG:HH21	1.85	0.41
4:1D:237:ASN:HB3	8:1H:284:GLN:HE22	1.86	0.41
4:1D:284:ASP:O	4:1D:306:GLN:HG3	2.21	0.41
5:1E:88:THR:HG23	7:1G:177:ARG:NH1	2.36	0.41
6:1F:205:LEU:HB3	6:1F:207:PRO:HD2	2.03	0.41
7:1G:377:ILE:HG12	7:1G:450:MET:HB3	2.03	0.41
7:1G:601:ARG:NE	7:1G:614:ASP:OD2	2.52	0.41
8:1H:5:ASN:ND2	26:1a:23:THR:OG1	2.39	0.41
8:1H:28:LEU:HG	8:1H:275:ALA:HB2	2.03	0.41
9:1I:70:TYR:OH	18:1R:68:HIS:HB3	2.20	0.41
9:1I:143:THR:OG1	9:1I:146:GLU:HG3	2.21	0.41
10:1J:68:PHE:CD1	10:1J:68:PHE:C	2.99	0.41
11:1K:70:GLU:OE1	14:1N:34:GLU:OE2	2.39	0.41
12:1L:89:PHE:HB2	12:1L:326:PHE:CZ	2.48	0.41
12:1L:105:MET:HE2	12:1L:105:MET:HB2	1.88	0.41
12:1L:201:ILE:O	12:1L:206:ASN:ND2	2.47	0.41
12:1L:306:THR:HG23	12:1L:332:HIS:HE1	1.85	0.41
12:1L:374:ILE:HD12	12:1L:375:ILE:N	2.36	0.41
12:1L:378:LEU:CD1	12:1L:386:LEU:HD22	2.48	0.41
12:1L:384:PRO:HB2	12:1L:385:TYR:CD2	2.56	0.41
12:1L:393:ASP:OD1	12:1L:393:ASP:N	2.54	0.41
13:1M:123:GLU:O	13:1M:126:LEU:HG	2.21	0.41
13:1M:175:ASN:HD21	13:1M:177:LEU:HB2	1.85	0.41
13:1M:391:ILE:O	13:1M:392:THR:C	2.62	0.41
16:1P:93:ASN:OD1	16:1P:93:ASN:C	2.64	0.41
16:1P:127:GLU:CD	16:1P:128:LYS:HG3	2.46	0.41
17:1Q:31:LYS:HB3	17:1Q:31:LYS:HE2	1.89	0.41
20:1T:6:LEU:HD12	20:1T:84:LYS:HE2	2.03	0.41
20:1T:22:TYR:OH	20:1T:46:ASP:OD2	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:9:GLU:H	20:1U:9:GLU:CD	2.23	0.41
21:1V:107:PRO:HD2	21:1V:110:GLN:HG3	2.03	0.41
24:1Y:89:TYR:CE2	24:1Y:125:LYS:HB2	2.55	0.41
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	2.03	0.41
28:1c:38:ASP:OD2	28:1c:38:ASP:N	2.53	0.41
32:1g:75:THR:HG21	33:1h:36:VAL:HG21	2.02	0.41
32:1g:81:PRO:HB3	33:1h:67:PHE:CZ	2.55	0.41
34:1i:5:PRO:CA	34:1i:8:LYS:HG2	2.49	0.41
34:1i:84:TYR:O	34:1i:88:HIS:HB2	2.21	0.41
34:1i:99:ARG:HH11	41:1p:117:GLY:HA3	1.86	0.41
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.20	0.41
37:1l:53:ARG:HH22	37:1l:58:ARG:HD2	1.84	0.41
37:1l:114:PHE:C	37:1l:114:PHE:HD1	2.29	0.41
37:1l:138:LEU:HD21	40:1o:55:ARG:CB	2.49	0.41
38:1m:33:ALA:C	39:1n:149:ARG:HH22	2.27	0.41
38:1m:53:PRO:CB	39:1n:129:ARG:HE	2.33	0.41
39:1n:26:LEU:HD12	39:1n:26:LEU:HA	1.86	0.41
39:1n:44:ARG:HA	39:1n:44:ARG:HD2	1.96	0.41
41:1p:27:ASN:HD22	41:1p:29:VAL:HG22	1.85	0.41
41:1p:93:ARG:NH1	41:1p:93:ARG:HB3	2.36	0.41
41:1p:145:LEU:HD23	41:1p:145:LEU:HA	1.88	0.41
3:1C:28:TYR:OH	3:1C:67:HIS:NE2	2.33	0.41
3:1C:137:MET:HB3	3:1C:162:PHE:HB2	2.03	0.41
3:1C:177:ASP:HB3	3:1C:180:VAL:HG22	2.03	0.41
4:1D:115:GLU:O	4:1D:119:SER:OG	2.27	0.41
4:1D:427:GLU:O	4:1D:430:ARG:HD3	2.21	0.41
7:1G:27:LEU:HD21	7:1G:39:ARG:HH22	1.86	0.41
7:1G:202:ILE:HD13	7:1G:202:ILE:HA	1.89	0.41
7:1G:380:VAL:HG11	7:1G:429:LEU:HD11	2.03	0.41
7:1G:704:CYS:SG	9:1I:103:SER:HA	2.61	0.41
9:1I:3:LYS:HB3	9:1I:3:LYS:HE3	1.89	0.41
9:1I:12:MET:CE	27:1b:9:LYS:HE2	2.51	0.41
10:1J:5:ILE:HD13	10:1J:5:ILE:HA	1.97	0.41
10:1J:86:ASN:OD1	10:1J:87:LYS:N	2.54	0.41
12:1L:407:TRP:HB2	37:1l:115:MET:HE1	2.03	0.41
12:1L:439:PRO:HG2	20:1U:57:GLU:HB2	2.02	0.41
12:1L:528:TYR:CG	37:1l:101:MET:HB2	2.55	0.41
15:1O:129:TYR:CE2	15:1O:166:PRO:HD3	2.56	0.41
15:1O:154:GLU:OE1	15:1O:154:GLU:N	2.53	0.41
20:1U:44:SER:O	20:1U:48:VAL:HG23	2.21	0.41
20:1U:49:GLU:HG2	39:1n:19:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:13:LEU:HD23	21:1V:13:LEU:HA	1.92	0.41
23:1X:33:ALA:HB2	23:1X:119:PRO:HG3	2.02	0.41
23:1X:105:LYS:O	23:1X:108:GLU:HG3	2.21	0.41
51:1a:101:CDL:CA3	42:1q:9:ARG:HD3	2.51	0.41
27:1b:37:TYR:O	27:1b:40:TYR:HB2	2.21	0.41
28:1c:5:ARG:HG3	28:1c:6:GLU:O	2.21	0.41
29:1d:95:LYS:HE3	29:1d:95:LYS:HB3	2.00	0.41
31:1f:34:LEU:HD22	33:1h:93:ILE:HG13	2.03	0.41
34:1i:25:GLN:HG3	39:1n:174:ARG:HD3	2.02	0.41
35:1j:27:PHE:CD1	35:1j:27:PHE:C	2.99	0.41
35:1j:29:SER:CA	35:1j:32:MET:HE3	2.51	0.41
37:1l:132:GLN:HB3	37:1l:155:HIS:CG	2.56	0.41
4:1D:343:GLU:OE1	4:1D:343:GLU:N	2.54	0.40
6:1F:45:THR:HG22	6:1F:49:LEU:HD23	2.03	0.40
6:1F:347:ILE:O	6:1F:351:ILE:HG12	2.21	0.40
7:1G:601:ARG:NH1	7:1G:605:GLU:OE1	2.42	0.40
8:1H:285:LEU:HD12	8:1H:286:MET:HG2	2.03	0.40
50:1H:701:U10:H301	50:1H:701:U10:H322	1.70	0.40
12:1L:281:GLY:O	12:1L:285:THR:HG23	2.20	0.40
12:1L:426:ILE:HA	12:1L:429:PHE:CD1	2.57	0.40
12:1L:480:THR:HG21	40:1o:90:GLU:HB2	2.04	0.40
12:1L:525:MET:HE3	37:1l:95:PRO:HG2	2.03	0.40
12:1L:539:TYR:HA	37:1l:83:MET:CE	2.48	0.40
13:1M:72:LEU:O	13:1M:75:LEU:HB2	2.21	0.40
14:1N:312:LYS:HZ3	15:1O:292:VAL:HG11	1.86	0.40
14:1N:326:LEU:HB3	14:1N:327:PRO:HD3	2.03	0.40
15:1O:24:VAL:HG13	15:1O:166:PRO:HA	2.04	0.40
16:1P:162:GLU:OE1	16:1P:162:GLU:N	2.53	0.40
16:1P:234:ASN:HB2	16:1P:236:TYR:HE1	1.87	0.40
16:1P:260:HIS:O	16:1P:264:ARG:HG2	2.21	0.40
22:1W:24:ASP:HB3	22:1W:26:ASN:OD1	2.22	0.40
22:1W:35:LEU:HG	22:1W:67:PHE:HZ	1.86	0.40
22:1W:54:ILE:HD12	22:1W:54:ILE:O	2.21	0.40
23:1X:11:ASP:O	23:1X:60:LYS:NZ	2.37	0.40
27:1b:7:PHE:CD1	27:1b:8:LEU:HD23	2.57	0.40
30:1e:81:GLN:HE22	30:1e:85:LEU:HD23	1.86	0.40
30:1e:82:ARG:HE	30:1e:82:ARG:HB3	1.70	0.40
30:1e:91:TYR:OH	30:1e:94:PRO:HD3	2.21	0.40
33:1h:11:ILE:O	33:1h:11:ILE:HD12	2.21	0.40
33:1h:48:GLY:HA2	41:1p:55:HIS:CD2	2.56	0.40
34:1i:8:LYS:O	34:1i:9:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:75:LEU:HD11	34:1i:79:TRP:CZ2	2.55	0.40
37:1l:60:PRO:HA	37:1l:70:ARG:HD3	2.03	0.40
2:1B:141:PRO:HG3	16:1P:61:PRO:HG3	2.02	0.40
3:1C:86:ARG:HH22	21:1V:113:TRP:HB2	1.87	0.40
3:1C:127:ALA:O	3:1C:131:GLU:HG2	2.21	0.40
4:1D:399:LEU:HD23	4:1D:399:LEU:HA	1.90	0.40
5:1E:104:THR:HB	6:1F:349:ARG:HH21	1.85	0.40
7:1G:258:ILE:HD11	7:1G:579:ARG:HE	1.86	0.40
8:1H:102:VAL:HG13	8:1H:150:LEU:HD13	2.04	0.40
10:1J:128:TYR:O	25:1Z:121:MET:HB3	2.21	0.40
12:1L:136:ASN:HA	12:1L:197:ASP:HA	2.02	0.40
12:1L:244:SER:OG	12:1L:299:LYS:NZ	2.48	0.40
12:1L:495:ILE:HA	12:1L:498:PHE:HB2	2.04	0.40
14:1N:168:GLY:HA3	14:1N:181:TYR:CE1	2.56	0.40
14:1N:330:ILE:O	14:1N:334:THR:HG23	2.20	0.40
20:1U:12:LYS:O	20:1U:12:LYS:HD2	2.20	0.40
24:1Y:21:ALA:HB1	24:1Y:71:LEU:HD22	2.02	0.40
25:1Z:53:TRP:NE1	25:1Z:57:ARG:HD2	2.35	0.40
28:1c:36:LYS:HA	28:1c:39:VAL:HG12	2.04	0.40
46:1d:201:PC1:H32	46:1d:201:PC1:H321	1.69	0.40
42:1q:7:LEU:HD13	42:1q:7:LEU:HA	1.92	0.40
1:1A:51:PHE:CE1	4:1D:70:GLY:HA2	2.57	0.40
2:1B:87:ILE:HA	2:1B:114:VAL:O	2.20	0.40
4:1D:168:PHE:CD2	8:1H:34:ARG:HD3	2.56	0.40
4:1D:349:PHE:CE2	9:1I:82:LEU:HD21	2.57	0.40
6:1F:93:LEU:O	6:1F:134:ALA:HA	2.21	0.40
8:1H:75:PRO:HG3	8:1H:215:TYR:CE2	2.44	0.40
12:1L:100:ILE:CG2	12:1L:341:MET:HE3	2.50	0.40
12:1L:307:SER:HA	12:1L:310:LEU:HD23	2.04	0.40
12:1L:338:MET:CE	12:1L:458:LEU:HA	2.51	0.40
12:1L:341:MET:HE1	12:1L:457:LEU:HD12	2.02	0.40
12:1L:492:ILE:HD12	12:1L:493:VAL:N	2.36	0.40
14:1N:124:LEU:HD23	14:1N:124:LEU:HA	1.90	0.40
14:1N:258:SER:OG	14:1N:333:SER:O	2.37	0.40
18:1R:43:LEU:HD23	18:1R:43:LEU:HA	1.94	0.40
19:1S:56:GLU:H	19:1S:56:GLU:HG2	1.68	0.40
20:1U:17:TYR:CZ	20:1U:21:LEU:HD12	2.57	0.40
21:1V:93:MET:HE3	21:1V:93:MET:HB2	1.95	0.40
21:1V:95:ARG:HB2	21:1V:95:ARG:CZ	2.51	0.40
25:1Z:97:ILE:C	25:1Z:98:MET:HE2	2.46	0.40
25:1Z:128:ARG:HB3	25:1Z:132:GLU:OE1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:1c:5:ARG:HB3	28:1c:5:ARG:CZ	2.51	0.40
1:1A:87:MET:C	1:1A:87:MET:SD	3.04	0.40
3:1C:16:ASP:HB2	3:1C:20:LYS:NZ	2.36	0.40
4:1D:62:LEU:HD13	4:1D:425:PHE:CE1	2.56	0.40
4:1D:150:HIS:HB3	4:1D:304:MET:HE2	2.03	0.40
8:1H:222:MET:O	8:1H:225:MET:HB2	2.22	0.40
10:1J:20:PHE:CE2	10:1J:33:LEU:HD12	2.56	0.40
12:1L:15:LEU:HD13	12:1L:125:LEU:CD1	2.52	0.40
12:1L:40:VAL:HG11	12:1L:97:THR:OG1	2.21	0.40
12:1L:145:GLU:O	12:1L:149:ILE:HG13	2.21	0.40
14:1N:41:ILE:N	14:1N:42:PRO:HD2	2.36	0.40
14:1N:312:LYS:HD3	15:1O:75:GLY:HA2	2.02	0.40
17:1Q:15:GLU:H	17:1Q:15:GLU:CD	2.29	0.40
18:1R:93:GLN:O	18:1R:95:HIS:N	2.54	0.40
21:1V:17:GLU:C	21:1V:17:GLU:OE1	2.64	0.40
23:1X:37:LYS:HB3	23:1X:37:LYS:HE2	1.85	0.40
25:1Z:83:VAL:HG23	25:1Z:124:LEU:HD21	2.03	0.40
25:1Z:97:ILE:HG23	25:1Z:98:MET:CE	2.52	0.40
51:1a:101:CDL:H331	51:1a:101:CDL:H182	2.04	0.40
30:1e:81:GLN:O	30:1e:85:LEU:HG	2.21	0.40
30:1e:88:GLU:O	30:1e:90:LYS:NZ	2.43	0.40
46:1f:101:PC1:H322	46:1f:101:PC1:H31	1.73	0.40
33:1h:86:ASN:O	33:1h:90:THR:OG1	2.39	0.40
34:1i:40:TRP:HB2	34:1i:43:GLU:OE1	2.21	0.40
37:1l:42:MET:SD	38:1m:85:THR:HG22	2.61	0.40
37:1l:69:LEU:HD23	37:1l:69:LEU:H	1.87	0.40
38:1m:65:ILE:C	38:1m:65:ILE:HD12	2.46	0.40
39:1n:176:ARG:HA	39:1n:176:ARG:HD3	1.86	0.40
3:1C:49:GLU:OE2	3:1C:106:ARG:NH2	2.50	0.40
8:1H:220:PHE:CD1	8:1H:220:PHE:C	2.99	0.40
9:1I:53:GLU:OE1	42:1q:34:ARG:NH1	2.54	0.40
11:1K:64:LEU:HD23	11:1K:64:LEU:HA	1.84	0.40
12:1L:274:GLN:O	12:1L:278:LEU:HG	2.22	0.40
12:1L:450:LEU:HD11	12:1L:454:ILE:HD11	2.03	0.40
12:1L:574:SER:OG	14:1N:171:ASN:HB2	2.22	0.40
12:1L:577:VAL:O	12:1L:580:GLN:NE2	2.54	0.40
13:1M:197:LEU:HD12	13:1M:197:LEU:HA	1.96	0.40
13:1M:262:LEU:HD23	13:1M:299:VAL:HA	2.04	0.40
14:1N:123:SER:OG	14:1N:125:GLN:OE1	2.40	0.40
15:1O:23:LYS:HB2	15:1O:25:ILE:HD11	2.03	0.40
15:1O:253:ASP:HA	15:1O:256:PHE:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:63:ASP:OD2	21:1V:66:LYS:NZ	2.44	0.40
23:1X:31:TYR:HE1	23:1X:66:ALA:HA	1.86	0.40
23:1X:46:ARG:HH22	23:1X:55:CYS:HB2	1.86	0.40
31:1f:43:LEU:HD21	41:1p:67:PHE:CD1	2.56	0.40
32:1g:93:ALA:HB1	41:1p:101:ILE:HD13	2.03	0.40
34:1i:8:LYS:HA	34:1i:8:LYS:CE	2.47	0.40
35:1j:36:ILE:HD12	35:1j:37:LEU:H	1.87	0.40
37:1l:79:TRP:HA	38:1m:67:TRP:HE1	1.86	0.40
39:1n:21:ARG:HB3	39:1n:70:PHE:CZ	2.57	0.40
39:1n:121:ARG:HH21	39:1n:125:LYS:NZ	2.20	0.40
42:1q:29:ARG:HE	42:1q:29:ARG:HB3	1.77	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1A	113/115 (98%)	102 (90%)	9 (8%)	2 (2%)	6	26
2	1B	153/258 (59%)	141 (92%)	12 (8%)	0	100	100
3	1C	207/264 (78%)	195 (94%)	12 (6%)	0	100	100
4	1D	427/476 (90%)	409 (96%)	18 (4%)	0	100	100
5	1E	212/249 (85%)	190 (90%)	21 (10%)	1 (0%)	24	54
6	1F	430/464 (93%)	416 (97%)	14 (3%)	0	100	100
7	1G	697/727 (96%)	656 (94%)	39 (6%)	2 (0%)	36	65
8	1H	316/318 (99%)	301 (95%)	11 (4%)	4 (1%)	9	33
9	1I	174/239 (73%)	171 (98%)	3 (2%)	0	100	100
10	1J	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	21	50
11	1K	96/98 (98%)	92 (96%)	3 (3%)	1 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	1L	604/606 (100%)	550 (91%)	53 (9%)	1 (0%)	43	71
13	1M	457/459 (100%)	436 (95%)	21 (5%)	0	100	100
14	1N	345/347 (99%)	326 (94%)	19 (6%)	0	100	100
15	1O	318/357 (89%)	297 (93%)	21 (7%)	0	100	100
16	1P	340/377 (90%)	318 (94%)	22 (6%)	0	100	100
17	1Q	127/175 (73%)	119 (94%)	8 (6%)	0	100	100
18	1R	94/123 (76%)	92 (98%)	2 (2%)	0	100	100
19	1S	85/99 (86%)	76 (89%)	9 (11%)	0	100	100
20	1T	83/156 (53%)	77 (93%)	6 (7%)	0	100	100
20	1U	84/156 (54%)	82 (98%)	2 (2%)	0	100	100
21	1V	113/116 (97%)	102 (90%)	11 (10%)	0	100	100
22	1W	113/128 (88%)	105 (93%)	8 (7%)	0	100	100
23	1X	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
24	1Y	137/141 (97%)	133 (97%)	4 (3%)	0	100	100
25	1Z	139/144 (96%)	132 (95%)	7 (5%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
28	1c	47/76 (62%)	42 (89%)	5 (11%)	0	100	100
29	1d	117/123 (95%)	108 (92%)	9 (8%)	0	100	100
30	1e	97/106 (92%)	90 (93%)	7 (7%)	0	100	100
31	1f	55/135 (41%)	52 (94%)	3 (6%)	0	100	100
32	1g	98/154 (64%)	91 (93%)	7 (7%)	0	100	100
33	1h	136/189 (72%)	129 (95%)	7 (5%)	0	100	100
34	1i	124/128 (97%)	114 (92%)	10 (8%)	0	100	100
35	1j	69/105 (66%)	64 (93%)	5 (7%)	0	100	100
36	1k	79/98 (81%)	76 (96%)	3 (4%)	0	100	100
37	1l	154/186 (83%)	140 (91%)	12 (8%)	2 (1%)	9	33
38	1m	126/129 (98%)	118 (94%)	8 (6%)	0	100	100
39	1n	170/179 (95%)	162 (95%)	8 (5%)	0	100	100
40	1o	120/137 (88%)	113 (94%)	7 (6%)	0	100	100
41	1p	171/176 (97%)	162 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	1q	143/145 (99%)	134 (94%)	9 (6%)	0	100	100
43	1r	90/114 (79%)	87 (97%)	3 (3%)	0	100	100
44	1s	43/471 (9%)	39 (91%)	4 (9%)	0	100	100
All	All	8194/9744 (84%)	7703 (94%)	477 (6%)	14 (0%)	44	71

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1A	109	LYS
8	1H	68	ILE
8	1H	92	PRO
8	1H	282	TYR
1	1A	46	SER
37	1l	44	TYR
5	1E	157	ASN
7	1G	416	THR
12	1L	562	LEU
8	1H	208	VAL
7	1G	186	TYR
11	1K	2	PRO
37	1l	51	PRO
10	1J	5	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1A	99/99 (100%)	95 (96%)	4 (4%)	28	53
2	1B	131/212 (62%)	126 (96%)	5 (4%)	29	54
3	1C	190/227 (84%)	177 (93%)	13 (7%)	14	40
4	1D	371/405 (92%)	356 (96%)	15 (4%)	28	53
5	1E	183/207 (88%)	180 (98%)	3 (2%)	55	68
6	1F	346/368 (94%)	336 (97%)	10 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1G	588/610 (96%)	559 (95%)	29 (5%)	22	49
8	1H	274/274 (100%)	262 (96%)	12 (4%)	25	51
9	1I	151/201 (75%)	148 (98%)	3 (2%)	48	65
10	1J	140/140 (100%)	131 (94%)	9 (6%)	16	42
11	1K	84/84 (100%)	73 (87%)	11 (13%)	4	16
12	1L	539/539 (100%)	513 (95%)	26 (5%)	23	50
13	1M	408/408 (100%)	385 (94%)	23 (6%)	19	46
14	1N	310/310 (100%)	299 (96%)	11 (4%)	32	56
15	1O	283/307 (92%)	273 (96%)	10 (4%)	32	56
16	1P	296/323 (92%)	282 (95%)	14 (5%)	23	50
17	1Q	117/152 (77%)	108 (92%)	9 (8%)	12	37
18	1R	79/97 (81%)	70 (89%)	9 (11%)	5	21
19	1S	77/82 (94%)	73 (95%)	4 (5%)	21	48
20	1T	79/133 (59%)	76 (96%)	3 (4%)	29	54
20	1U	79/133 (59%)	75 (95%)	4 (5%)	21	48
21	1V	100/101 (99%)	93 (93%)	7 (7%)	14	40
22	1W	107/112 (96%)	99 (92%)	8 (8%)	12	38
23	1X	153/154 (99%)	143 (94%)	10 (6%)	15	42
24	1Y	101/102 (99%)	97 (96%)	4 (4%)	28	53
25	1Z	123/124 (99%)	118 (96%)	5 (4%)	27	52
26	1a	58/58 (100%)	54 (93%)	4 (7%)	14	40
27	1b	69/70 (99%)	65 (94%)	4 (6%)	18	45
28	1c	45/66 (68%)	44 (98%)	1 (2%)	45	63
29	1d	107/109 (98%)	104 (97%)	3 (3%)	38	60
30	1e	87/94 (93%)	84 (97%)	3 (3%)	32	57
31	1f	54/113 (48%)	52 (96%)	2 (4%)	30	55
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	74
33	1h	121/158 (77%)	112 (93%)	9 (7%)	13	38
34	1i	119/120 (99%)	111 (93%)	8 (7%)	15	41
35	1j	62/84 (74%)	57 (92%)	5 (8%)	11	36
36	1k	63/76 (83%)	62 (98%)	1 (2%)	55	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	1l	141/161 (88%)	130 (92%)	11 (8%)	11	37
38	1m	113/114 (99%)	104 (92%)	9 (8%)	11	36
39	1n	156/160 (98%)	152 (97%)	4 (3%)	40	61
40	1o	110/120 (92%)	104 (94%)	6 (6%)	19	46
41	1p	154/156 (99%)	148 (96%)	6 (4%)	28	53
42	1q	131/131 (100%)	119 (91%)	12 (9%)	8	29
43	1r	85/98 (87%)	81 (95%)	4 (5%)	23	50
44	1s	44/351 (12%)	42 (96%)	2 (4%)	24	51
All	All	7219/8272 (87%)	6863 (95%)	356 (5%)	24	49

All (356) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	34	THR
1	1A	69	ILE
1	1A	84	LEU
1	1A	97	LEU
2	1B	34	ASP
2	1B	62	MET
2	1B	83	SER
2	1B	103	VAL
2	1B	126	TYR
3	1C	42	VAL
3	1C	43	SER
3	1C	44	CYS
3	1C	73	LYS
3	1C	83	VAL
3	1C	97	LEU
3	1C	109	THR
3	1C	111	THR
3	1C	172	VAL
3	1C	188	VAL
3	1C	198	ASP
3	1C	199	LEU
3	1C	201	SER
4	1D	8	VAL
4	1D	73	VAL
4	1D	110	SER
4	1D	152	MET

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Mol	Chain	Res	Type
4	1D	159	LEU
4	1D	161	ILE
4	1D	199	VAL
4	1D	208	LEU
4	1D	246	THR
4	1D	258	VAL
4	1D	307	SER
4	1D	312	SER
4	1D	325	VAL
4	1D	399	LEU
4	1D	422	ASP
5	1E	53	LEU
5	1E	66	MET
5	1E	104	THR
6	1F	63	SER
6	1F	82	MET
6	1F	83	ASN
6	1F	110	ILE
6	1F	218	CYS
6	1F	227	THR
6	1F	233	THR
6	1F	253	THR
6	1F	262	VAL
6	1F	336	VAL
7	1G	11	VAL
7	1G	65	VAL
7	1G	73	VAL
7	1G	86	SER
7	1G	123	PHE
7	1G	131	LEU
7	1G	209	THR
7	1G	227	SER
7	1G	323	VAL
7	1G	366	THR
7	1G	377	ILE
7	1G	390	LEU
7	1G	398	SER
7	1G	461	SER
7	1G	467	LEU
7	1G	480	SER
7	1G	483	VAL
7	1G	531	CYS

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Mol	Chain	Res	Type
7	1G	532	ILE
7	1G	533	THR
7	1G	536	ASP
7	1G	567	THR
7	1G	583	THR
7	1G	617	ASP
7	1G	666	LEU
7	1G	667	THR
7	1G	669	LYS
7	1G	692	THR
7	1G	693	GLU
8	1H	20	LEU
8	1H	58	LYS
8	1H	68	ILE
8	1H	103	LEU
8	1H	110	SER
8	1H	111	LEU
8	1H	188	SER
8	1H	209	SER
8	1H	233	MET
8	1H	256	THR
8	1H	266	LEU
8	1H	285	LEU
9	1I	41	LEU
9	1I	107	THR
9	1I	114	THR
10	1J	33	LEU
10	1J	35	VAL
10	1J	46	ASN
10	1J	52	LEU
10	1J	66	VAL
10	1J	67	VAL
10	1J	82	VAL
10	1J	161	LEU
10	1J	165	VAL
11	1K	3	LEU
11	1K	4	VAL
11	1K	24	SER
11	1K	29	SER
11	1K	54	THR
11	1K	61	ILE
11	1K	63	LEU

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Mol	Chain	Res	Type
11	1K	69	CYS
11	1K	77	LEU
11	1K	79	VAL
11	1K	97	GLN
12	1L	11	THR
12	1L	12	LEU
12	1L	20	MET
12	1L	31	LEU
12	1L	36	VAL
12	1L	41	SER
12	1L	99	SER
12	1L	127	THR
12	1L	196	TRP
12	1L	206	ASN
12	1L	244	SER
12	1L	293	ILE
12	1L	307	SER
12	1L	340	PHE
12	1L	346	ILE
12	1L	482	MET
12	1L	508	THR
12	1L	511	LEU
12	1L	519	THR
12	1L	553	LEU
12	1L	565	THR
12	1L	571	MET
12	1L	574	SER
12	1L	590	SER
12	1L	598	SER
12	1L	606	GLU
13	1M	15	THR
13	1M	28	THR
13	1M	41	LEU
13	1M	53	SER
13	1M	55	THR
13	1M	84	LEU
13	1M	86	LYS
13	1M	98	MET
13	1M	100	ILE
13	1M	115	LEU
13	1M	116	ILE
13	1M	212	LEU

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Mol	Chain	Res	Type
13	1M	244	MET
13	1M	274	SER
13	1M	292	SER
13	1M	305	THR
13	1M	321	LEU
13	1M	349	GLN
13	1M	354	LEU
13	1M	363	SER
13	1M	367	LEU
13	1M	389	SER
13	1M	431	THR
14	1N	34	GLU
14	1N	57	THR
14	1N	65	THR
14	1N	70	LEU
14	1N	161	SER
14	1N	173	THR
14	1N	183	SER
14	1N	233	THR
14	1N	242	SER
14	1N	281	LEU
14	1N	335	LEU
15	1O	14	THR
15	1O	71	VAL
15	1O	78	SER
15	1O	105	LEU
15	1O	136	GLU
15	1O	154	GLU
15	1O	164	LEU
15	1O	176	VAL
15	1O	283	THR
15	1O	289	SER
16	1P	15	SER
16	1P	88	SER
16	1P	90	VAL
16	1P	102	LYS
16	1P	151	VAL
16	1P	170	ASP
16	1P	171	ILE
16	1P	184	SER
16	1P	214	ILE
16	1P	237	LEU

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Mol	Chain	Res	Type
16	1P	280	THR
16	1P	297	LEU
16	1P	323	THR
16	1P	331	MET
17	1Q	11	ILE
17	1Q	13	VAL
17	1Q	47	SER
17	1Q	83	VAL
17	1Q	88	THR
17	1Q	97	GLU
17	1Q	102	SER
17	1Q	105	VAL
17	1Q	110	VAL
18	1R	7	THR
18	1R	12	THR
18	1R	26	VAL
18	1R	49	VAL
18	1R	50	SER
18	1R	54	SER
18	1R	56	VAL
18	1R	79	THR
18	1R	90	GLN
19	1S	15	LEU
19	1S	41	VAL
19	1S	50	LEU
19	1S	84	ASP
20	1T	16	LEU
20	1T	25	ILE
20	1T	40	LEU
20	1U	20	LYS
20	1U	37	MET
20	1U	51	ILE
20	1U	69	LYS
21	1V	10	LEU
21	1V	11	VAL
21	1V	29	LYS
21	1V	51	THR
21	1V	68	GLU
21	1V	88	SER
21	1V	109	ASN
22	1W	52	LEU
22	1W	55	SER

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Mol	Chain	Res	Type
22	1W	70	ASN
22	1W	73	VAL
22	1W	85	LYS
22	1W	93	THR
22	1W	101	THR
22	1W	126	HIS
23	1X	5	GLU
23	1X	23	VAL
23	1X	44	LEU
23	1X	88	ILE
23	1X	113	LYS
23	1X	127	VAL
23	1X	130	VAL
23	1X	132	THR
23	1X	170	THR
23	1X	171	MET
24	1Y	15	THR
24	1Y	36	SER
24	1Y	84	ASP
24	1Y	104	THR
25	1Z	4	SER
25	1Z	30	LEU
25	1Z	31	SER
25	1Z	127	LEU
25	1Z	134	LEU
26	1a	6	LEU
26	1a	16	LEU
26	1a	50	ARG
26	1a	54	ILE
27	1b	17	VAL
27	1b	31	LEU
27	1b	51	ASN
27	1b	56	LEU
28	1c	46	ASN
29	1d	13	PHE
29	1d	34	MET
29	1d	108	THR
30	1e	37	LYS
30	1e	69	GLN
30	1e	90	LYS
31	1f	5	GLN
31	1f	31	ASP

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Mol	Chain	Res	Type
32	1g	67	SER
33	1h	10	ILE
33	1h	24	LEU
33	1h	79	PHE
33	1h	84	GLU
33	1h	97	GLU
33	1h	107	GLU
33	1h	114	MET
33	1h	127	THR
33	1h	136	SER
34	1i	33	VAL
34	1i	39	VAL
34	1i	57	LYS
34	1i	78	VAL
34	1i	96	VAL
34	1i	102	ARG
34	1i	103	ILE
34	1i	108	THR
35	1j	17	LEU
35	1j	20	SER
35	1j	44	SER
35	1j	48	LEU
35	1j	63	GLU
36	1k	61	SER
37	1l	3	HIS
37	1l	5	THR
37	1l	29	MET
37	1l	44	TYR
37	1l	49	LYS
37	1l	58	ARG
37	1l	91	THR
37	1l	128	VAL
37	1l	136	ASN
37	1l	154	VAL
37	1l	158	ILE
38	1m	2	PHE
38	1m	45	GLU
38	1m	49	GLN
38	1m	56	LEU
38	1m	106	THR
38	1m	116	GLN
38	1m	121	ASP

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Mol	Chain	Res	Type
38	1m	126	ILE
38	1m	127	SER
39	1n	10	THR
39	1n	52	ASN
39	1n	67	GLU
39	1n	84	SER
40	1o	19	LEU
40	1o	24	PHE
40	1o	50	LEU
40	1o	91	HIS
40	1o	107	LEU
40	1o	116	GLN
41	1p	30	THR
41	1p	32	LEU
41	1p	61	TYR
41	1p	97	VAL
41	1p	102	VAL
41	1p	128	LEU
42	1q	6	VAL
42	1q	35	VAL
42	1q	37	THR
42	1q	39	VAL
42	1q	80	SER
42	1q	94	THR
42	1q	104	THR
42	1q	107	LYS
42	1q	111	THR
42	1q	118	SER
42	1q	125	VAL
42	1q	129	THR
43	1r	2	SER
43	1r	15	SER
43	1r	54	CYS
43	1r	107	LYS
44	1s	60	LYS
44	1s	72	SER

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

Mol	Chain	Res	Type
1	1A	83	ASN
2	1B	94	ASN

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Mol	Chain	Res	Type
3	1C	53	HIS
3	1C	71	GLN
3	1C	95	ASN
4	1D	13	GLN
4	1D	421	GLN
6	1F	326	GLN
6	1F	398	GLN
6	1F	438	GLN
7	1G	82	ASN
7	1G	308	GLN
7	1G	365	ASN
7	1G	392	ASN
7	1G	430	GLN
7	1G	665	GLN
8	1H	287	HIS
12	1L	109	HIS
12	1L	135	ASN
12	1L	175	ASN
12	1L	199	GLN
12	1L	296	ASN
12	1L	320	ASN
12	1L	348	HIS
12	1L	446	ASN
12	1L	524	ASN
12	1L	541	ASN
13	1M	83	HIS
13	1M	175	ASN
13	1M	251	ASN
13	1M	415	GLN
13	1M	425	ASN
14	1N	36	ASN
14	1N	63	GLN
14	1N	134	GLN
14	1N	150	ASN
14	1N	221	HIS
15	1O	92	ASN
15	1O	180	GLN
15	1O	294	GLN
16	1P	58	HIS
16	1P	67	GLN
16	1P	180	ASN
16	1P	203	GLN

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Mol	Chain	Res	Type
16	1P	306	GLN
16	1P	321	HIS
17	1Q	6	GLN
18	1R	36	ASN
19	1S	85	GLN
24	1Y	133	GLN
27	1b	10	ASN
28	1c	35	HIS
29	1d	46	ASN
29	1d	79	GLN
30	1e	20	GLN
30	1e	44	HIS
31	1f	10	HIS
32	1g	36	ASN
32	1g	41	ASN
34	1i	12	GLN
34	1i	51	GLN
37	1l	78	HIS
38	1m	32	GLN
38	1m	74	ASN
39	1n	61	GLN
39	1n	138	GLN
40	1o	53	GLN
40	1o	64	GLN
40	1o	81	HIS
40	1o	116	GLN
41	1p	90	GLN
41	1p	103	ASN
41	1p	123	ASN
41	1p	160	GLN
42	1q	135	GLN
43	1r	8	GLN
43	1r	20	GLN
43	1r	28	GLN
43	1r	35	GLN
43	1r	46	HIS
43	1r	109	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.03	1 (12%)
12	FME	1L	1	12	8,9,10	0.55	0	8,9,11	0.89	1 (12%)
10	FME	1J	1	10	8,9,10	0.57	0	8,9,11	0.97	1 (12%)
34	SAC	1i	1	-	7,8,9	0.57	0	7,9,11	1.14	1 (14%)
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.99	1 (12%)
11	FME	1K	1	30,11	8,9,10	0.83	0	8,9,11	4.24	2 (25%)
14	FME	1N	1	14	8,9,10	0.55	0	8,9,11	0.99	1 (12%)
1	FME	1A	1	1	8,9,10	0.55	0	8,9,11	1.13	1 (12%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	1H	1	8	-	2/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
10	FME	1J	1	10	-	1/7/9/11	-
34	SAC	1i	1	-	-	1/7/8/10	-
13	FME	1M	1	13	-	1/7/9/11	-
11	FME	1K	1	30,11	-	4/7/9/11	-
14	FME	1N	1	14	-	2/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	1K	1	FME	CA-N-CN	-11.67	104.87	122.82
34	1i	1	SAC	O-C-CA	-2.96	117.17	124.77
10	1J	1	FME	O-C-CA	-2.69	117.86	124.77
8	1H	1	FME	O-C-CA	-2.68	117.87	124.77
1	1A	1	FME	O-C-CA	-2.60	118.08	124.77
13	1M	1	FME	O-C-CA	-2.56	118.17	124.77
14	1N	1	FME	O-C-CA	-2.42	118.56	124.77
12	1L	1	FME	O-C-CA	-2.40	118.60	124.77
11	1K	1	FME	O-C-CA	-2.22	119.05	124.77

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	1H	1	FME	O1-CN-N-CA
11	1K	1	FME	O1-CN-N-CA
11	1K	1	FME	O-C-CA-CB
14	1N	1	FME	O1-CN-N-CA
14	1N	1	FME	CB-CA-N-CN
34	1i	1	SAC	C-CA-N-C1A
13	1M	1	FME	C-CA-CB-CG
11	1K	1	FME	N-CA-CB-CG
11	1K	1	FME	C-CA-CB-CG
10	1J	1	FME	N-CA-CB-CG
8	1H	1	FME	CB-CA-N-CN

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	1J	1	FME	1	0
34	1i	1	SAC	3	0
13	1M	1	FME	2	0
11	1K	1	FME	3	0
1	1A	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
47	FES	1E	301	5	0,4,4	-	-	-		
52	3PE	1Y	202	24	34,34,50	0.37	0	37,39,55	0.85	1 (2%)
58	MYR	1l	201	-	13,14,15	0.30	0	12,13,15	0.35	0
46	PC1	1Y	201	-	45,45,53	0.28	0	51,53,61	0.35	0
47	FES	1G	803	7	0,4,4	-	-	-		
45	SF4	1G	802	7	0,12,12	-	-	-		
45	SF4	1I	202	9	0,12,12	-	-	-		
57	EHZ	1W	201	-	31,36,37	0.18	0	36,44,47	1.02	1 (2%)
46	PC1	1d	201	30,29	38,38,53	0.32	0	44,46,61	0.48	0
55	NDP	1P	501	-	51,52,52	0.53	0	71,80,80	0.76	2 (2%)
51	CDL	1a	101	42,26	60,60,99	0.50	0	66,72,111	0.86	5 (7%)
46	PC1	1q	201	42	47,47,53	0.28	0	53,55,61	0.32	0
46	PC1	1B	202	2	33,33,53	0.32	0	39,41,61	0.61	1 (2%)
50	U10	1H	701	-	63,63,63	0.49	0	78,79,79	0.94	5 (6%)
57	EHZ	1n	201	-	31,36,37	0.21	0	36,44,47	1.13	1 (2%)
52	3PE	1N	401	-	37,37,50	0.30	0	40,42,55	0.43	0
48	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.65	1 (2%)
52	3PE	1L	701	12	41,41,50	0.30	0	44,46,55	0.34	0
45	SF4	1G	801	7	0,12,12	-	-	-		
51	CDL	1N	402	14	66,66,99	0.31	0	72,78,111	0.38	0
51	CDL	1H	702	8	50,50,99	0.36	0	56,62,111	0.67	1 (1%)
46	PC1	1M	501	-	34,34,53	0.32	0	40,42,61	0.36	0
45	SF4	1F	502	6	0,12,12	-	-	-		
45	SF4	1I	201	9	0,12,12	-	-	-		
45	SF4	1B	201	2	0,12,12	-	-	-		
53	GTP	1O	401	54	33,34,34	0.57	0	50,54,54	0.60	0
46	PC1	1f	101	31	33,33,53	0.30	0	39,41,61	0.38	0
52	3PE	1f	102	31	50,50,50	0.29	0	53,55,55	1.03	4 (7%)

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
47	FES	1E	301	5	-	-	0/1/1/1
52	3PE	1Y	202	24	-	9/38/38/54	-
58	MYR	1I	201	-	-	0/12/12/13	-
46	PC1	1Y	201	-	-	6/49/49/57	-
47	FES	1G	803	7	-	-	0/1/1/1
45	SF4	1G	802	7	-	-	0/6/5/5
45	SF4	1I	202	9	-	-	0/6/5/5
57	EHZ	1W	201	-	-	6/42/44/45	-
46	PC1	1d	201	30,29	-	9/42/42/57	-
55	NDP	1P	501	-	-	3/34/77/77	0/5/5/5
51	CDL	1a	101	42,26	-	15/71/71/110	-
46	PC1	1q	201	42	-	11/51/51/57	-
46	PC1	1B	202	2	-	13/37/37/57	-
50	U10	1H	701	-	-	17/63/87/87	0/1/1/1
57	EHZ	1n	201	-	-	8/42/44/45	-
52	3PE	1N	401	-	-	9/41/41/54	-
52	3PE	1L	701	12	-	4/45/45/54	-
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
51	CDL	1N	402	14	-	10/76/76/110	-
45	SF4	1G	801	7	-	-	0/6/5/5
51	CDL	1H	702	8	-	7/61/61/110	-
46	PC1	1M	501	-	-	0/38/38/57	-
45	SF4	1F	502	6	-	-	0/6/5/5
45	SF4	1I	201	9	-	-	0/6/5/5
45	SF4	1B	201	2	-	-	0/6/5/5
53	GTP	1O	401	54	-	4/22/38/38	0/3/3/3
46	PC1	1f	101	31	-	5/36/36/57	-
52	3PE	1f	102	31	-	13/54/54/54	-

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1n	201	EHZ	C10-S1-C9	6.23	120.27	101.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	1f	102	3PE	O21-C21-C22	5.21	122.76	111.48
57	1W	201	EHZ	C10-S1-C9	5.21	117.24	101.84
55	1P	501	NDP	P2B-O2B-C2B	-4.11	112.46	123.43
50	1H	701	U10	O3-C3-C2	3.49	128.41	116.64
50	1H	701	U10	O4-C4-C5	3.42	128.17	116.64
52	1Y	202	3PE	O21-C21-C22	3.34	118.70	111.48
51	1H	702	CDL	OB6-CB5-C51	3.17	118.34	111.48
50	1H	701	U10	O4-C4-C3	-3.05	112.11	123.64
50	1H	701	U10	O3-C3-C4	-2.95	112.48	123.64
52	1f	102	3PE	O21-C21-O22	-2.94	116.84	123.70
51	1a	101	CDL	OA6-CA4-CA3	2.64	117.82	108.34
50	1H	701	U10	C7-C6-C1	-2.50	120.61	124.89
51	1a	101	CDL	OA6-CA5-OA7	-2.48	117.90	123.70
52	1f	102	3PE	O21-C2-C3	2.39	116.92	108.34
52	1f	102	3PE	C2-O21-C21	2.32	123.35	117.80
55	1P	501	NDP	O4D-C1D-C2D	-2.23	101.83	106.62
51	1a	101	CDL	OA6-CA5-C11	2.20	116.24	111.48
48	1F	501	FMN	C4-N3-C2	-2.08	121.95	125.64
51	1a	101	CDL	OA8-CA6-CA4	2.01	114.19	108.40
46	1B	202	PC1	O12-P-O14	2.01	121.78	112.44
51	1a	101	CDL	OA4-PA1-OA3	2.01	121.78	112.44

There are no chirality outliers.

All (150) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	1B	202	PC1	C11-O13-P-O12
46	1B	202	PC1	C1-O11-P-O12
46	1B	202	PC1	C1-O11-P-O13
46	1B	202	PC1	O32-C31-O31-C3
46	1B	202	PC1	C32-C31-O31-C3
46	1Y	201	PC1	C11-O13-P-O14
46	1Y	201	PC1	C1-O11-P-O14
46	1d	201	PC1	O13-C11-C12-N
46	1d	201	PC1	C2-C1-O11-P
46	1d	201	PC1	O32-C31-O31-C3
46	1d	201	PC1	C32-C31-O31-C3
46	1f	101	PC1	O32-C31-O31-C3
46	1f	101	PC1	C32-C31-O31-C3
46	1q	201	PC1	C11-O13-P-O14
51	1H	702	CDL	C1-CA2-OA2-PA1
51	1H	702	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
51	1H	702	CDL	OB7-CB5-OB6-CB4
51	1H	702	CDL	C51-CB5-OB6-CB4
51	1N	402	CDL	CB2-OB2-PB2-OB4
51	1N	402	CDL	CB2-OB2-PB2-OB5
51	1a	101	CDL	CA4-CA3-OA5-PA1
51	1a	101	CDL	CB3-OB5-PB2-OB2
51	1a	101	CDL	CB3-OB5-PB2-OB3
52	1Y	202	3PE	C12-C11-O13-P
52	1Y	202	3PE	O22-C21-O21-C2
52	1Y	202	3PE	C22-C21-O21-C2
52	1f	102	3PE	O22-C21-O21-C2
52	1f	102	3PE	C22-C21-O21-C2
57	1W	201	EHZ	O2-C9-S1-C10
57	1W	201	EHZ	C8-C9-S1-C10
57	1n	201	EHZ	C16-C17-C20-O6
57	1n	201	EHZ	C18-C17-C20-O6
57	1n	201	EHZ	C19-C17-C20-O6
57	1n	201	EHZ	O2-C9-S1-C10
57	1n	201	EHZ	C8-C9-S1-C10
50	1H	701	U10	C30-C29-C31-C32
50	1H	701	U10	C40-C39-C41-C42
50	1H	701	U10	C45-C44-C46-C47
50	1H	701	U10	C28-C29-C31-C32
50	1H	701	U10	C34-C36-C37-C38
52	1L	701	3PE	C2-C1-O11-P
50	1H	701	U10	C38-C39-C41-C42
50	1H	701	U10	C43-C44-C46-C47
51	1a	101	CDL	CA5-C11-C12-C13
50	1H	701	U10	C4-C3-O3-C3M
50	1H	701	U10	C3-C4-O4-C4M
51	1a	101	CDL	O1-C1-CB2-OB2
50	1H	701	U10	C2-C3-O3-C3M
51	1a	101	CDL	CA7-C31-C32-C33
51	1a	101	CDL	CA2-C1-CB2-OB2
52	1f	102	3PE	C2-C1-O11-P
57	1W	201	EHZ	C5-C6-C7-O1
52	1f	102	3PE	O21-C2-C3-O31
50	1H	701	U10	C5-C4-O4-C4M
51	1a	101	CDL	C11-CA5-OA6-CA4
46	1q	201	PC1	C3A-C3B-C3C-C3D
52	1f	102	3PE	C22-C23-C24-C25
57	1W	201	EHZ	C12-C13-C14-N2

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Mol	Chain	Res	Type	Atoms
46	1q	201	PC1	C32-C33-C34-C35
51	1N	402	CDL	OB6-CB4-CB6-OB8
51	1a	101	CDL	OB6-CB4-CB6-OB8
52	1Y	202	3PE	C32-C33-C34-C35
51	1a	101	CDL	OA5-CA3-CA4-CA6
51	1a	101	CDL	OA5-CA3-CA4-OA6
46	1q	201	PC1	C39-C3A-C3B-C3C
52	1N	401	3PE	C34-C35-C36-C37
52	1L	701	3PE	O21-C2-C3-O31
52	1N	401	3PE	O31-C31-C32-C33
51	1N	402	CDL	C55-C56-C57-C58
48	1F	501	FMN	C4'-C5'-O5'-P
46	1d	201	PC1	C35-C36-C37-C38
52	1f	102	3PE	C27-C28-C29-C2A
52	1f	102	3PE	C23-C24-C25-C26
46	1B	202	PC1	C1-C2-C3-O31
51	1N	402	CDL	CB3-CB4-CB6-OB8
51	1a	101	CDL	CB3-CB4-CB6-OB8
52	1L	701	3PE	C1-C2-C3-O31
52	1N	401	3PE	C1-C2-C3-O31
46	1q	201	PC1	C35-C36-C37-C38
46	1B	202	PC1	O21-C2-C3-O31
51	1N	402	CDL	OA5-CA3-CA4-OA6
52	1f	102	3PE	O11-C1-C2-O21
46	1Y	201	PC1	C12-C11-O13-P
46	1d	201	PC1	C12-C11-O13-P
46	1q	201	PC1	C12-C11-O13-P
52	1f	102	3PE	C12-C11-O13-P
57	1W	201	EHZ	C21-C22-C23-C24
46	1Y	201	PC1	O13-C11-C12-N
53	1O	401	GTP	PA-O3A-PB-O1B
52	1N	401	3PE	C21-C22-C23-C24
46	1f	101	PC1	C35-C36-C37-C38
46	1d	201	PC1	C22-C23-C24-C25
52	1N	401	3PE	O21-C2-C3-O31
46	1B	202	PC1	C11-O13-P-O14
46	1B	202	PC1	C11-O13-P-O11
46	1B	202	PC1	C1-O11-P-O14
46	1f	101	PC1	C11-O13-P-O14
51	1H	702	CDL	CA3-OA5-PA1-OA2
51	1N	402	CDL	CA2-OA2-PA1-OA3
51	1N	402	CDL	CB3-OB5-PB2-OB3

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Mol	Chain	Res	Type	Atoms
51	1a	101	CDL	CA2-OA2-PA1-OA3
51	1a	101	CDL	CB3-OB5-PB2-OB4
52	1N	401	3PE	C1-O11-P-O13
52	1N	401	3PE	C11-O13-P-O14
52	1Y	202	3PE	C1-O11-P-O14
52	1Y	202	3PE	O13-C11-C12-N
53	1O	401	GTP	C5'-O5'-PA-O1A
46	1Y	201	PC1	C33-C34-C35-C36
51	1H	702	CDL	CA4-CA3-OA5-PA1
51	1N	402	CDL	CA4-CA3-OA5-PA1
51	1a	101	CDL	CB4-CB3-OB5-PB2
50	1H	701	U10	C9-C11-C12-C13
52	1Y	202	3PE	O11-C1-C2-O21
50	1H	701	U10	C20-C19-C21-C22
46	1Y	201	PC1	C27-C28-C29-C2A
50	1H	701	U10	C18-C19-C21-C22
55	1P	501	NDP	C2D-C1D-N1N-C6N
46	1q	201	PC1	C37-C38-C39-C3A
52	1f	102	3PE	C1-C2-C3-O31
46	1d	201	PC1	C1-C2-O21-C21
51	1N	402	CDL	OA5-CA3-CA4-CA6
46	1B	202	PC1	C31-C32-C33-C34
52	1f	102	3PE	C25-C26-C27-C28
55	1P	501	NDP	O4D-C1D-N1N-C6N
52	1N	401	3PE	O32-C31-C32-C33
52	1N	401	3PE	C37-C38-C39-C3A
57	1W	201	EHZ	C1-C21-C22-C23
55	1P	501	NDP	C2D-C1D-N1N-C2N
46	1B	202	PC1	C2-C1-O11-P
50	1H	701	U10	C29-C31-C32-C33
53	1O	401	GTP	PA-O3A-PB-O2B
57	1n	201	EHZ	C4-C5-C6-C7
52	1f	102	3PE	C26-C27-C28-C29
46	1q	201	PC1	C33-C34-C35-C36
52	1f	102	3PE	C38-C39-C3A-C3B
53	1O	401	GTP	O4'-C4'-C5'-O5'
46	1d	201	PC1	C33-C34-C35-C36
46	1q	201	PC1	O31-C31-C32-C33
50	1H	701	U10	C16-C17-C18-C19
46	1q	201	PC1	O32-C31-C32-C33
57	1n	201	EHZ	C21-C1-C2-C3
57	1n	201	EHZ	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
46	1q	201	PC1	C23-C24-C25-C26
46	1f	101	PC1	C37-C38-C39-C3A
50	1H	701	U10	C46-C47-C48-C49
46	1B	202	PC1	O31-C31-C32-C33
52	1Y	202	3PE	O21-C21-C22-C23
51	1H	702	CDL	C32-C31-CA7-OA8
52	1Y	202	3PE	C25-C26-C27-C28
52	1L	701	3PE	O21-C21-C22-C23

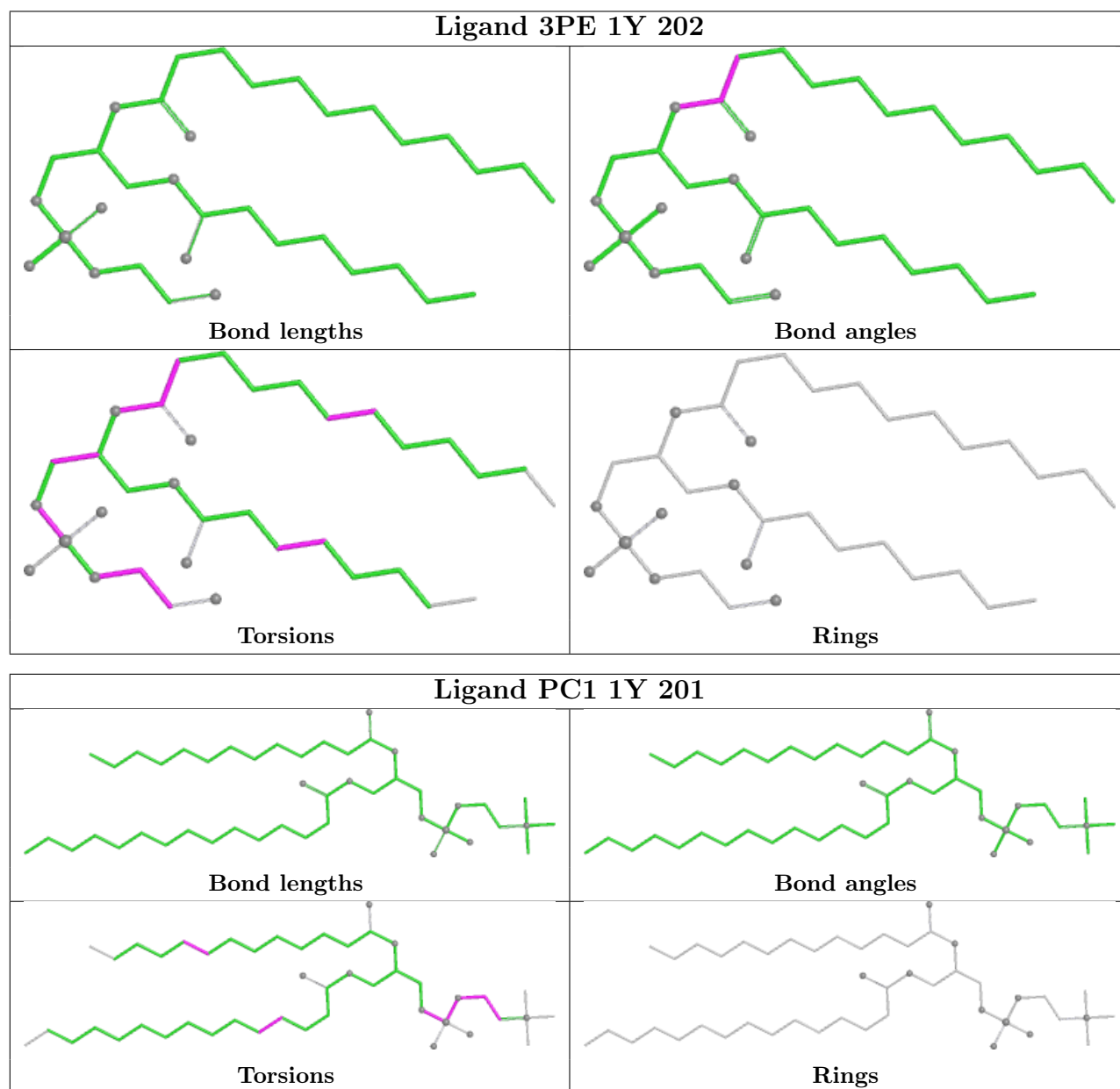
There are no ring outliers.

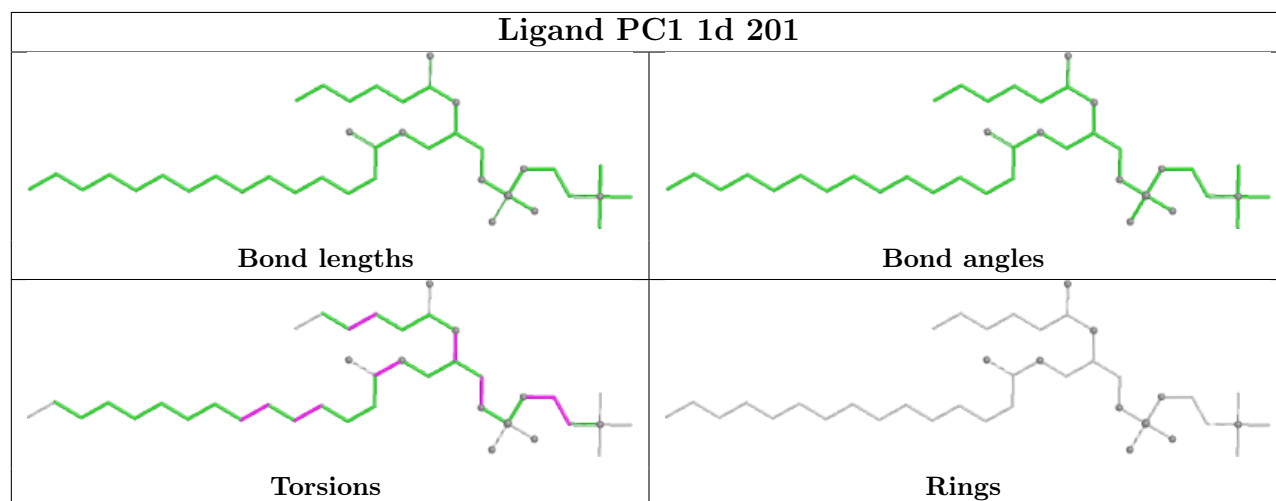
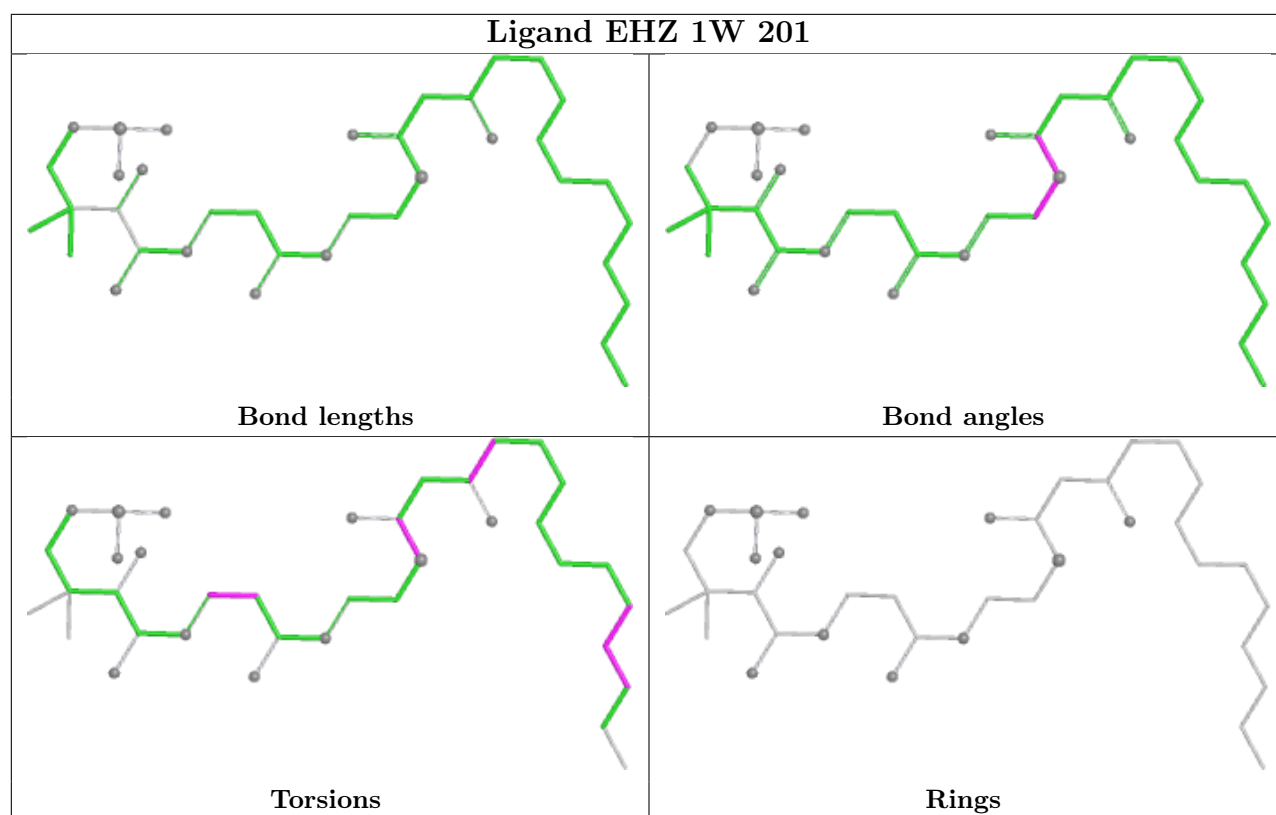
22 monomers are involved in 88 short contacts:

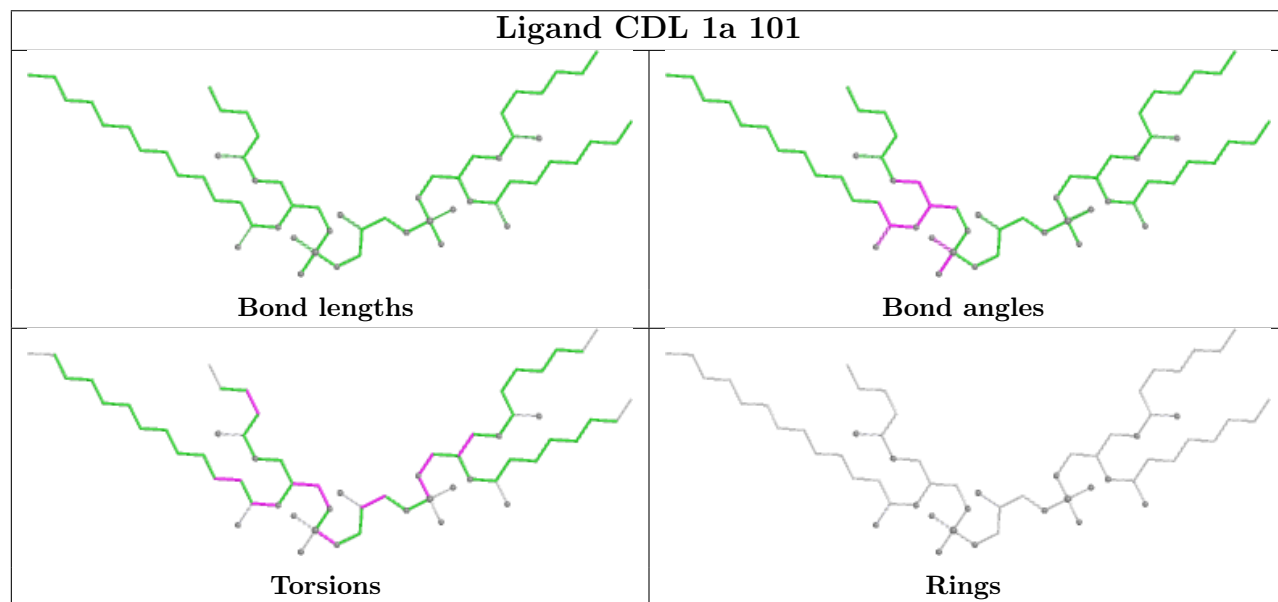
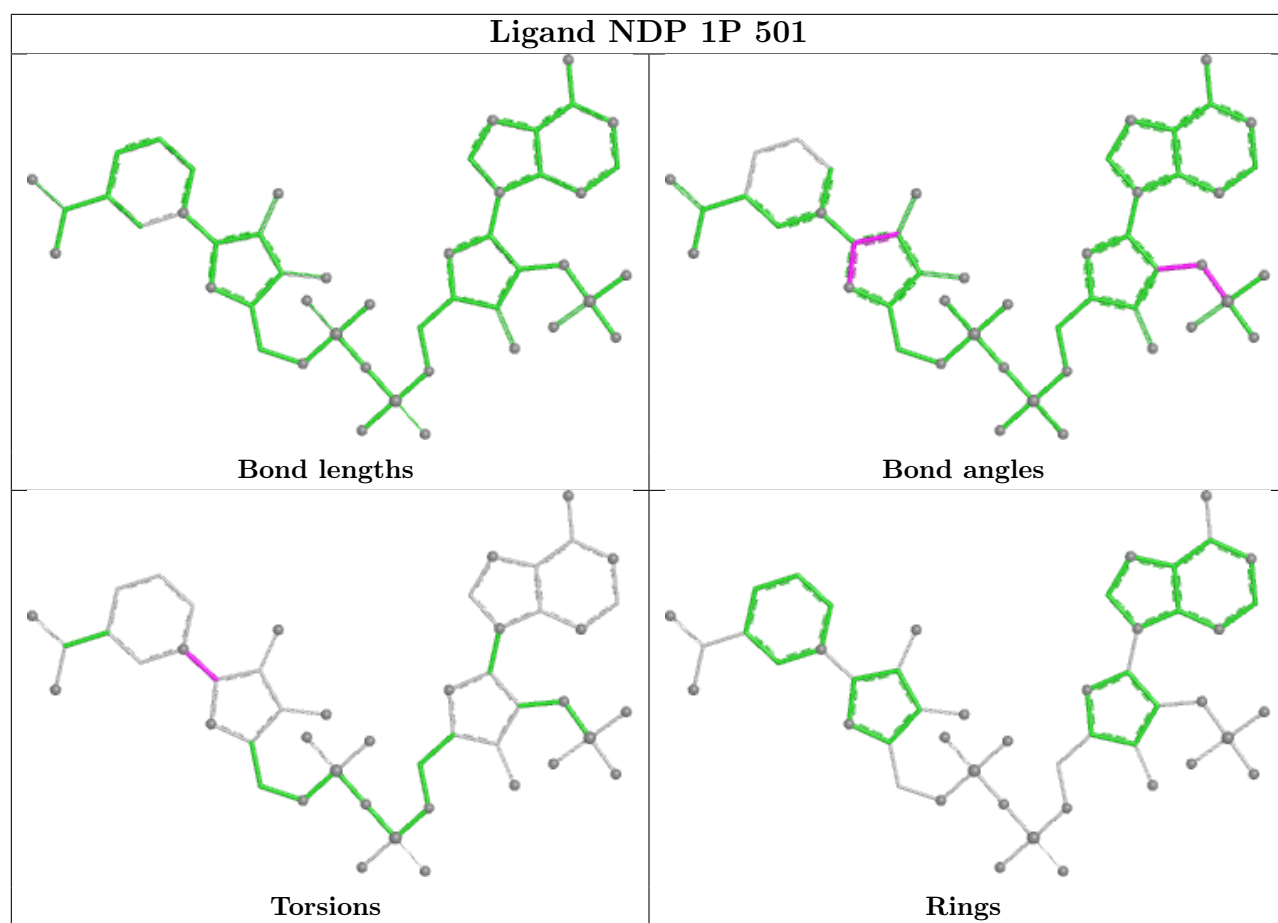
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	1E	301	FES	1	0
52	1Y	202	3PE	6	0
58	1l	201	MYR	2	0
46	1Y	201	PC1	2	0
57	1W	201	EHZ	2	0
46	1d	201	PC1	6	0
55	1P	501	NDP	5	0
51	1a	101	CDL	9	0
46	1q	201	PC1	1	0
46	1B	202	PC1	4	0
50	1H	701	U10	7	0
52	1N	401	3PE	8	0
48	1F	501	FMN	2	0
52	1L	701	3PE	5	0
51	1N	402	CDL	6	0
51	1H	702	CDL	2	0
46	1M	501	PC1	4	0
45	1F	502	SF4	1	0
45	1I	201	SF4	2	0
45	1B	201	SF4	2	0
46	1f	101	PC1	7	0
52	1f	102	3PE	4	0

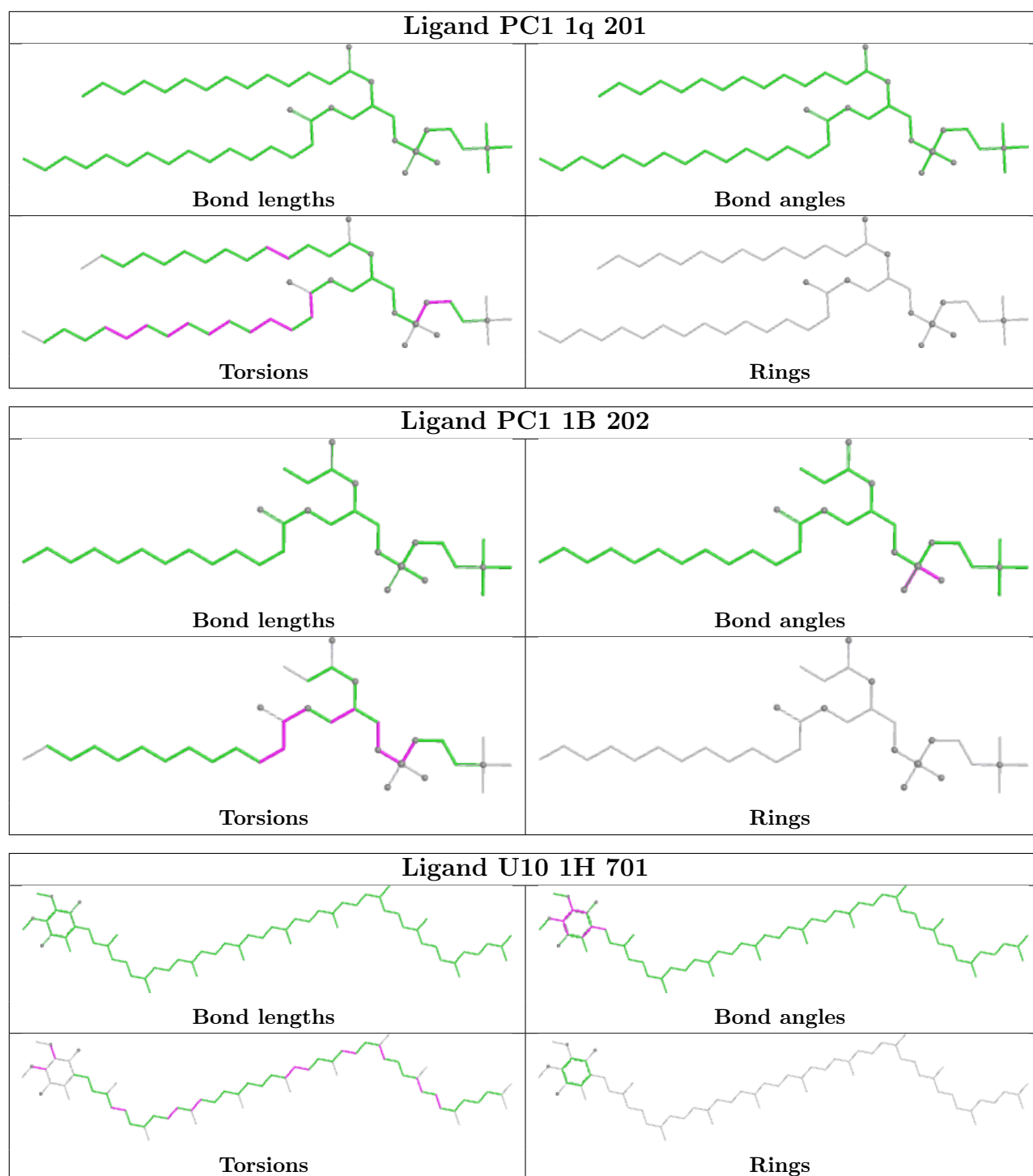
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

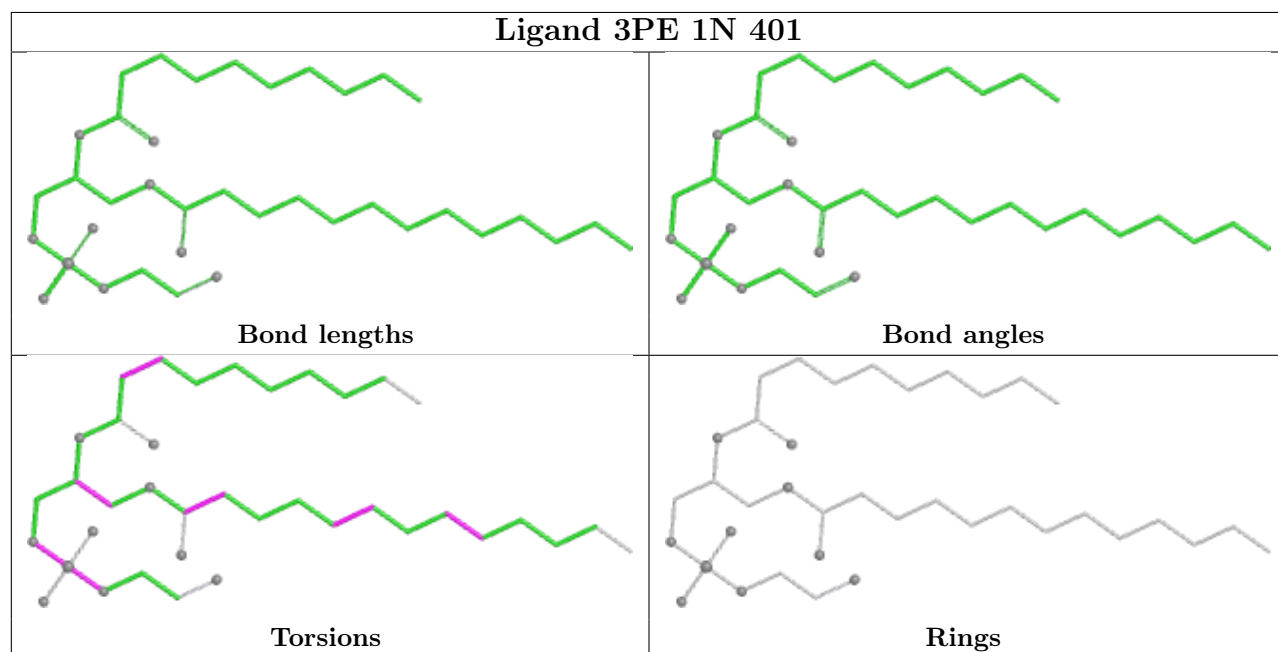
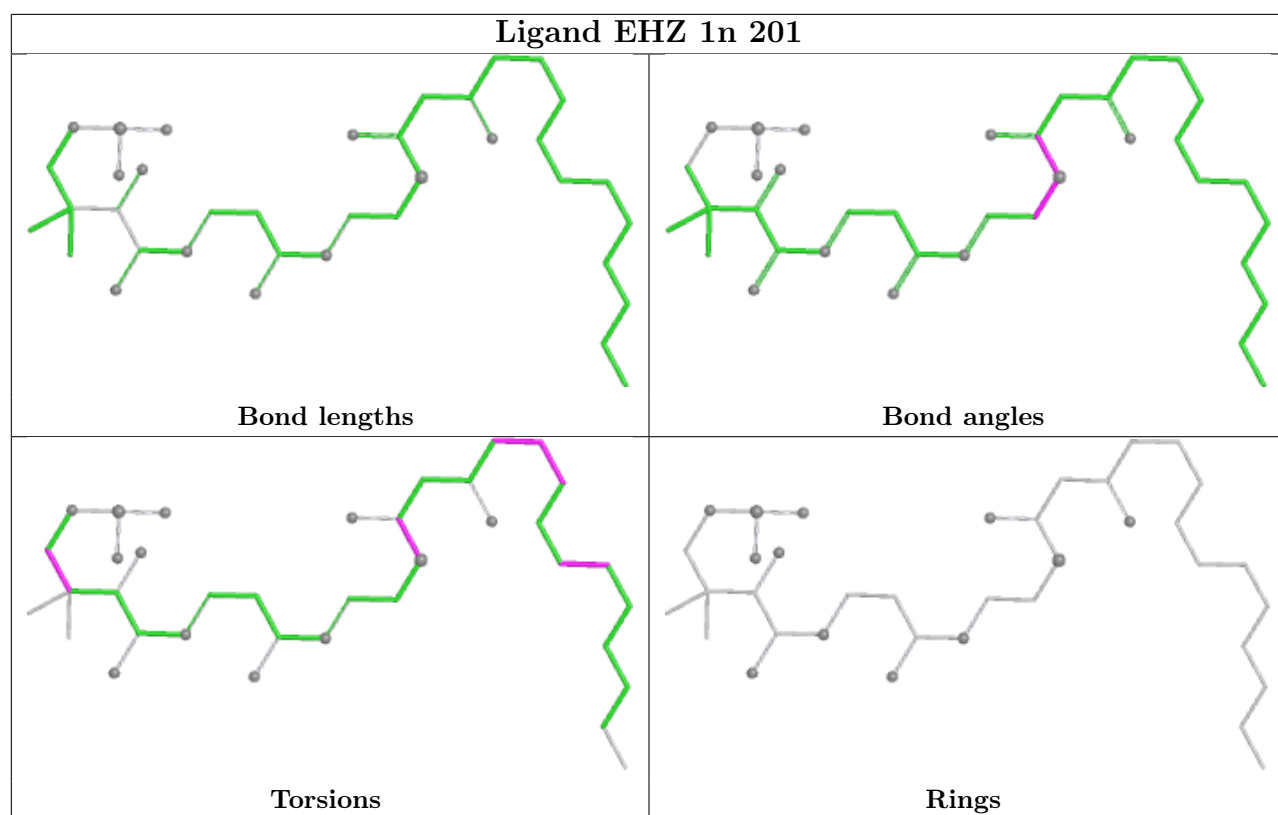
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

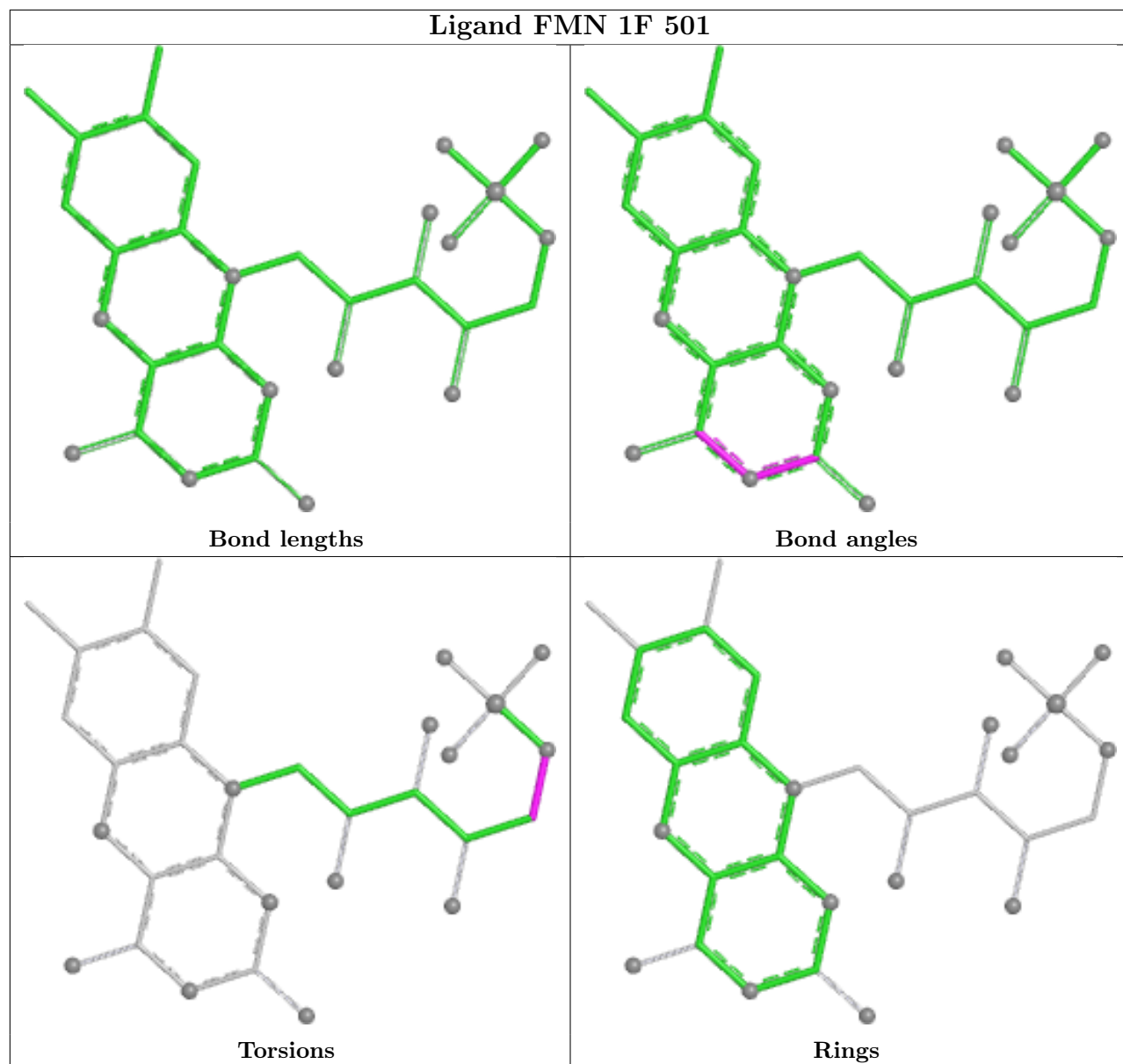


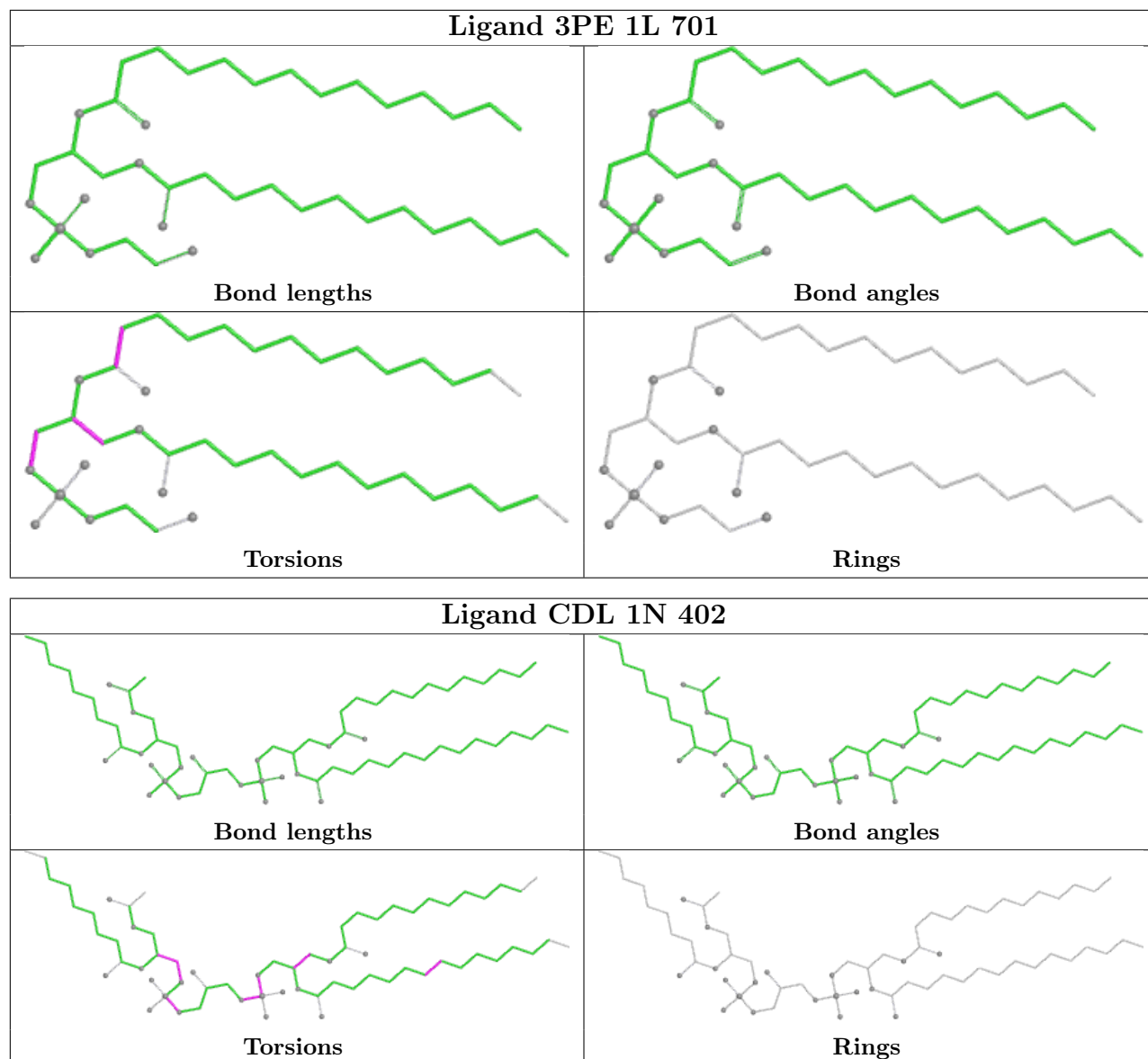


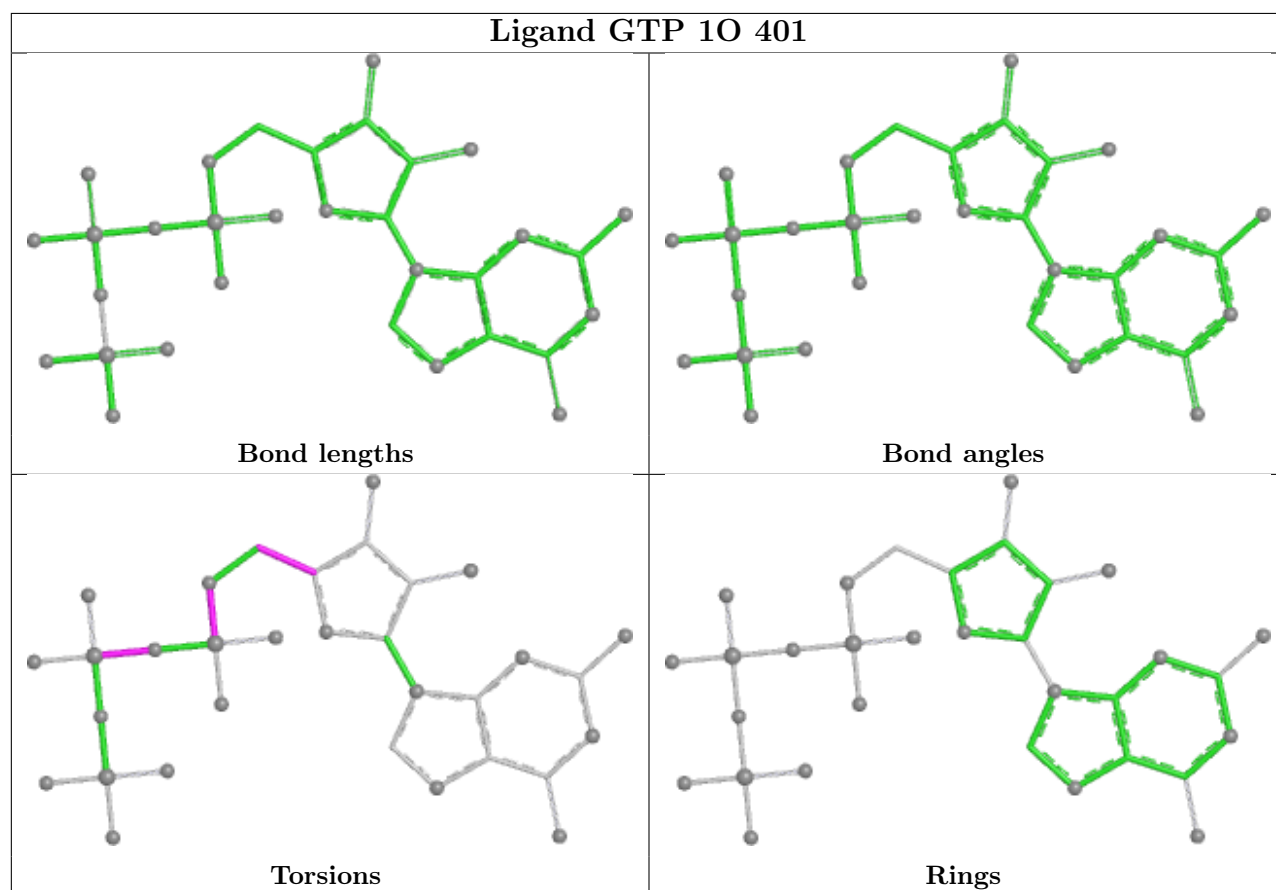
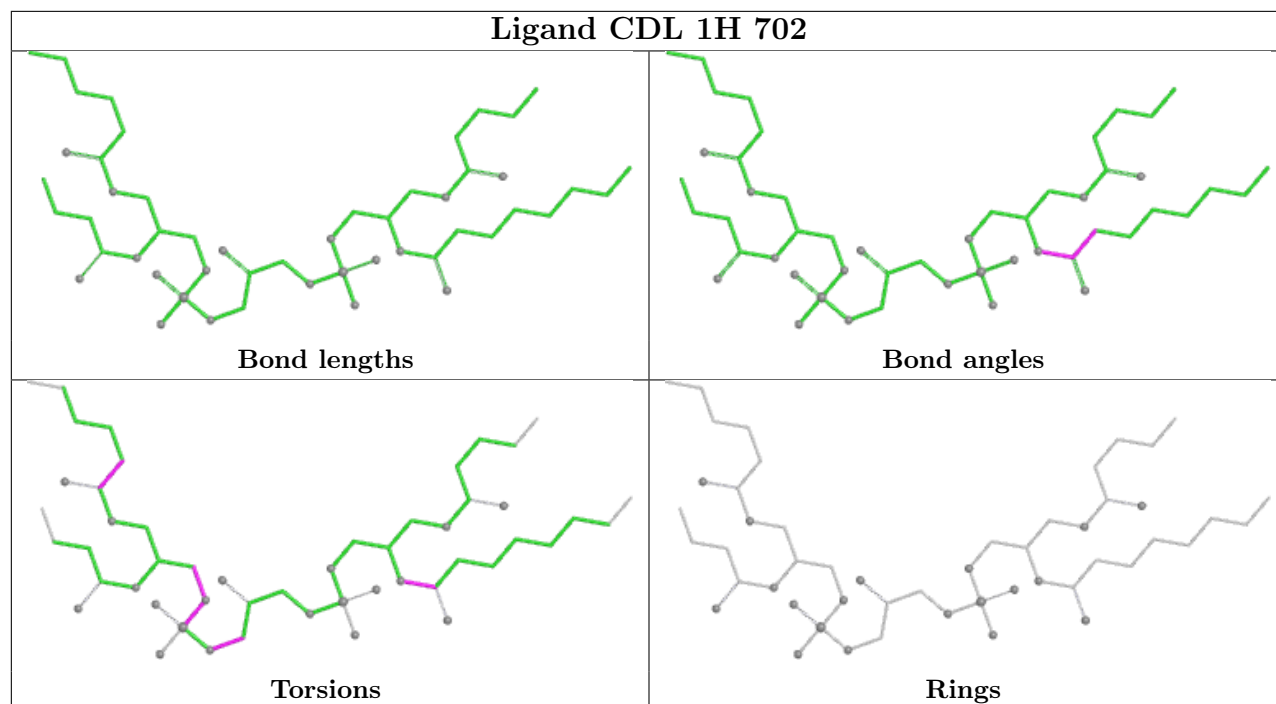


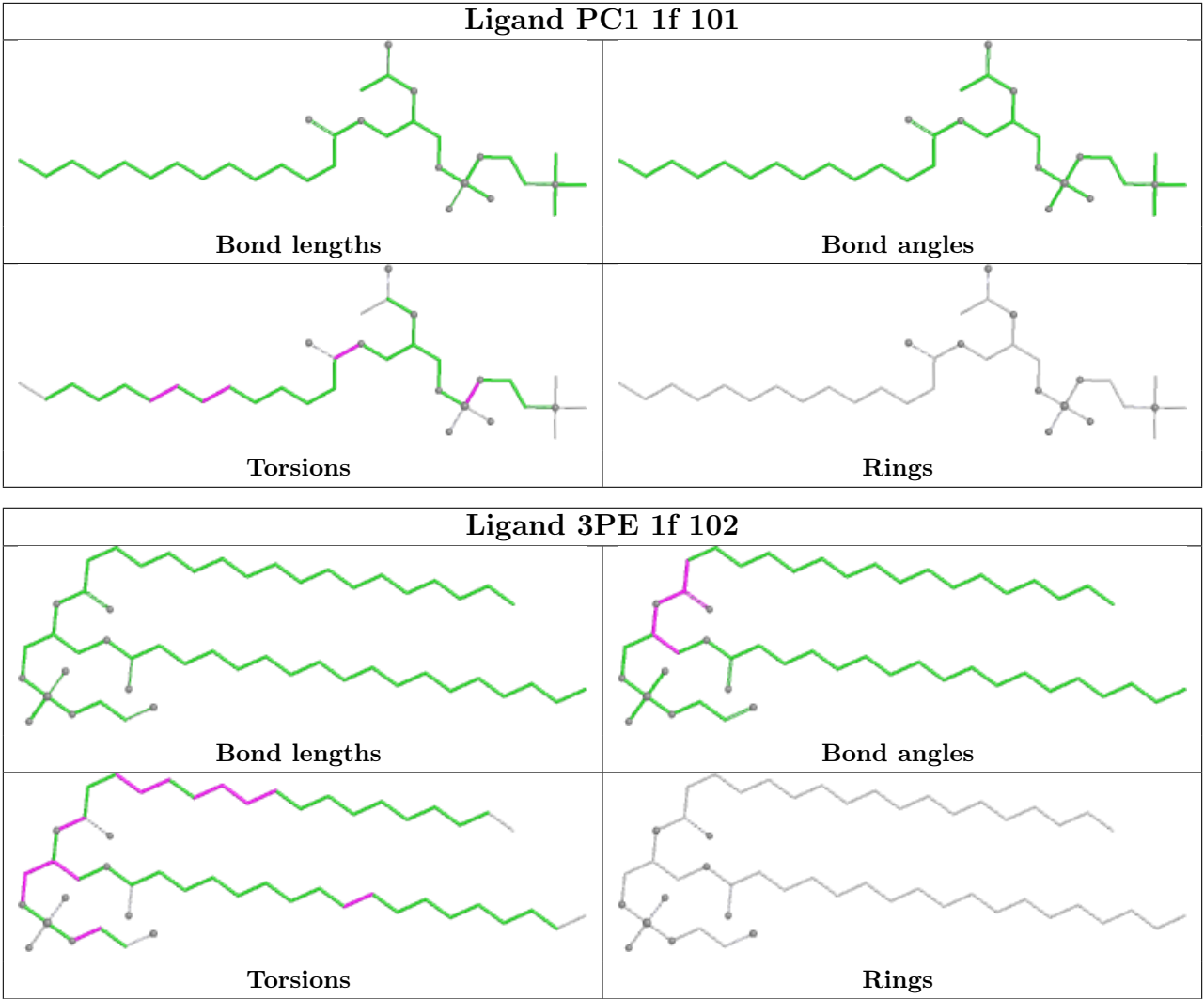












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1r	1:ALA	C	2:SER	N	7.81

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	li	1:SAC	C	2:GLY	N	3.21

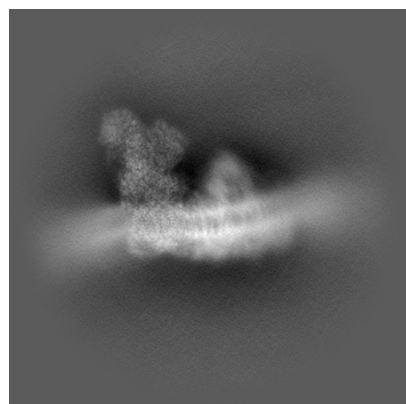
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42166. These allow visual inspection of the internal detail of the map and identification of artifacts.

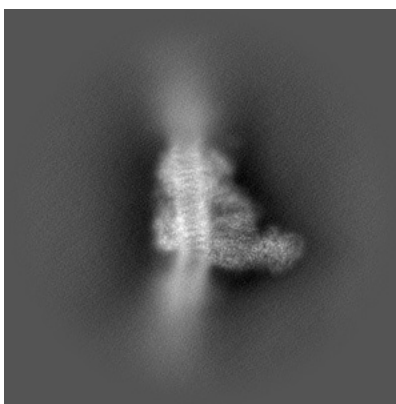
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

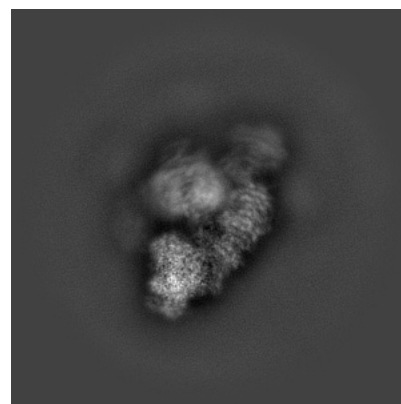
6.1.1 Primary map



X

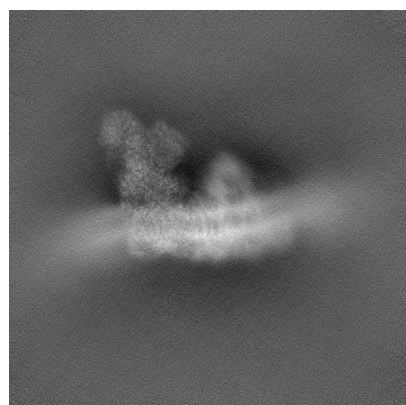


Y

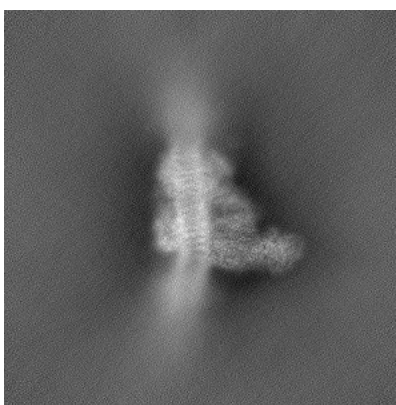


Z

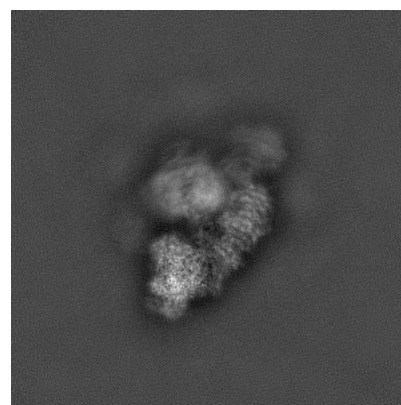
6.1.2 Raw map



X



Y

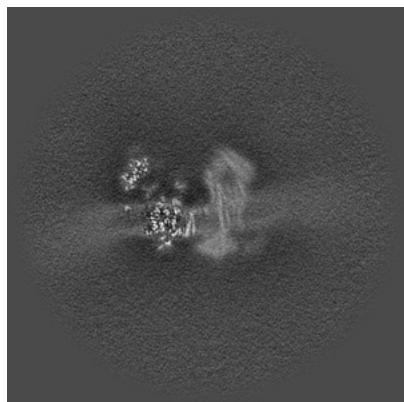


Z

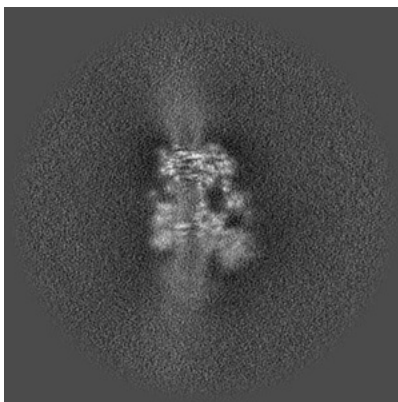
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

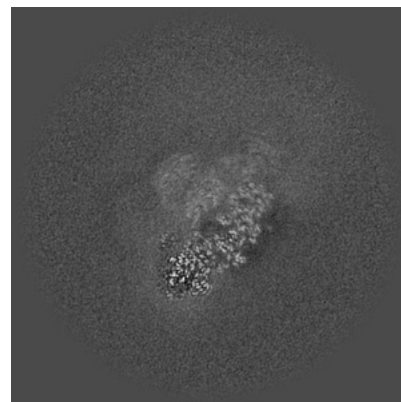
6.2.1 Primary map



X Index: 200

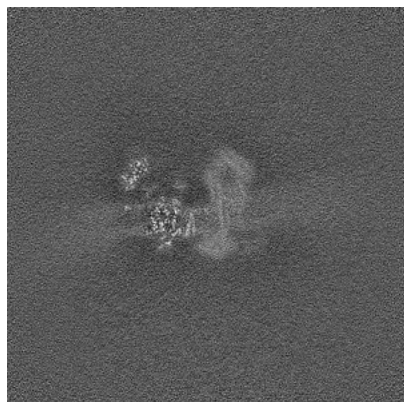


Y Index: 200

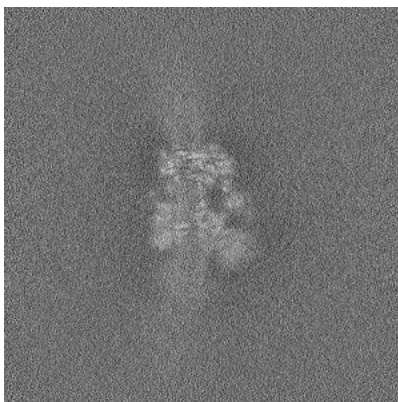


Z Index: 200

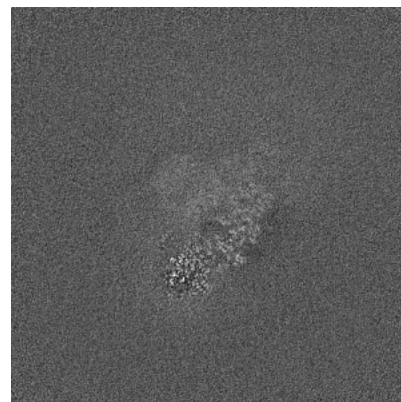
6.2.2 Raw map



X Index: 200



Y Index: 200

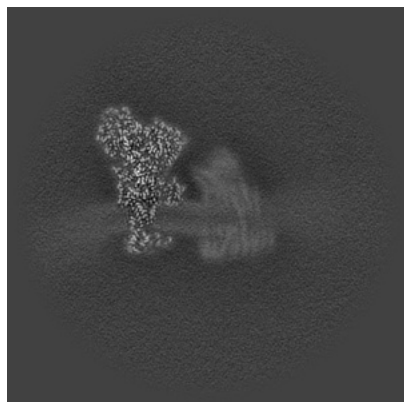


Z Index: 200

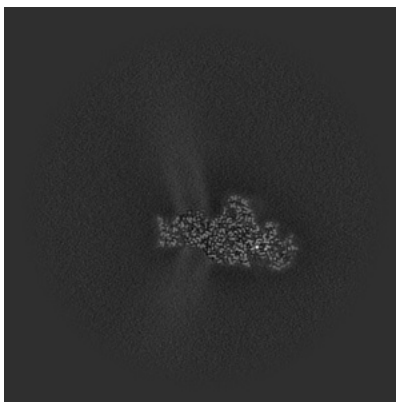
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

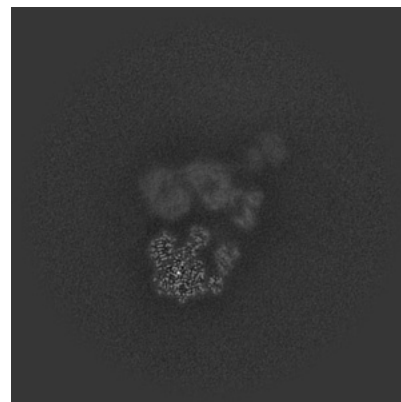
6.3.1 Primary map



X Index: 163

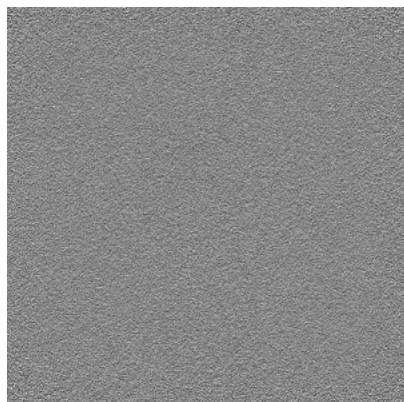


Y Index: 127

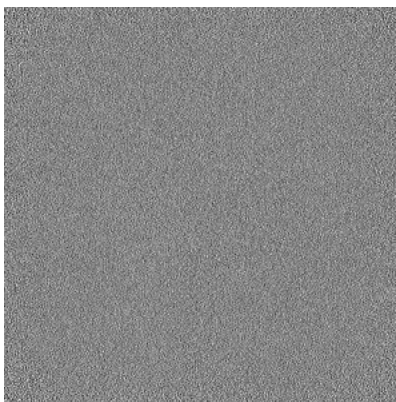


Z Index: 227

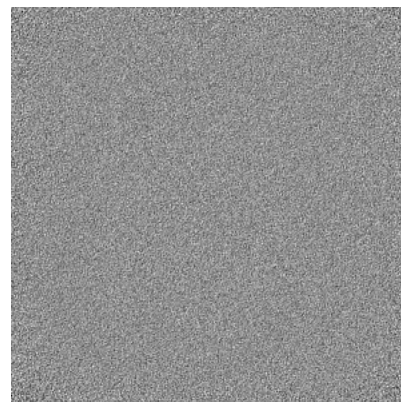
6.3.2 Raw map



X Index: 0



Y Index: 0

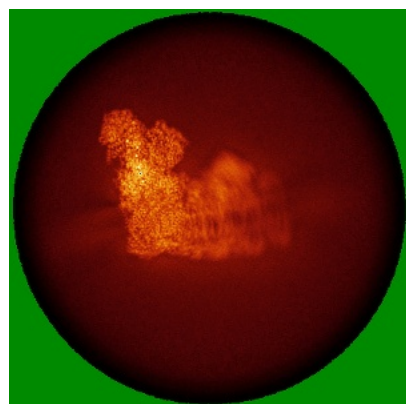


Z Index: 0

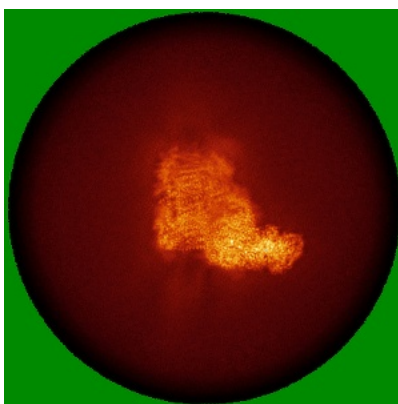
The images above show the largest variance slices of the map in three orthogonal directions.

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

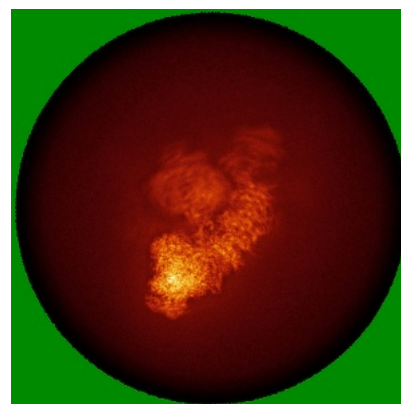
6.4.1 Primary map



X

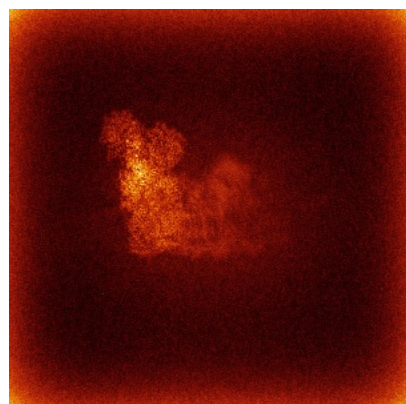


Y

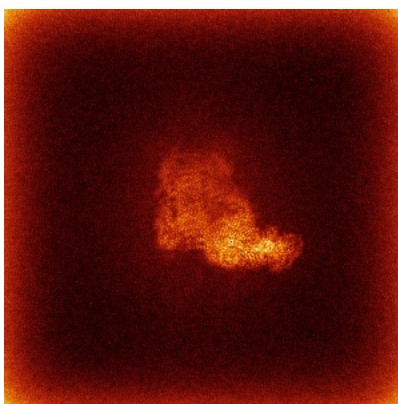


Z

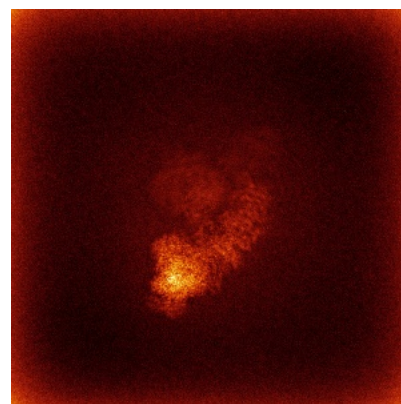
6.4.2 Raw map



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.

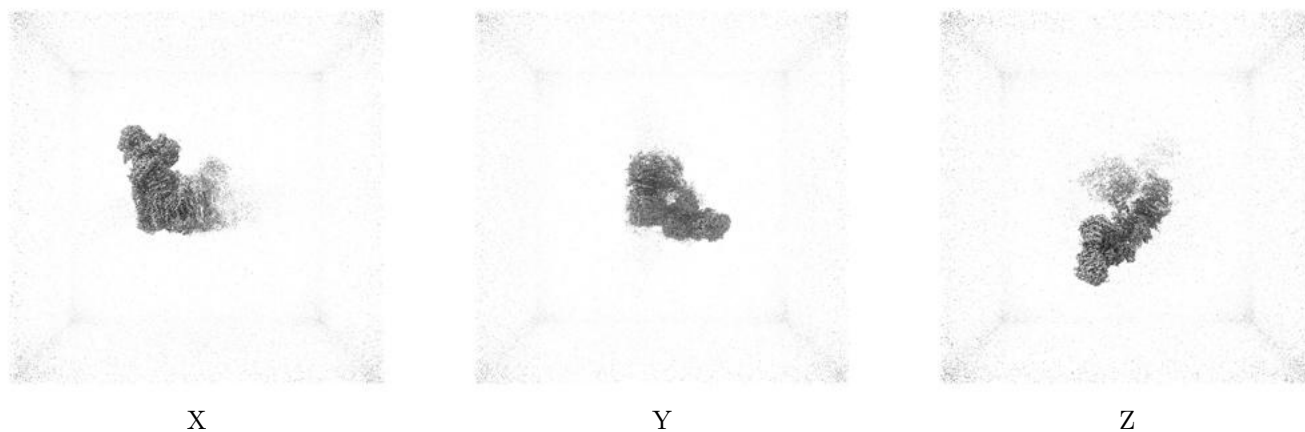
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. 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.

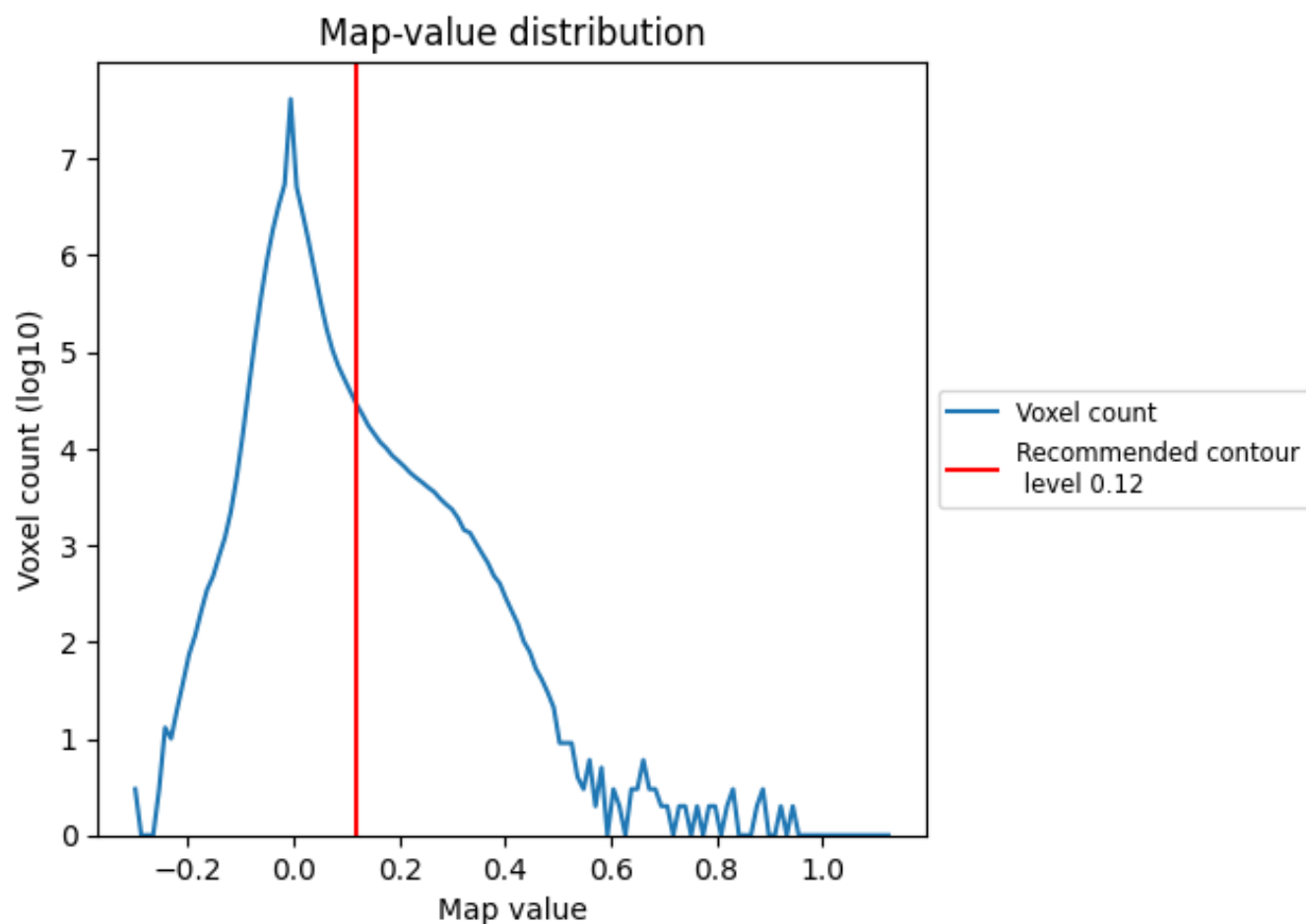
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

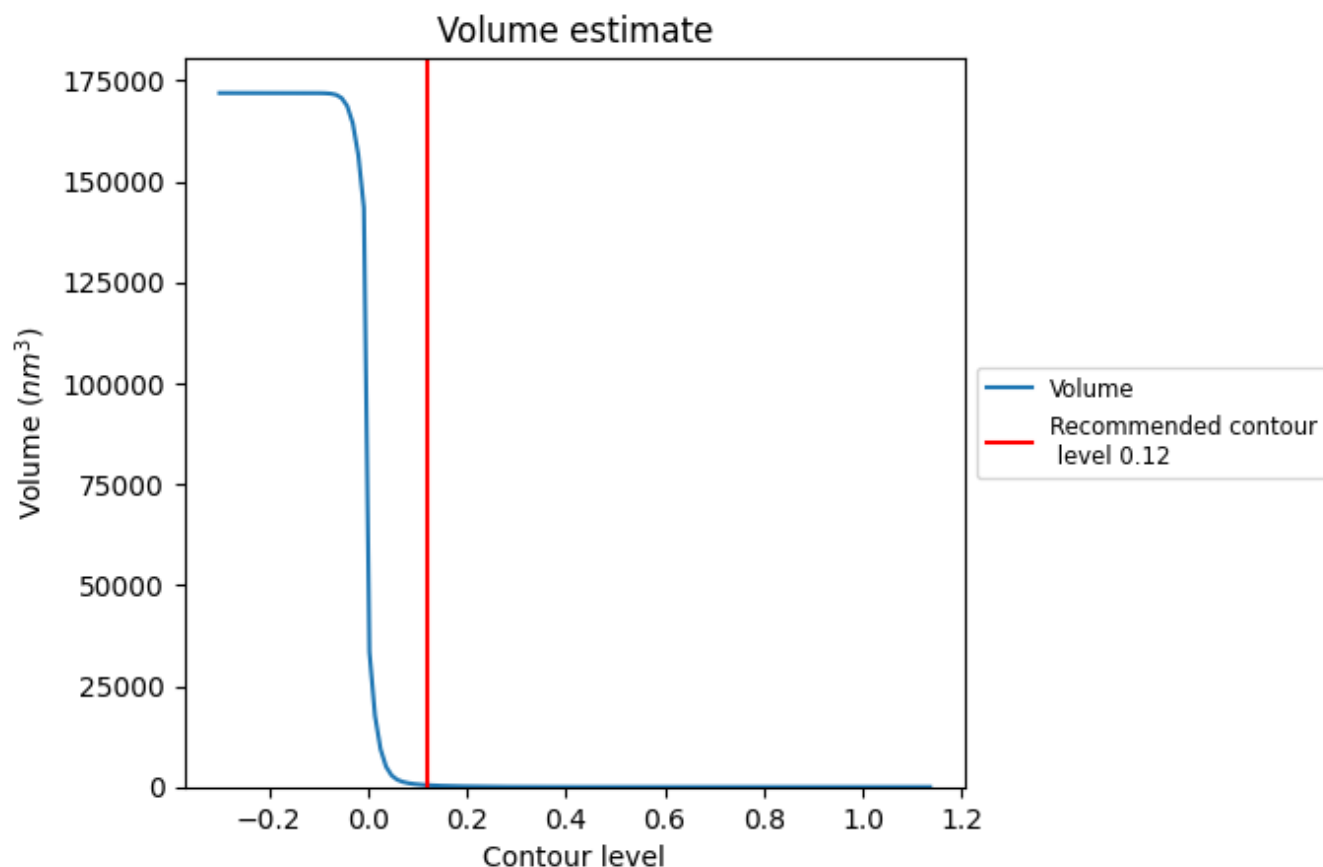
This section contains the results of statistical analysis of the map.

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.

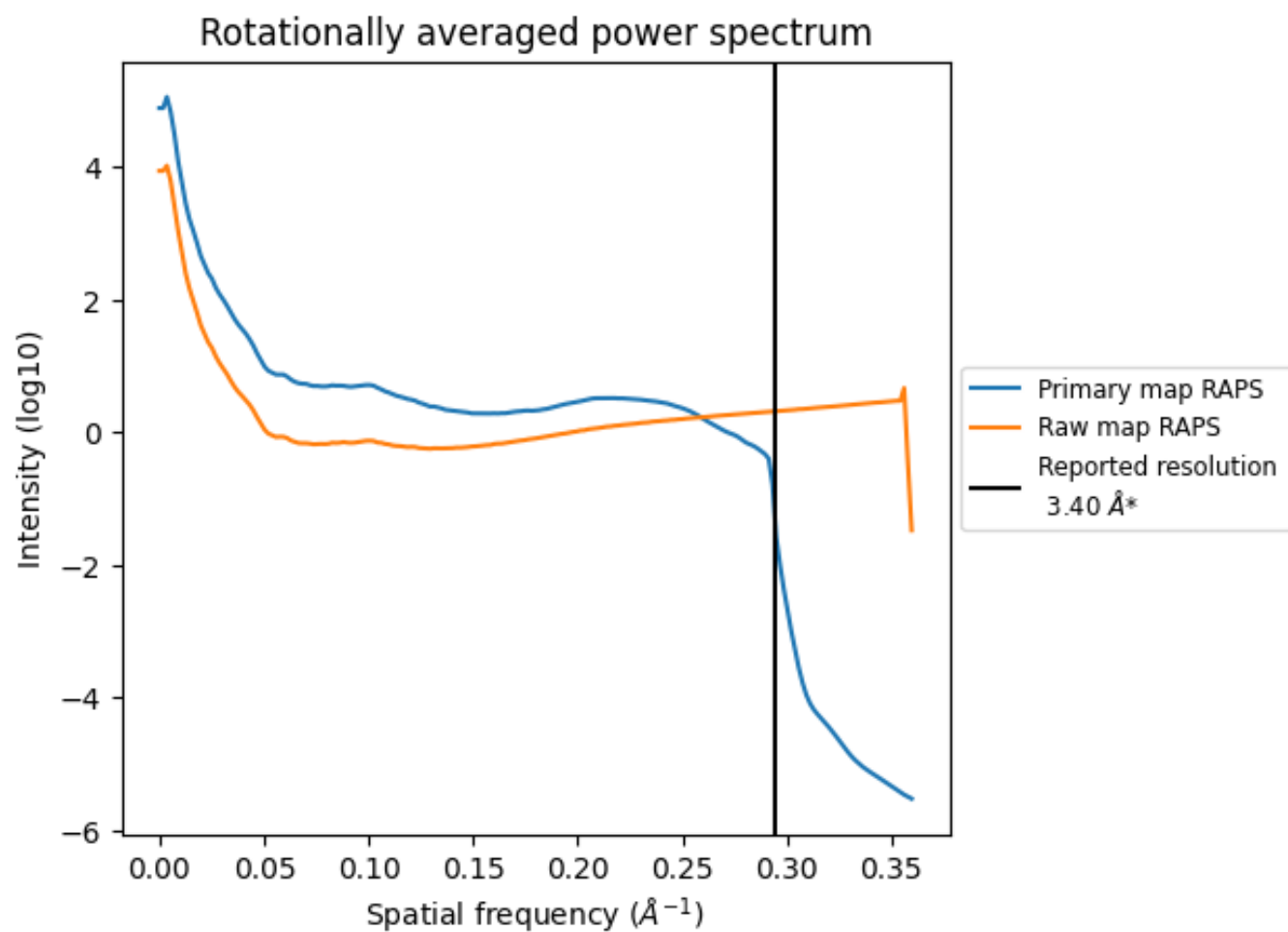
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm^3 ; this corresponds to an approximate mass of 397 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 [i](#)

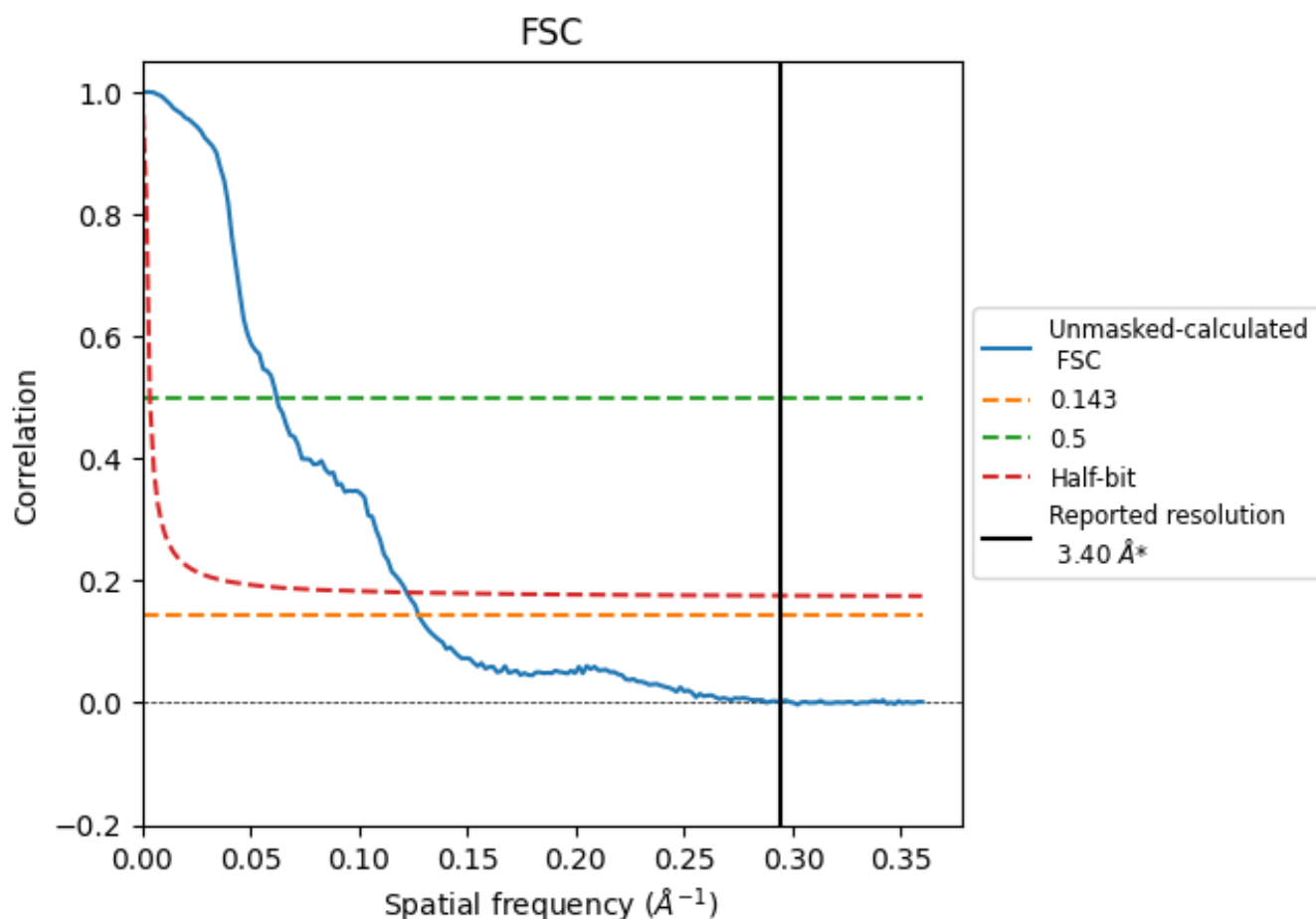


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.294 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

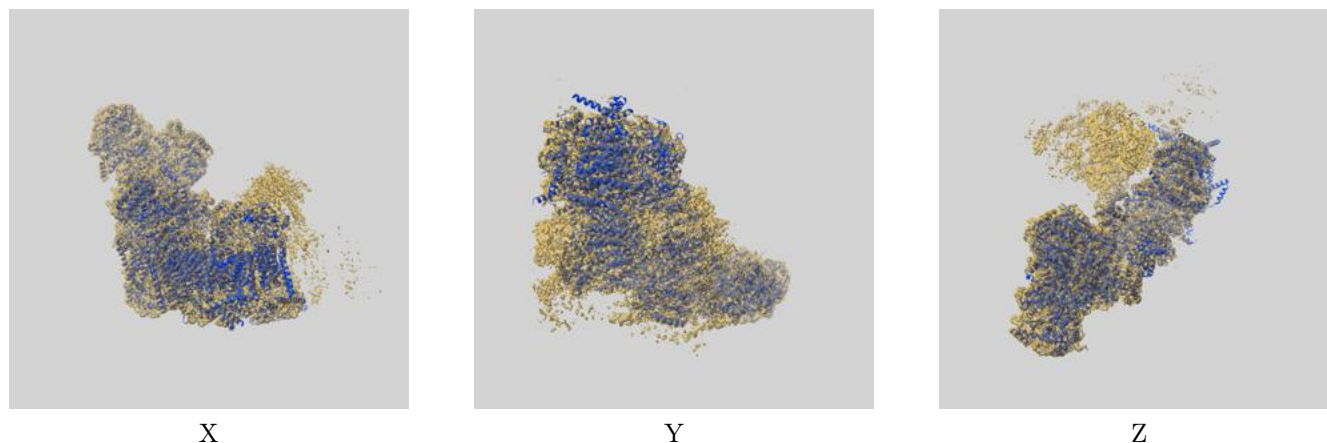
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.84	16.13	8.20

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

9 Map-model fit [i](#)

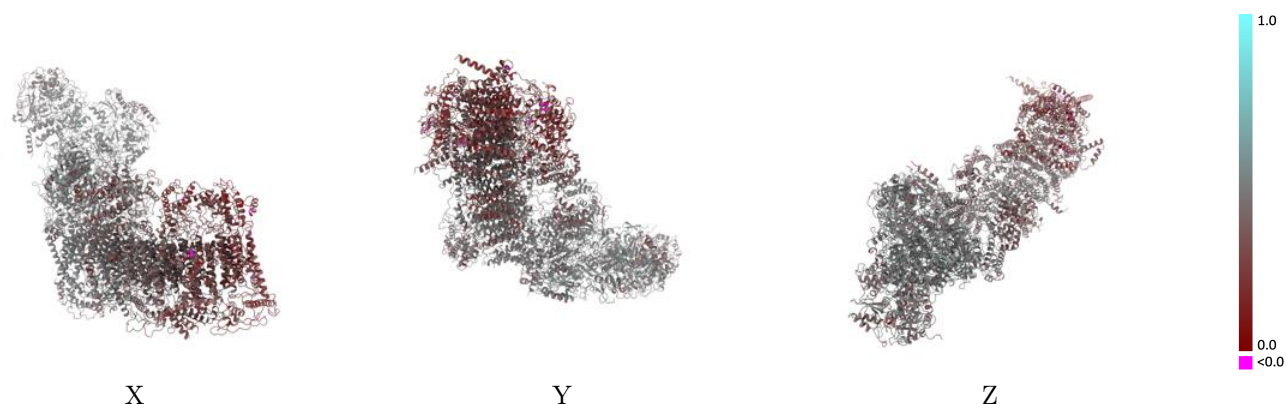
This section contains information regarding the fit between EMDB map EMD-42166 and PDB model 8UEP. Per-residue inclusion information can be found in section 3 on page 21.

9.1 Map-model overlay [i](#)



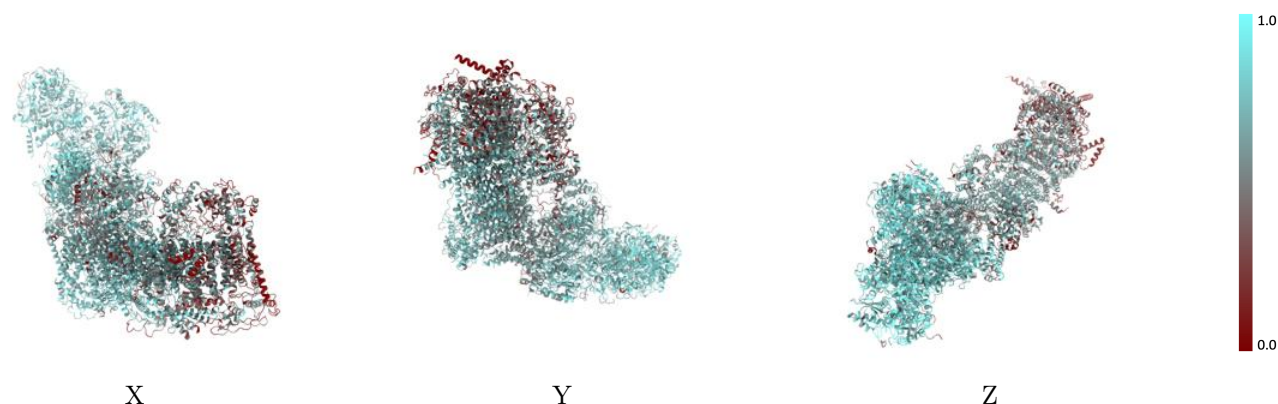
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



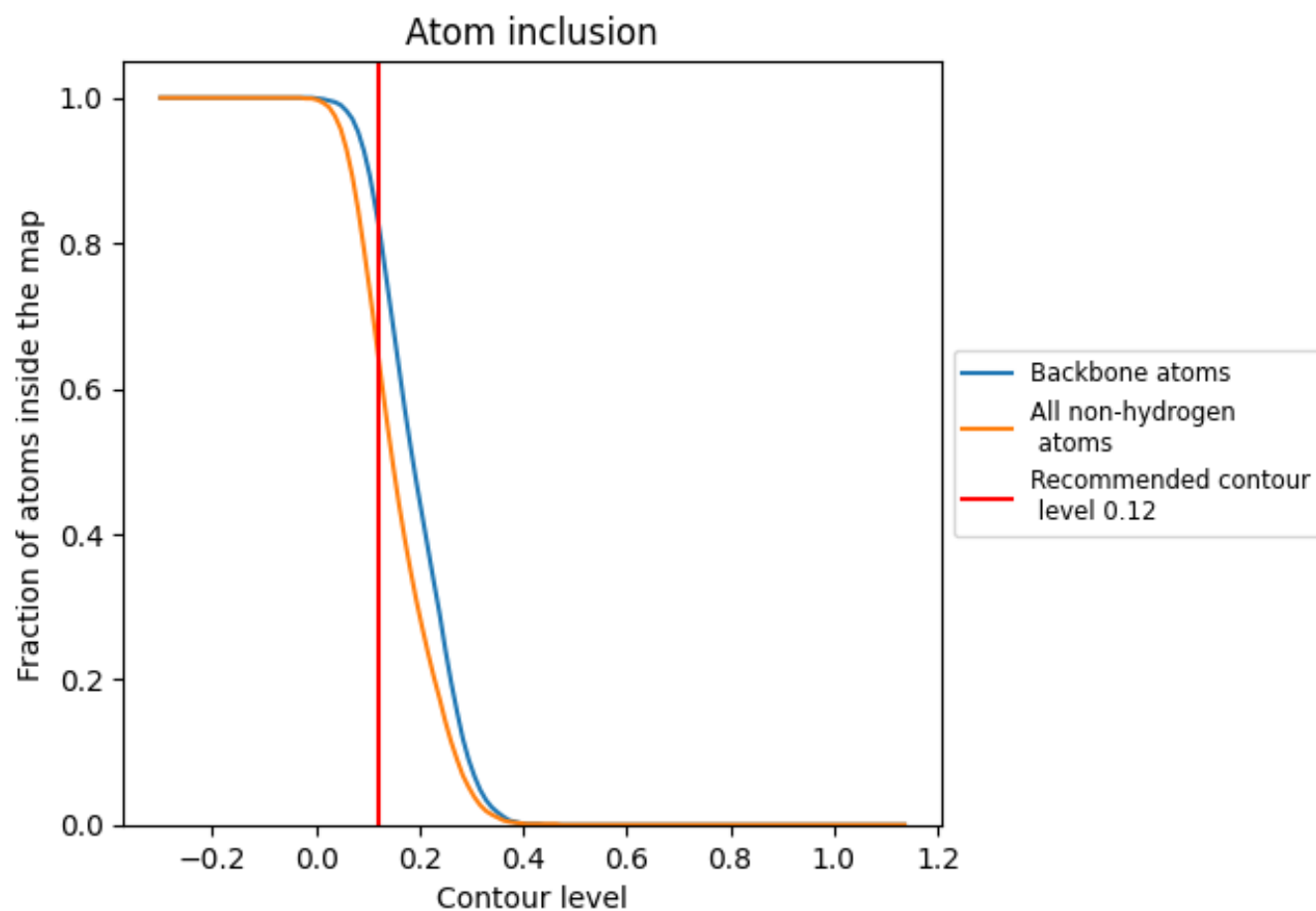
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.12).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 65% 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 (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6490	 0.4130
1A	 0.6190	 0.4620
1B	 0.7530	 0.4810
1C	 0.7670	 0.4940
1D	 0.7610	 0.4810
1E	 0.7770	 0.4460
1F	 0.7940	 0.4480
1G	 0.7830	 0.4730
1H	 0.6630	 0.4730
1I	 0.8070	 0.4910
1J	 0.6210	 0.4370
1K	 0.6650	 0.4370
1L	 0.4790	 0.3010
1M	 0.6600	 0.4060
1N	 0.7080	 0.4520
1O	 0.5280	 0.3750
1P	 0.6750	 0.4740
1Q	 0.6910	 0.4670
1R	 0.7510	 0.4850
1S	 0.7610	 0.4210
1T	 0.5180	 0.3760
1U	 0.3400	 0.2320
1V	 0.6910	 0.4410
1W	 0.6700	 0.4500
1X	 0.7690	 0.4430
1Y	 0.5890	 0.3600
1Z	 0.7630	 0.4580
1a	 0.7230	 0.4470
1b	 0.6980	 0.4570
1c	 0.5370	 0.3800
1d	 0.6950	 0.4330
1e	 0.7450	 0.4480
1f	 0.4430	 0.3640
1g	 0.5610	 0.3530
1h	 0.6400	 0.3960



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Chain	Atom inclusion	Q-score
1i	 0.3070	 0.2850
1j	 0.3090	 0.2890
1k	 0.2050	 0.2320
1l	 0.4730	 0.3000
1m	 0.4960	 0.3020
1n	 0.4620	 0.2680
1o	 0.4200	 0.2400
1p	 0.5510	 0.3410
1q	 0.7540	 0.4820
1r	 0.7780	 0.4880
1s	 0.7470	 0.4190