



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 09:41 AM EDT

PDB ID : 8UEW / pdb_00008uew
EMDB ID : EMD-42173
Title : In-situ complex I, Deactive class05
Authors : Zheng, W.; Zhu, J.; Zhang, K.
Deposited on : 2023-10-02
Resolution : 3.60 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

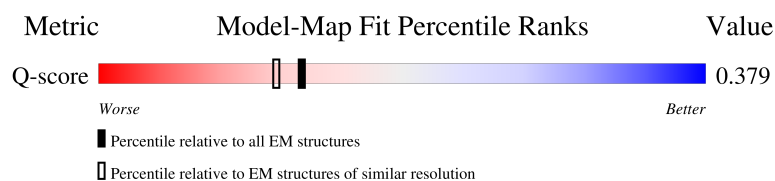
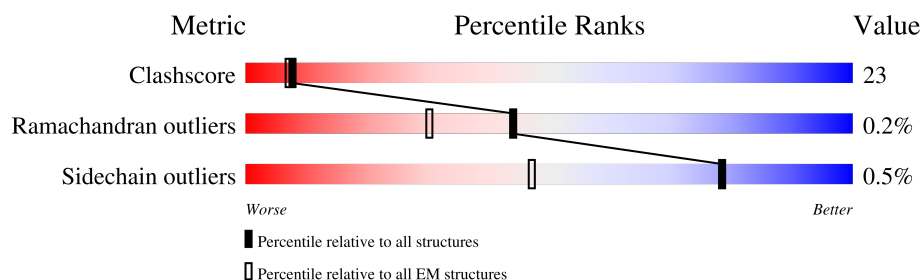
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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
1	FME	1A	1	-	-	X	-
46	SF4	1B	201	-	-	X	-
46	SF4	1I	201	-	-	X	-
46	SF4	1I	202	-	-	X	-
47	FES	1G	804	-	-	X	-

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 67472 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		

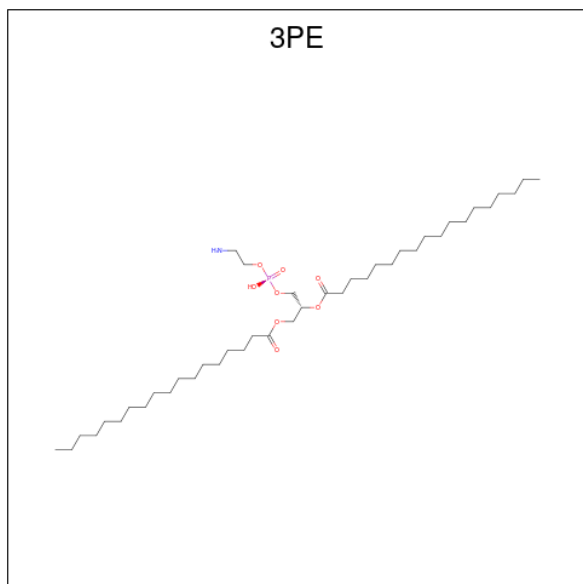
There is a discrepancy between the modelled and reference sequences:

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

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

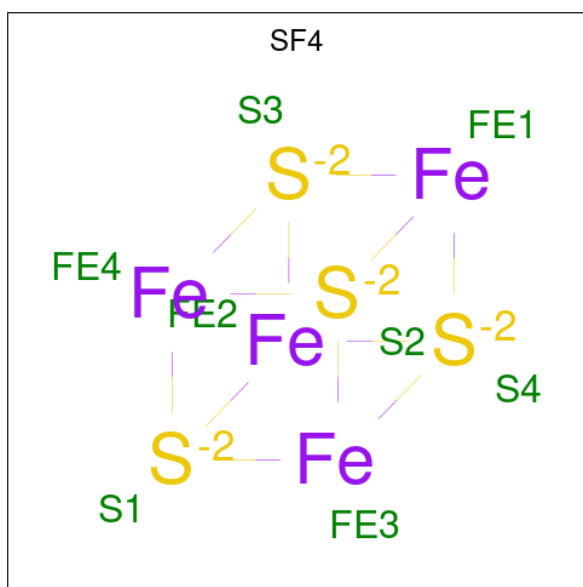
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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



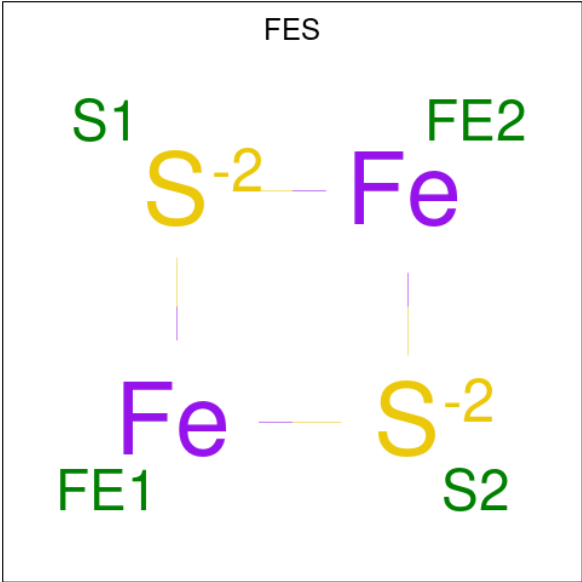
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



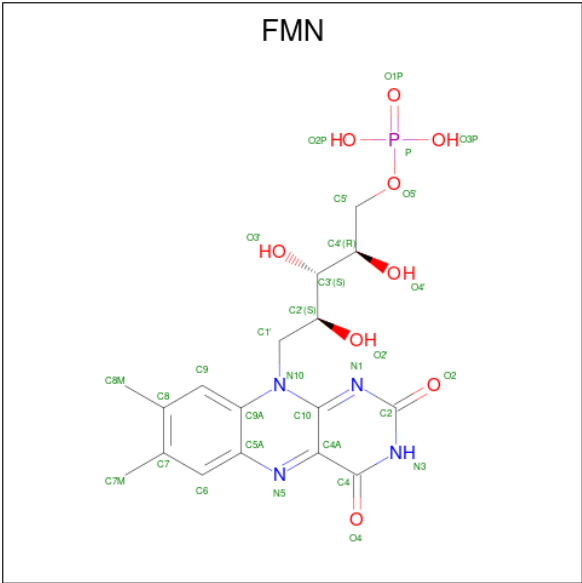
Mol	Chain	Residues	Atoms			AltConf
46	1B	1	Total	Fe	S	0
			8	4	4	
46	1F	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



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).

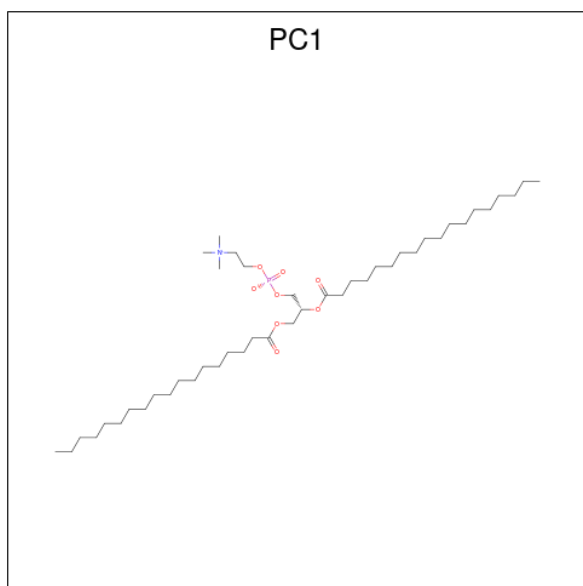


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

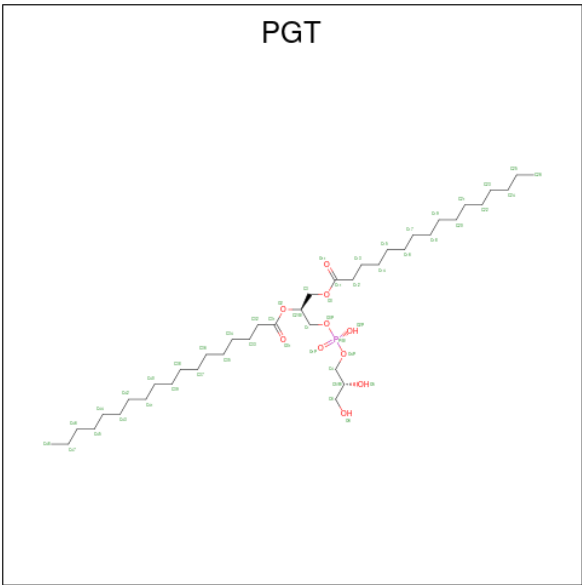
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

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



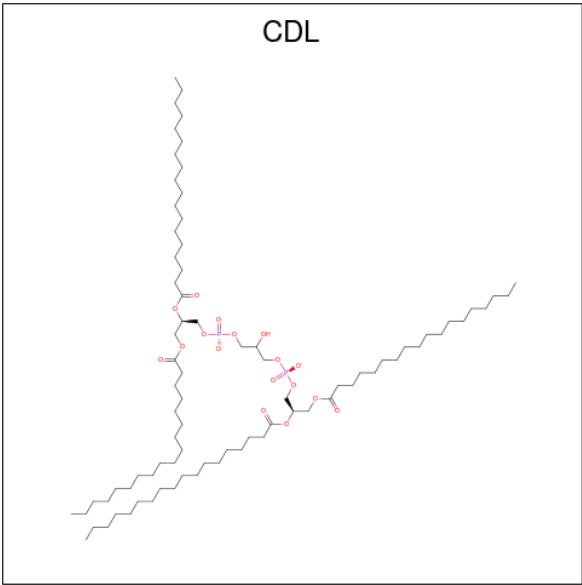
Mol	Chain	Residues	Atoms					AltConf
50	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 51 is (1S)-2-{{[(2R)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (CCD ID: PGT) (formula: $C_{40}H_{79}O_{10}P$).



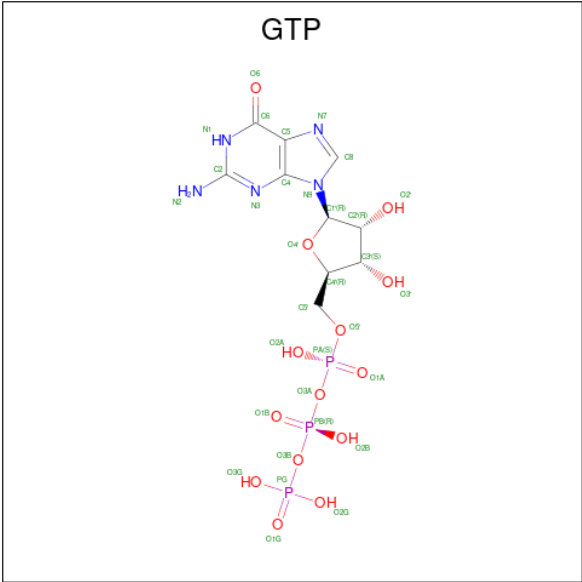
Mol	Chain	Residues	Atoms				AltConf
51	1M	1	Total	C	O	P	0
			51	40	10	1	

- Molecule 52 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$).



Mol	Chain	Residues	Atoms				AltConf
52	1N	1	Total	C	O	P	0
			77	58	17	2	
52	1r	1	Total	C	O	P	0
			61	42	17	2	

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

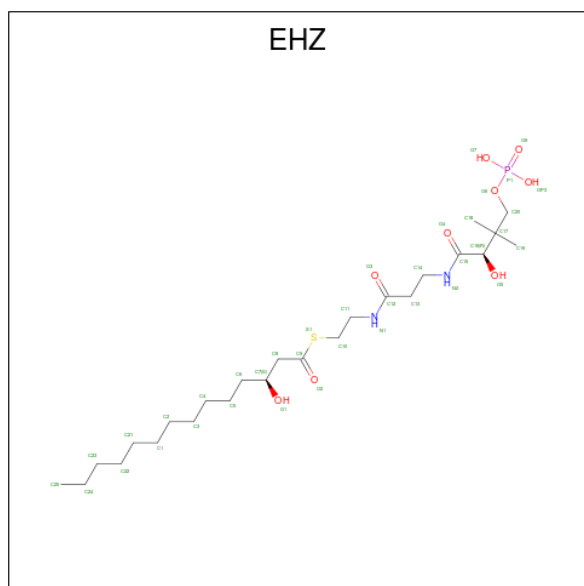


Mol	Chain	Residues	Atoms					AltConf
55	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

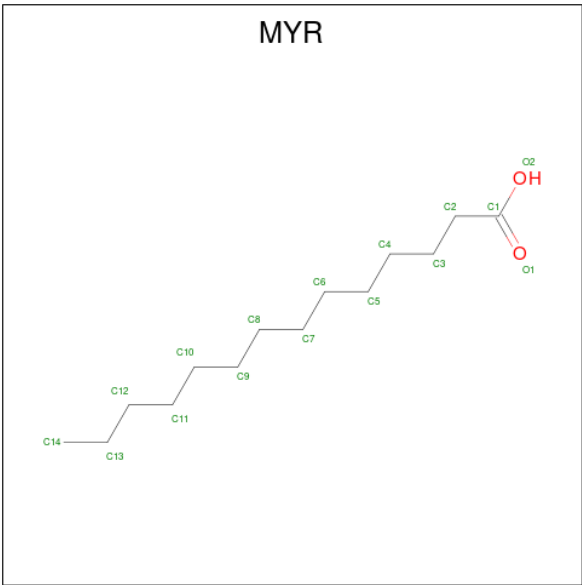
Mol	Chain	Residues	Atoms		AltConf
56	1R	1	Total	Zn	0
			1	1	

- 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).



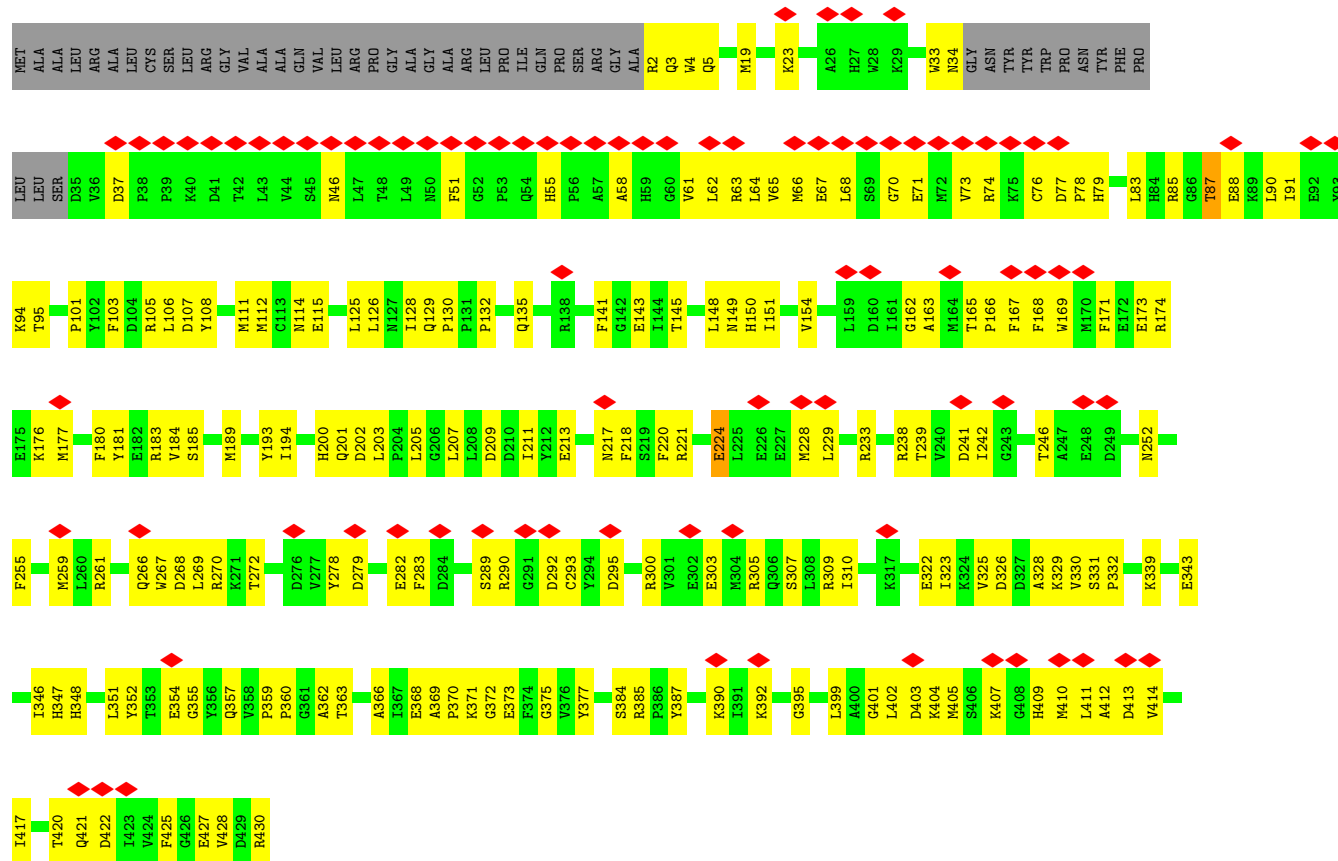
Mol	Chain	Residues	Atoms						AltConf
57	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
57	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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

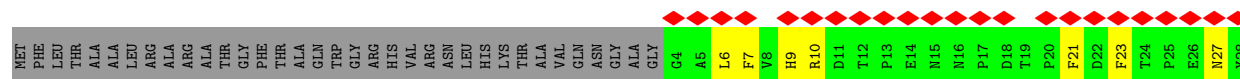
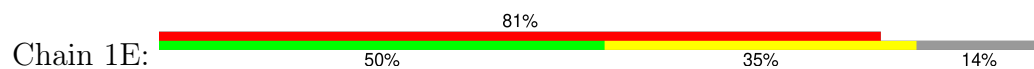


Mol	Chain	Residues	Atoms			AltConf
58	1l	1	Total	C	O	0
			15	14	1	

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

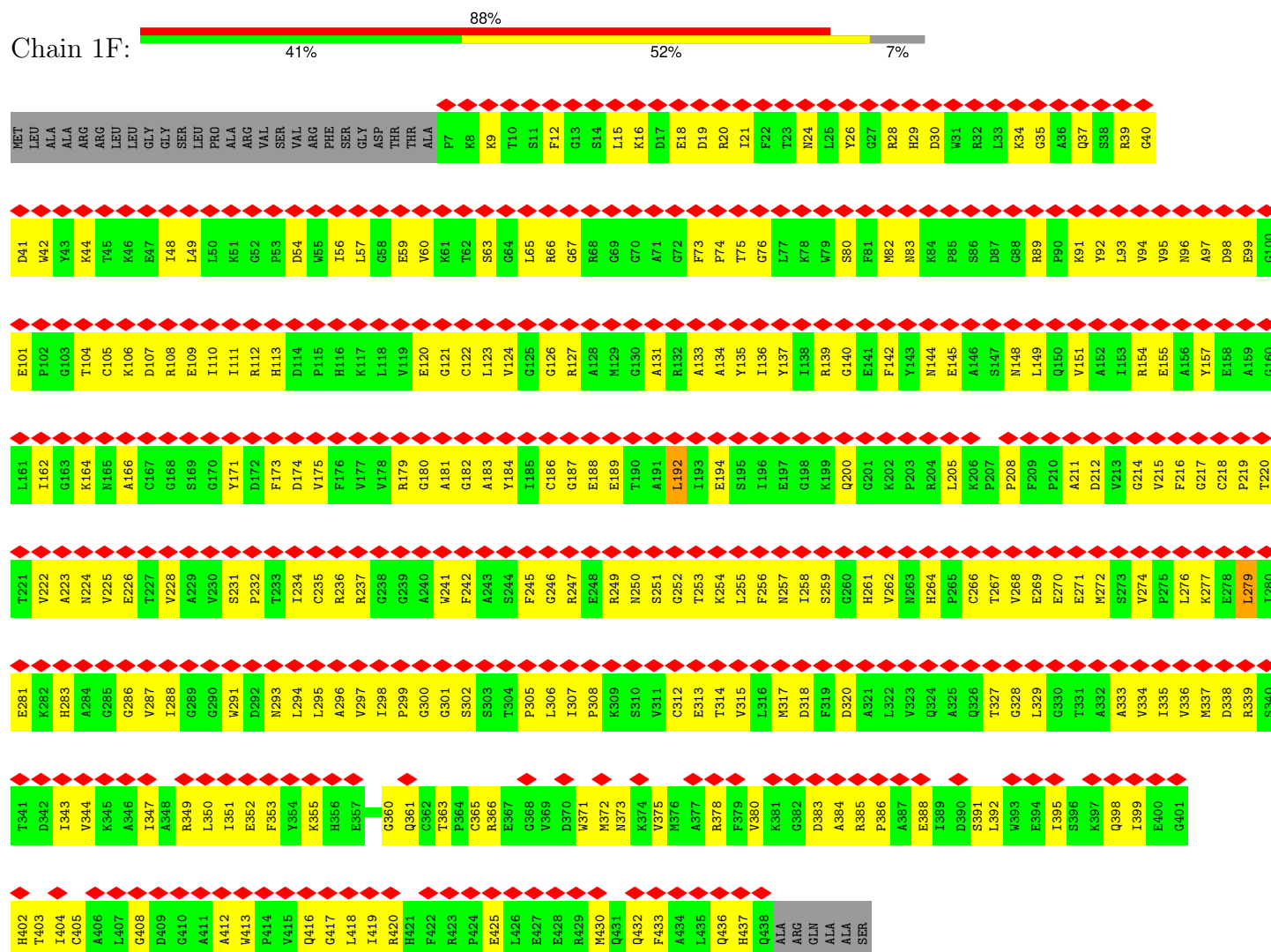


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



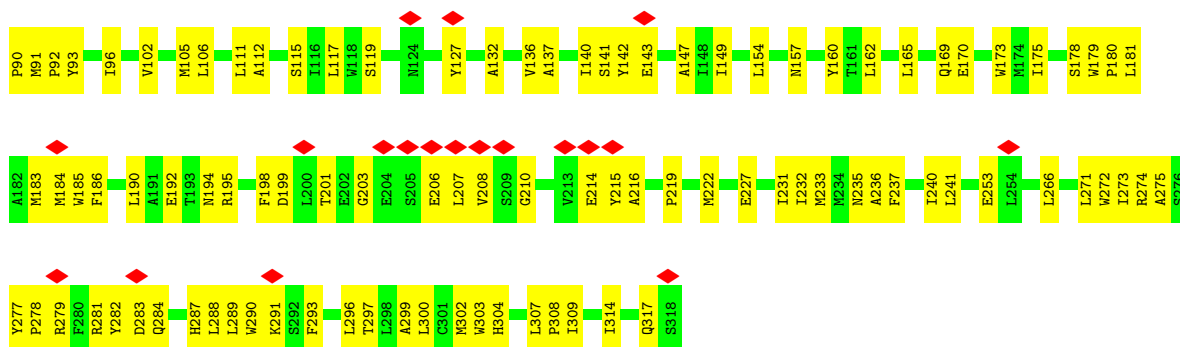


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

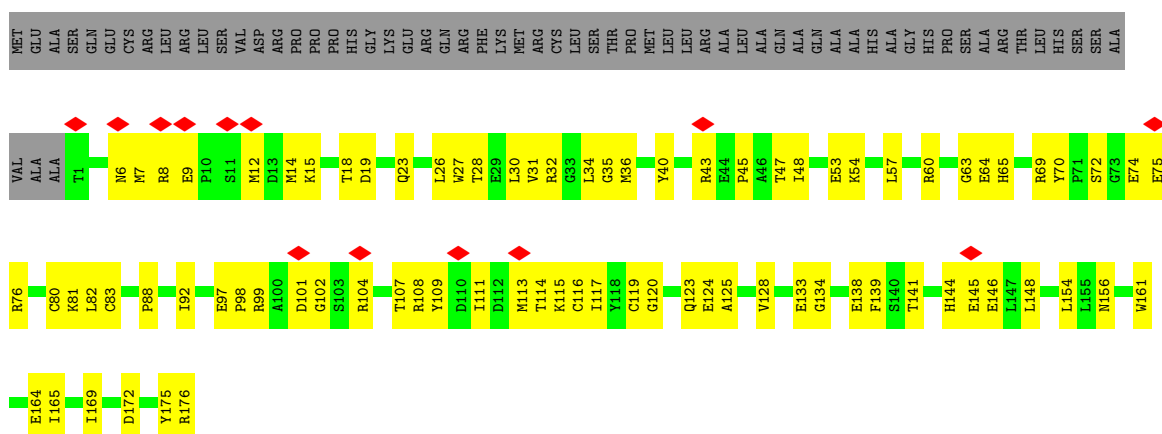


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

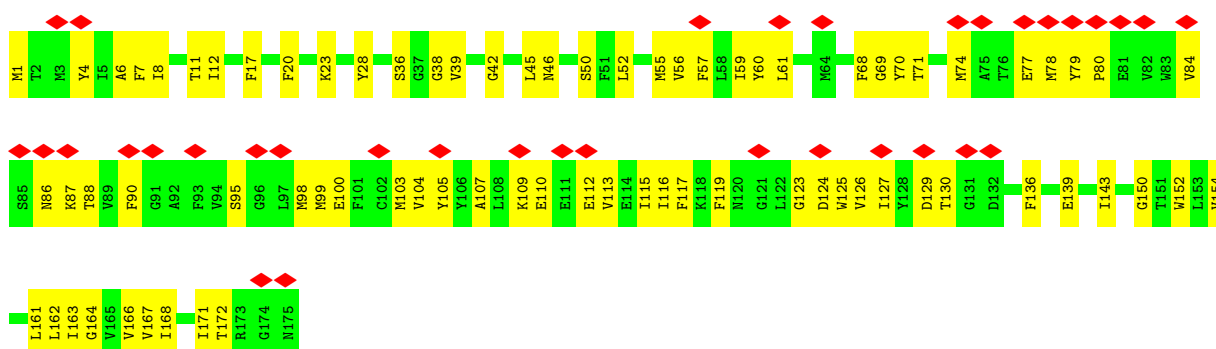




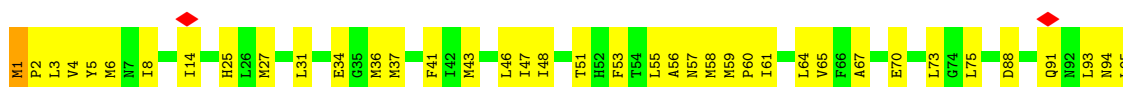
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

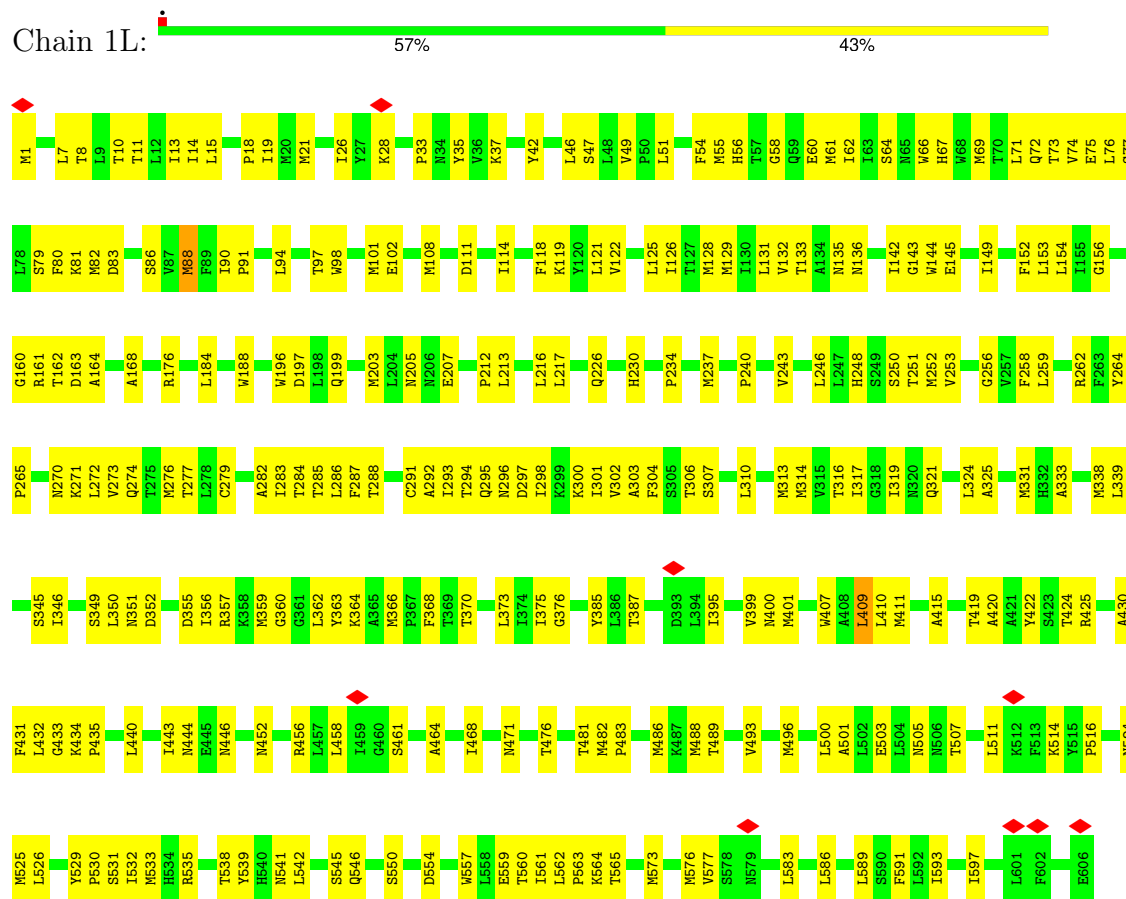


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

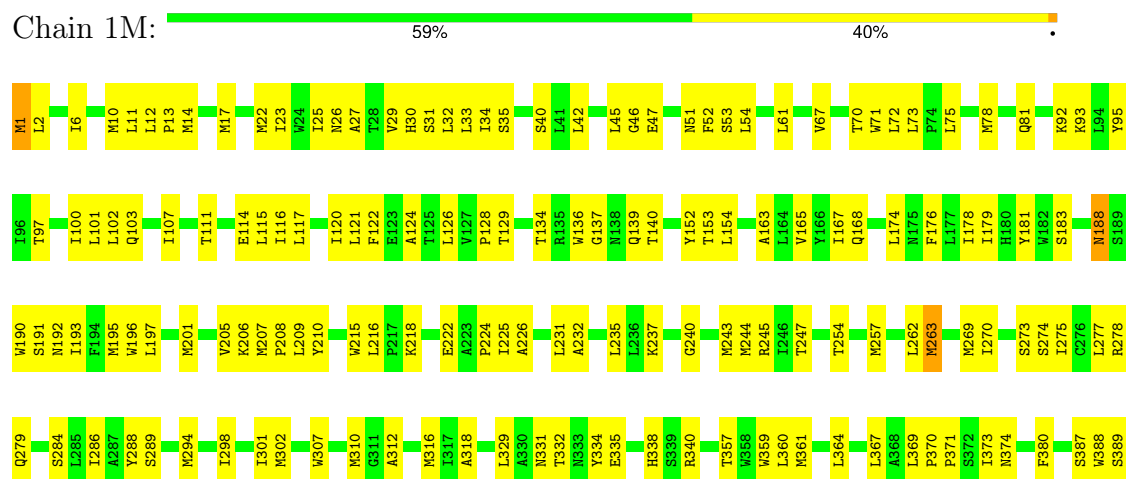




• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

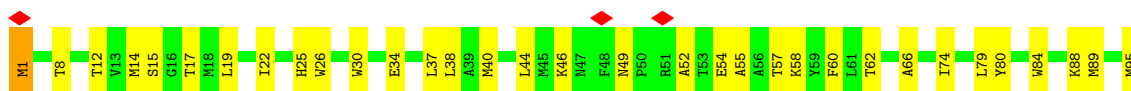


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

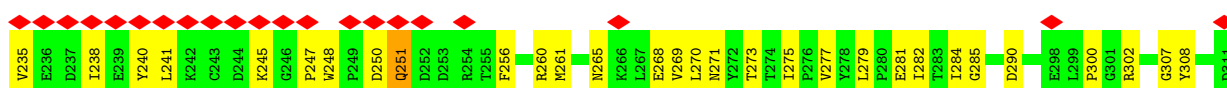
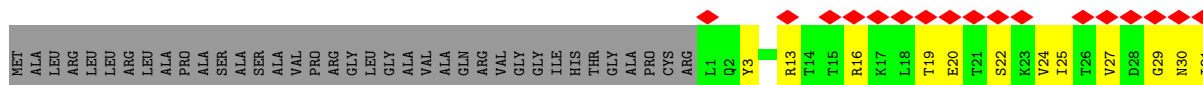
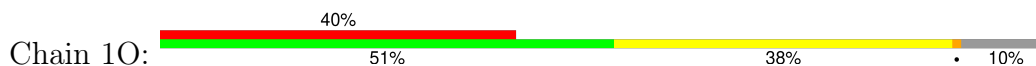


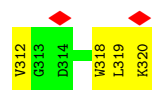


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

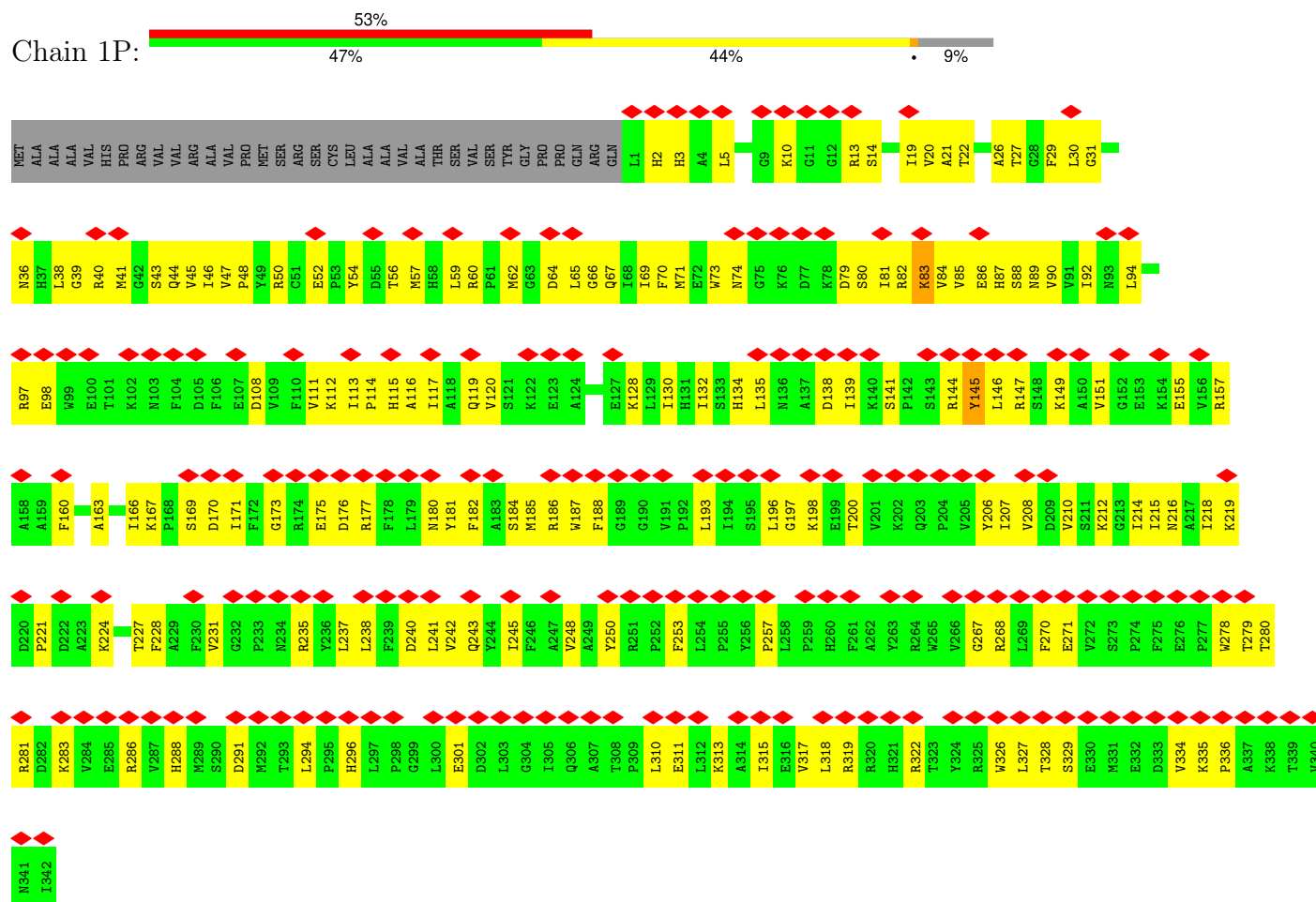


• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

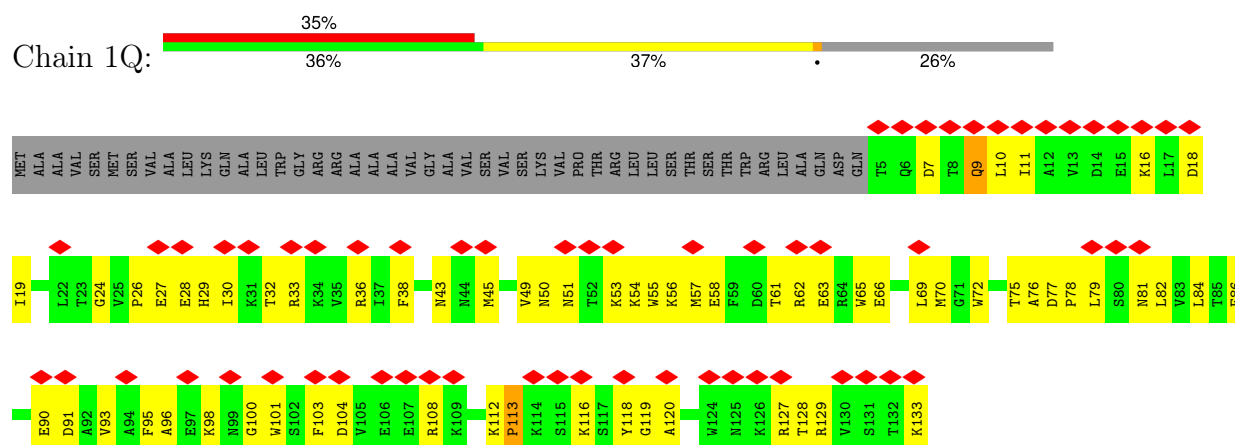




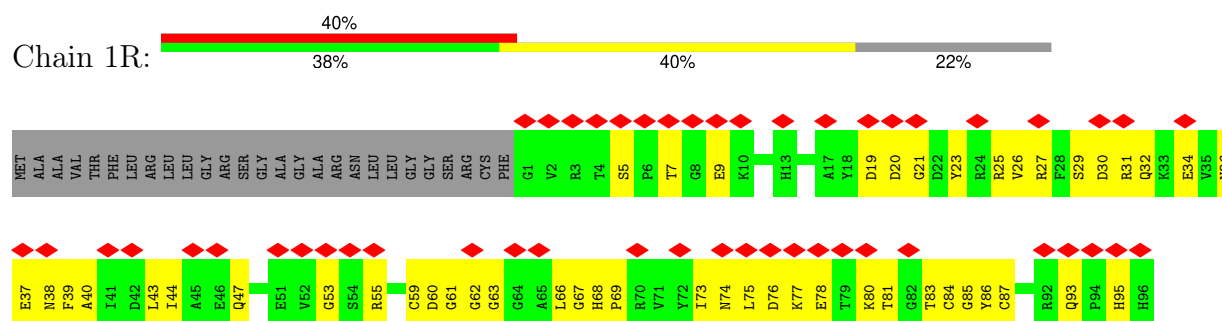
- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9



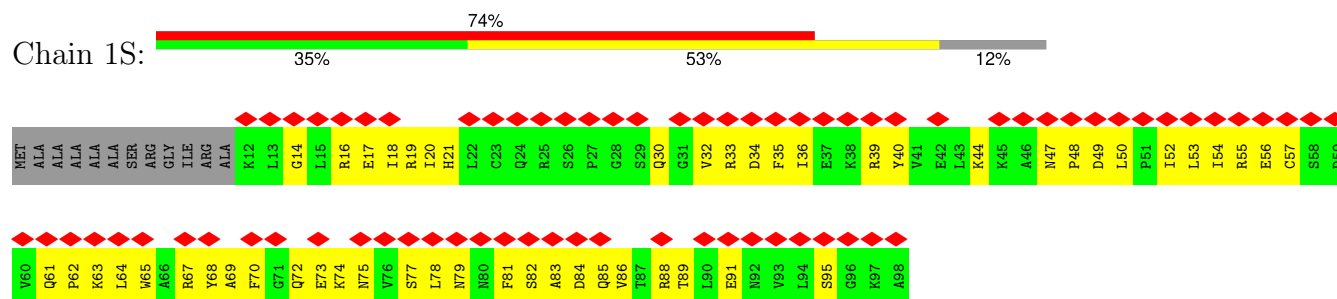
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



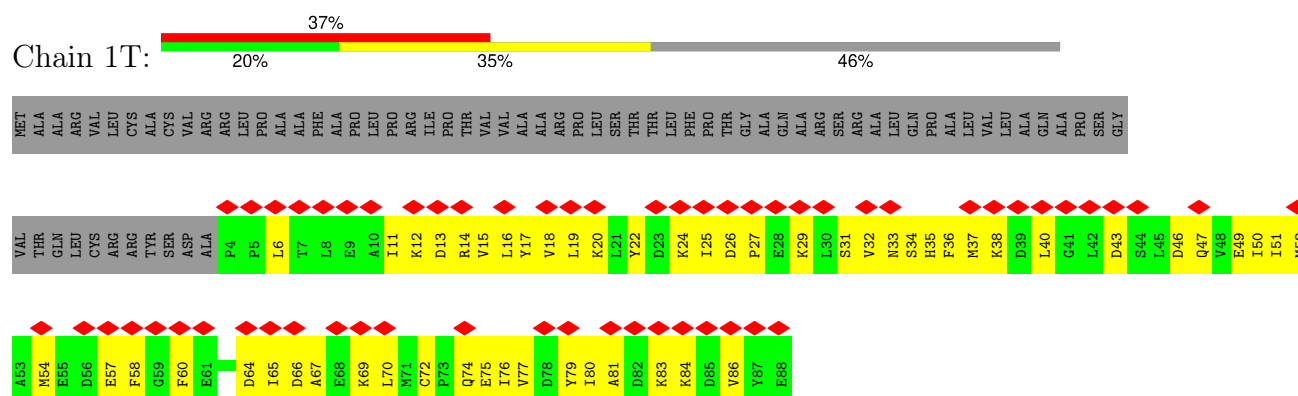
- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



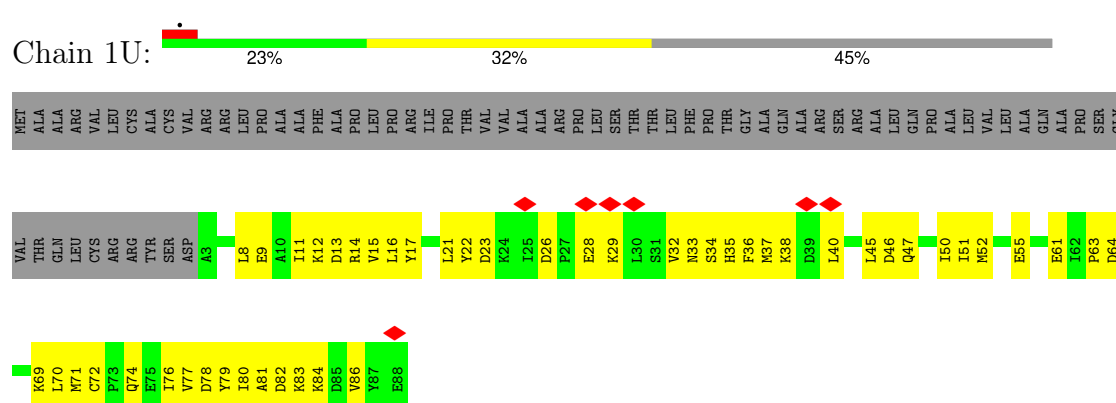
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



- Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

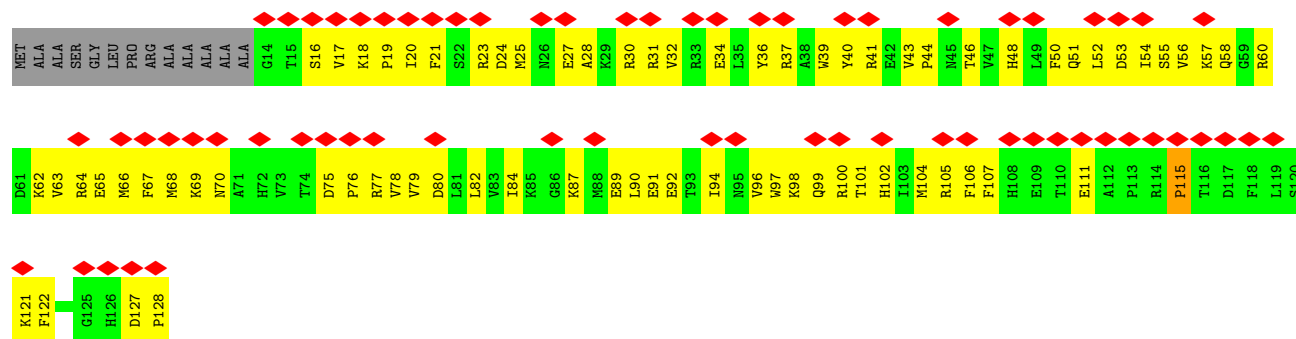


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

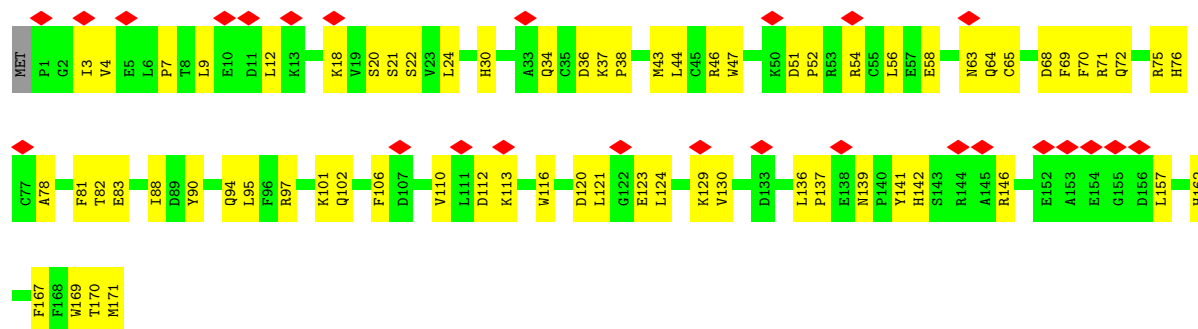




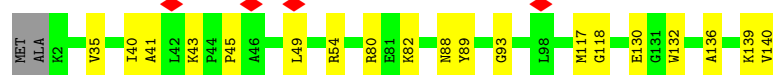
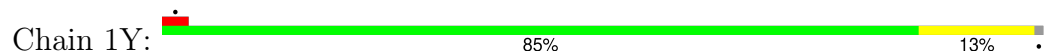
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



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

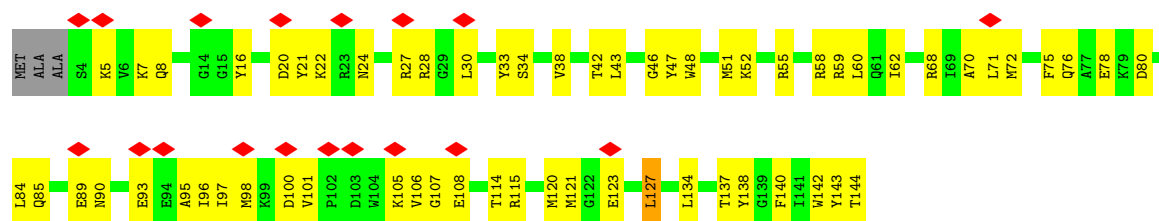


• Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



• Molecule 25: NADH:ubiquinone oxidoreductase subunit A13





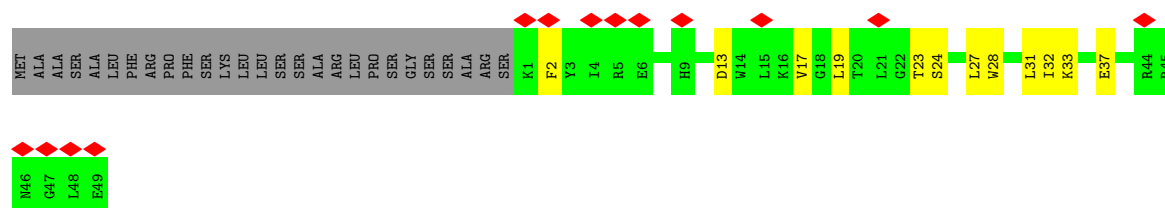
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



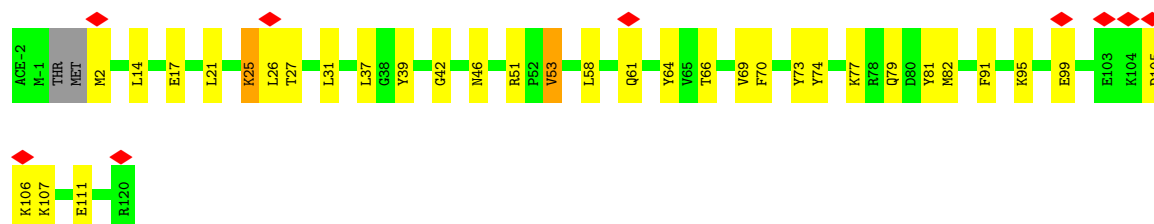
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



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

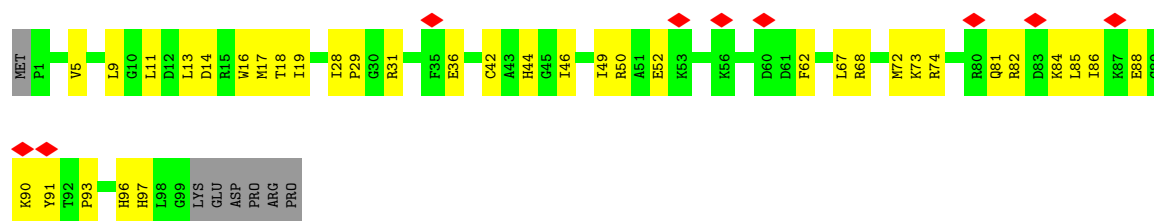


- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2

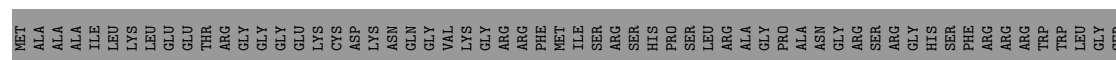


- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

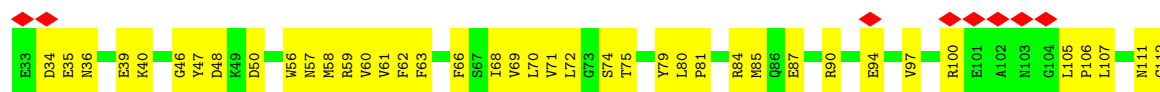
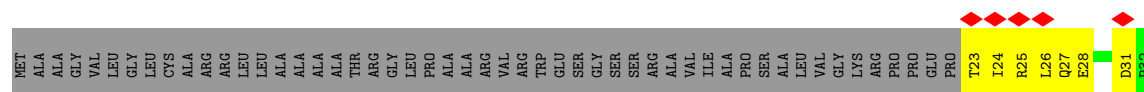




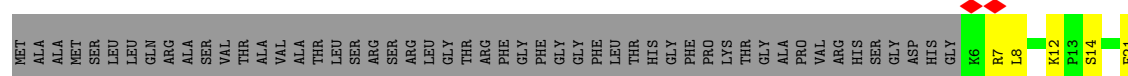
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



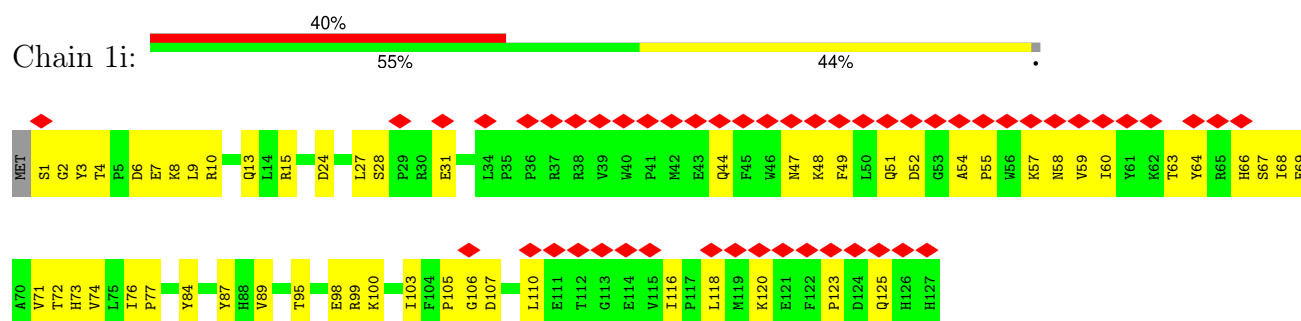
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



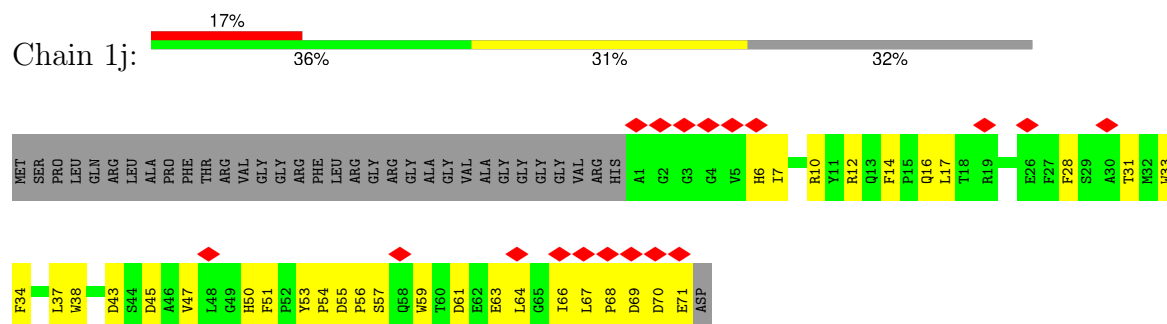
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



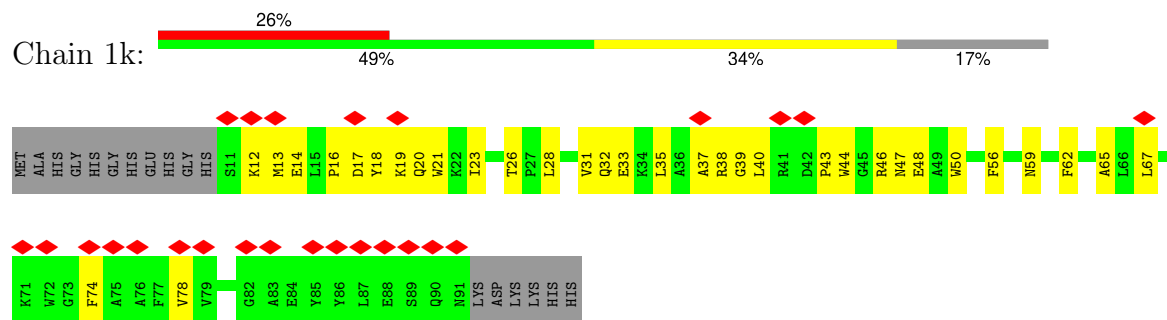
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



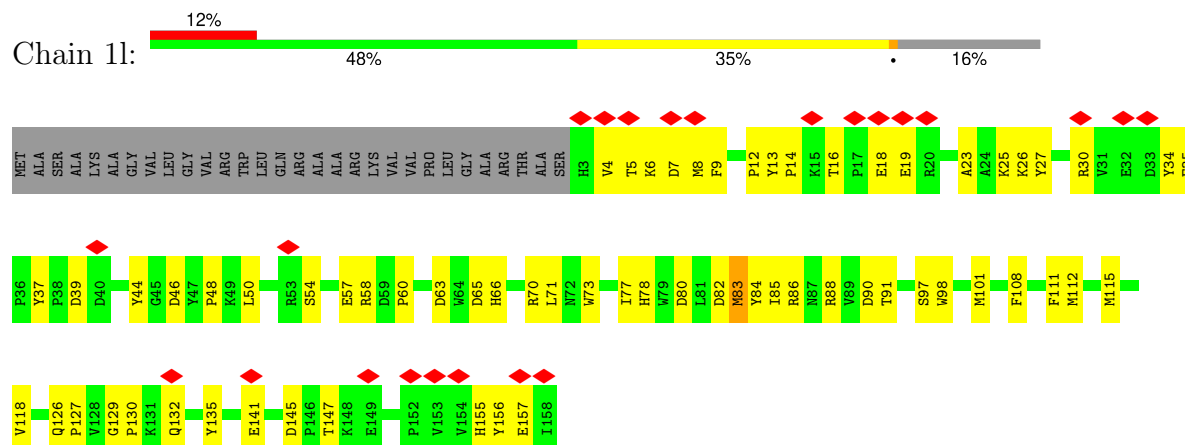
- Molecule 35: NADH:ubiquinone oxidoreductase subunit B2



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

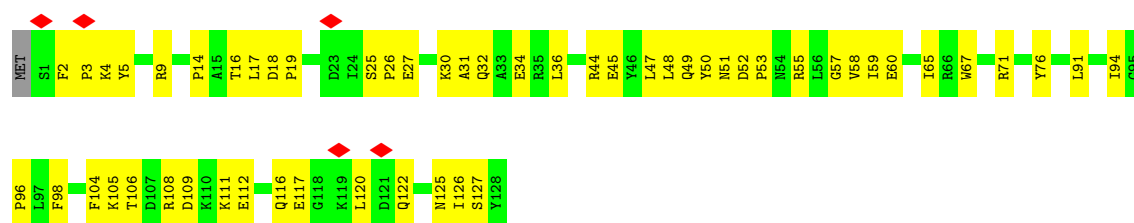


- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



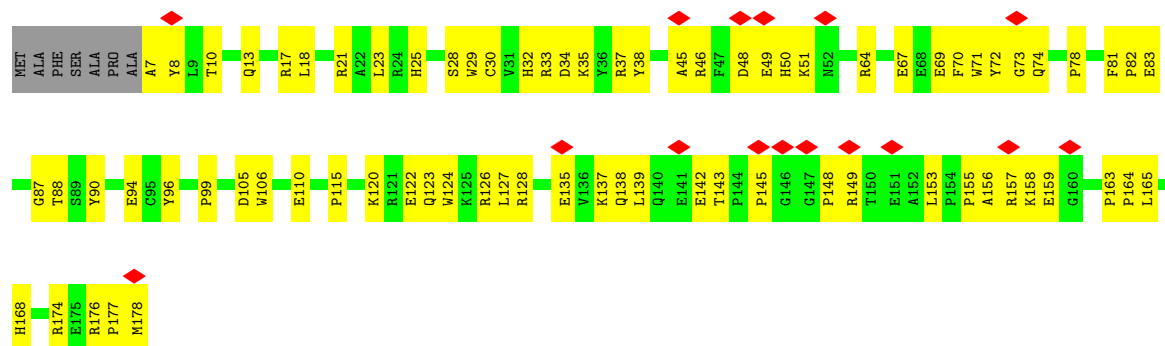
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain 1m: 



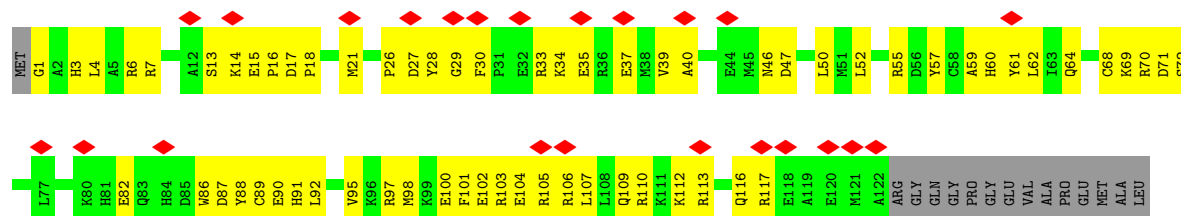
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain 1n: 



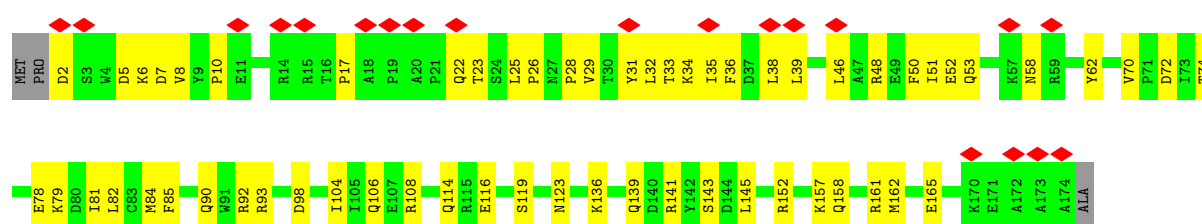
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain 1o: 



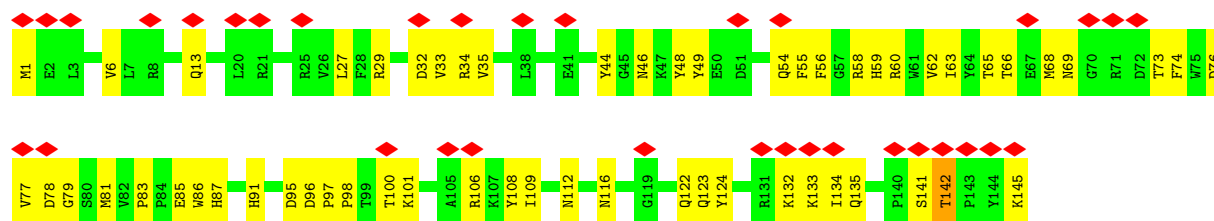
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain 1p: 

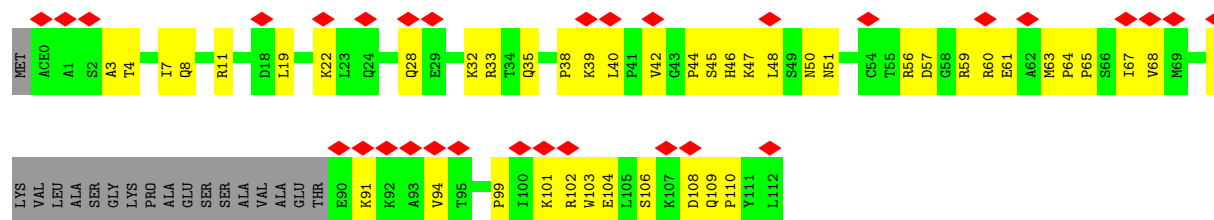


- Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

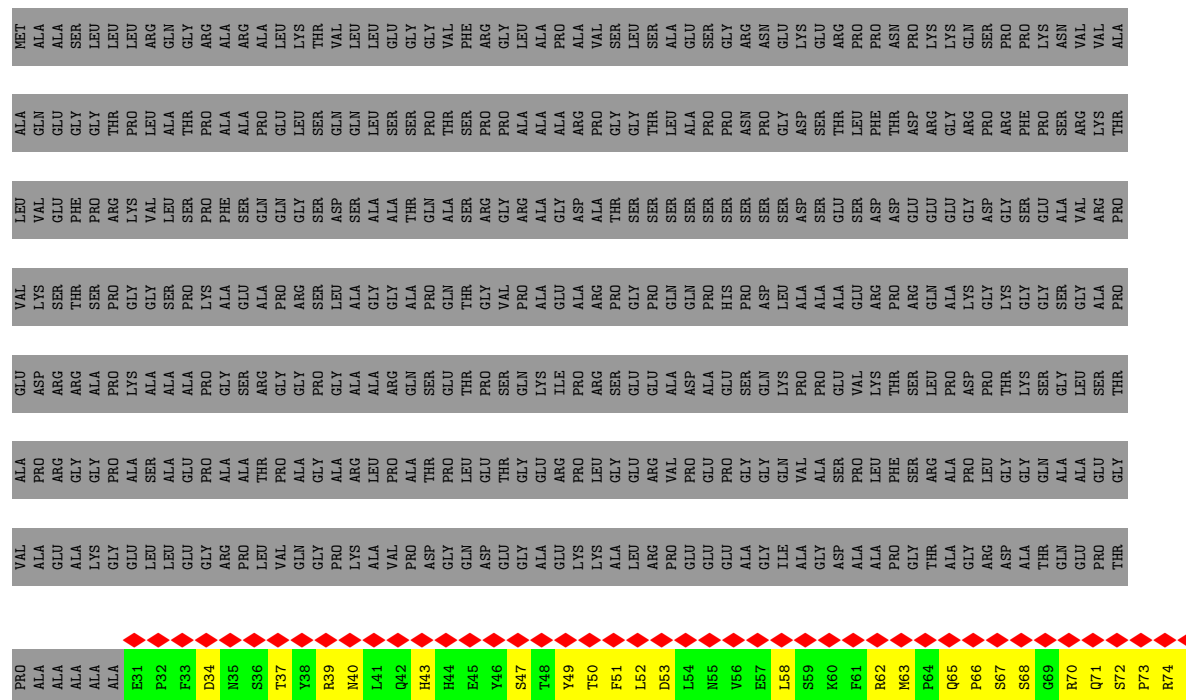
Chain 1q: 



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.599	Depositor
Minimum map value	-0.178	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.09	Depositor
Map size (Å)	425.6, 425.6, 425.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.33, 1.33, 1.33	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1A	0.18	0/930	0.50	1/1271 (0.1%)
2	1B	0.19	0/1273	0.44	0/1722
3	1C	0.16	0/1791	0.40	0/2439
4	1D	0.16	0/3545	0.38	0/4806
5	1E	0.17	0/1698	0.46	0/2311
6	1F	0.15	0/3401	0.36	0/4595
7	1G	0.14	0/5451	0.40	0/7387
8	1H	0.16	0/2566	0.38	0/3509
9	1I	0.19	0/1443	0.45	0/1952
10	1J	0.16	0/1364	0.44	0/1850
11	1K	0.17	0/751	0.43	0/1018
12	1L	0.16	0/4939	0.38	0/6718
13	1M	0.15	0/3713	0.33	0/5063
14	1N	0.16	0/2765	0.40	0/3758
15	1O	0.15	0/2650	0.42	1/3588 (0.0%)
16	1P	0.15	0/2828	0.39	0/3834
17	1Q	0.24	0/1070	0.59	2/1446 (0.1%)
18	1R	0.20	0/755	0.51	0/1018
19	1S	0.17	0/711	0.53	0/956
20	1T	0.16	0/701	0.47	0/946
20	1U	0.18	0/706	0.53	0/954
21	1V	0.19	0/946	0.52	0/1281
22	1W	0.24	0/995	0.67	1/1340 (0.1%)
23	1X	0.12	0/1436	0.30	0/1938
24	1Y	0.11	0/1037	0.35	0/1404
25	1Z	0.16	0/1199	0.42	0/1617
26	1a	0.17	0/577	0.35	0/777
27	1b	0.16	0/664	0.42	0/912
28	1c	0.16	0/430	0.43	0/581
29	1d	0.15	0/1024	0.40	0/1383
30	1e	0.13	0/836	0.33	0/1118
31	1f	0.21	0/499	0.48	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.18	0/858	0.47	0/1165
33	1h	0.15	0/1184	0.37	0/1603
34	1i	0.16	0/1131	0.44	0/1541
35	1j	0.13	0/627	0.38	0/858
36	1k	0.16	0/668	0.43	0/903
37	1l	0.16	0/1365	0.42	0/1867
38	1m	0.17	0/1092	0.41	0/1481
39	1n	0.12	0/1549	0.30	0/2098
40	1o	0.12	0/1069	0.33	0/1430
41	1p	0.11	0/1481	0.30	0/1997
42	1q	0.17	0/1253	0.42	0/1704
43	1r	0.16	0/782	0.48	0/1057
44	1s	0.13	0/394	0.38	0/533
All	All	0.16	0/68147	0.41	5/92402 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	1W	115	PRO	CA-N-CD	-9.65	98.49	112.00
17	1Q	113	PRO	CA-N-CD	-9.17	99.16	112.00
15	1O	165	PRO	CA-N-CD	-8.50	100.11	112.00
17	1Q	9	GLN	CB-CG-CD	5.09	121.25	112.60
1	1A	109	LYS	CA-CB-CG	5.04	124.17	114.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1A	916	0	950	70	0
2	1B	1242	0	1249	81	0
3	1C	1740	0	1691	112	0
4	1D	3452	0	3389	191	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	1E	1658	0	1662	93	0
6	1F	3325	0	3288	220	0
7	1G	5362	0	5387	304	0
8	1H	2504	0	2602	134	0
9	1I	1412	0	1364	95	0
10	1J	1339	0	1337	74	0
11	1K	750	0	798	45	0
12	1L	4818	0	4956	233	0
13	1M	3632	0	3836	172	0
14	1N	2712	0	2873	130	0
15	1O	2590	0	2555	128	0
16	1P	2751	0	2776	137	0
17	1Q	1047	0	1042	79	0
18	1R	741	0	704	47	0
19	1S	700	0	719	58	0
20	1T	689	0	687	49	0
20	1U	694	0	691	51	0
21	1V	927	0	972	77	0
22	1W	971	0	975	77	0
23	1X	1398	0	1378	73	0
24	1Y	1016	0	1020	20	0
25	1Z	1168	0	1161	68	0
26	1a	562	0	557	38	0
27	1b	643	0	645	25	0
28	1c	417	0	425	13	0
29	1d	996	0	990	31	0
30	1e	816	0	823	39	0
31	1f	487	0	496	21	0
32	1g	835	0	795	52	0
33	1h	1151	0	1164	54	0
34	1i	1100	0	1106	53	0
35	1j	601	0	546	39	0
36	1k	649	0	626	39	0
37	1l	1310	0	1204	65	0
38	1m	1062	0	1075	67	0
39	1n	1495	0	1434	76	0
40	1o	1045	0	1018	62	0
41	1p	1449	0	1416	61	0
42	1q	1212	0	1172	52	0
43	1r	767	0	791	52	0
44	1s	382	0	351	29	0
45	1A	47	0	71	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	1L	88	0	127	6	0
45	1N	51	0	82	3	0
45	1Y	82	0	118	9	0
46	1B	8	0	0	2	0
46	1F	8	0	0	1	0
46	1G	16	0	0	1	0
46	1I	16	0	0	4	0
47	1E	4	0	0	1	0
47	1G	4	0	0	3	0
48	1F	31	0	19	4	0
49	1G	1	0	0	0	0
50	1I	98	0	148	9	0
50	1J	35	0	44	0	0
50	1L	44	0	65	1	0
50	1f	46	0	69	2	0
51	1M	51	0	78	8	0
52	1N	77	0	98	2	0
52	1r	61	0	64	7	0
53	1O	32	0	12	3	0
54	1O	1	0	0	0	0
55	1P	48	0	26	7	0
56	1R	1	0	0	0	0
57	1W	37	0	0	0	0
57	1n	37	0	0	2	0
58	1l	15	0	27	1	0
All	All	67472	0	67744	3073	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 (3073) 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)
9:1I:119:CYS:HB2	46:1I:201:SF4:S2	2.02	0.98
12:1L:310:LEU:HA	12:1L:313:MET:HG3	1.48	0.95
12:1L:35:TYR:HH	34:1i:73:HIS:HE2	1.11	0.94
21:1V:43:TYR:HB3	21:1V:99:TRP:HH2	1.33	0.93
5:1E:111:ARG:HG3	5:1E:152:PRO:HD3	1.49	0.93
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.34	0.92
9:1I:43:ARG:HG2	43:1r:11:ARG:HE	1.35	0.92
43:1r:63:MET:HE3	43:1r:64:PRO:HD2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:68:HIS:CD2	18:1R:87:CYS:SG	2.63	0.90
7:1G:283:MET:HB3	7:1G:560:ILE:HB	1.53	0.89
16:1P:113:ILE:HD12	16:1P:114:PRO:HD3	1.55	0.89
2:1B:91:THR:HG21	4:1D:85:ARG:HD3	1.55	0.87
7:1G:59:ILE:HG22	7:1G:62:ALA:HB2	1.54	0.87
12:1L:128:MET:HE3	12:1L:251:THR:HG22	1.57	0.87
4:1D:163:ALA:H	8:1H:278:PRO:HA	1.40	0.85
12:1L:286:LEU:HD22	12:1L:411:MET:HE1	1.57	0.85
2:1B:69:MET:H	2:1B:69:MET:HE3	1.43	0.84
5:1E:121:GLN:HE22	5:1E:127:LYS:HA	1.43	0.84
9:1I:119:CYS:CB	46:1I:201:SF4:S2	2.65	0.84
6:1F:256:PHE:HZ	6:1F:272:MET:HA	1.42	0.83
6:1F:343:ILE:HD11	6:1F:425:GLU:HG2	1.62	0.82
18:1R:59:CYS:SG	18:1R:84:CYS:HB2	2.20	0.82
19:1S:62:PRO:HG2	19:1S:79:ASN:HA	1.60	0.82
20:1T:15:VAL:HG13	20:1T:54:MET:HE1	1.59	0.82
21:1V:91:ARG:NH1	21:1V:91:ARG:O	2.13	0.82
4:1D:162:GLY:HA3	8:1H:279:ARG:H	1.44	0.82
23:1X:94:GLN:HE22	26:1a:37:ARG:HE	1.26	0.81
14:1N:313:MET:H	14:1N:313:MET:HE2	1.44	0.81
20:1U:37:MET:SD	20:1U:38:LYS:NZ	2.52	0.81
38:1m:2:PHE:HD1	38:1m:3:PRO:HD2	1.43	0.81
2:1B:63:ALA:HA	2:1B:69:MET:HE1	1.63	0.81
7:1G:30:CYS:HB3	7:1G:35:MET:HB3	1.63	0.81
40:1o:106:ARG:HA	40:1o:109:GLN:HE22	1.46	0.81
44:1s:72:SER:OG	44:1s:75:HIS:ND1	2.15	0.80
8:1H:85:MET:HB3	8:1H:233:MET:HE3	1.64	0.79
19:1S:81:PHE:HE1	19:1S:85:GLN:HB2	1.47	0.79
8:1H:86:TRP:HA	8:1H:89:LEU:HD23	1.64	0.78
15:1O:247:PRO:O	15:1O:251:GLN:NE2	2.17	0.78
25:1Z:68:ARG:HE	25:1Z:72:MET:HE2	1.48	0.78
6:1F:365:CYS:HB2	46:1F:502:SF4:S2	2.24	0.77
38:1m:16:THR:HG23	38:1m:17:LEU:HD12	1.66	0.77
21:1V:37:ILE:HD12	21:1V:38:PRO:HD2	1.66	0.77
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.67	0.77
1:1A:52:SER:OG	1:1A:53:MET:N	2.16	0.77
7:1G:47:SER:OG	7:1G:48:VAL:N	2.16	0.77
5:1E:209:PRO:HA	6:1F:40:GLY:HA2	1.66	0.77
42:1q:60:ARG:HH12	42:1q:95:ASP:HA	1.50	0.76
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.66	0.76
7:1G:418:ARG:HD2	44:1s:75:HIS:HA	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:128:LEU:HD11	14:1N:213:LEU:HD13	1.66	0.75
6:1F:224:ASN:ND2	48:1F:501:FMN:O2	2.19	0.75
41:1p:78:GLU:HG3	41:1p:79:LYS:HG2	1.67	0.75
5:1E:162:GLU:OE1	6:1F:108:ARG:NH2	2.20	0.75
9:1I:19:ASP:HB3	50:1I:204:PC1:H131	1.69	0.75
30:1e:49:ILE:HD11	33:1h:118:GLY:HA3	1.69	0.75
38:1m:122:GLN:HB3	38:1m:125:ASN:HB3	1.69	0.75
6:1F:391:SER:OG	43:1r:48:LEU:O	2.03	0.75
7:1G:512:GLU:HA	7:1G:515:ARG:HE	1.51	0.74
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.20	0.74
31:1f:53:GLU:N	31:1f:53:GLU:OE1	2.20	0.74
25:1Z:5:LYS:HA	25:1Z:5:LYS:HE3	1.68	0.74
15:1O:116:LEU:HD23	15:1O:260:ARG:HG3	1.69	0.74
7:1G:45:ARG:HH22	7:1G:261:GLU:HG2	1.53	0.74
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	1.69	0.74
21:1V:19:PRO:HG2	21:1V:64:VAL:HG11	1.68	0.74
12:1L:532:ILE:HD11	37:1l:101:MET:HB3	1.69	0.74
4:1D:58:ALA:HB1	4:1D:62:LEU:HB3	1.70	0.74
12:1L:237:MET:HE3	12:1L:237:MET:HA	1.68	0.74
2:1B:139:ILE:HG22	2:1B:140:VAL:HG13	1.70	0.74
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	1.69	0.74
7:1G:168:GLY:HA2	7:1G:396:ARG:HH21	1.54	0.73
9:1I:108:ARG:NH1	17:1Q:70:MET:O	2.21	0.73
17:1Q:16:LYS:HE2	17:1Q:16:LYS:HA	1.68	0.73
20:1T:46:ASP:OD1	22:1W:64:ARG:NH2	2.21	0.73
16:1P:171:ILE:HG12	55:1P:501:NDP:H42N	1.68	0.73
20:1T:43:ASP:H	20:1T:46:ASP:HB2	1.53	0.73
21:1V:43:TYR:HB3	21:1V:99:TRP:CH2	2.21	0.73
23:1X:18:LYS:HA	26:1a:54:ILE:HD11	1.71	0.73
8:1H:141:SER:HB3	8:1H:290:TRP:HE1	1.53	0.73
12:1L:128:MET:HE1	12:1L:252:MET:HA	1.68	0.73
12:1L:359:MET:N	12:1L:359:MET:SD	2.62	0.72
7:1G:704:CYS:HB2	9:1I:104:ARG:H	1.52	0.72
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.21	0.72
14:1N:108:LEU:HB3	14:1N:161:SER:HB2	1.71	0.72
21:1V:57:MET:H	21:1V:57:MET:HE3	1.54	0.72
13:1M:318:ALA:HB2	13:1M:373:ILE:HG22	1.70	0.72
12:1L:407:TRP:HE1	37:1l:112:MET:HE1	1.55	0.72
19:1S:81:PHE:HD1	19:1S:82:SER:H	1.38	0.72
7:1G:362:TYR:OH	19:1S:55:ARG:NH2	2.23	0.72
12:1L:401:MET:HG3	12:1L:482:MET:HE2	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:111:LEU:HB2	8:1H:291:LYS:HE3	1.72	0.72
8:1H:67:SER:O	8:1H:69:SER:N	2.23	0.72
3:1C:189:GLU:HG2	16:1P:14:SER:HB3	1.72	0.71
22:1W:27:GLU:HA	22:1W:30:ARG:HB3	1.70	0.71
14:1N:120:GLN:HE21	14:1N:177:LYS:HE2	1.54	0.71
19:1S:17:GLU:HB3	19:1S:67:ARG:HB3	1.72	0.71
9:1L:70:TYR:HE2	18:1R:87:CYS:HA	1.55	0.71
12:1L:276:MET:HA	12:1L:279:CYS:HB2	1.72	0.71
21:1V:94:LEU:HB3	21:1V:95:ARG:HH12	1.55	0.71
7:1G:315:VAL:HG12	7:1G:521:VAL:HB	1.72	0.71
8:1H:102:VAL:HG21	8:1H:154:LEU:HD21	1.71	0.71
24:1Y:43:LYS:NZ	45:1Y:201:3PE:O31	2.24	0.71
42:1q:68:MET:HE2	42:1q:68:MET:HA	1.73	0.71
1:1A:33:LYS:O	2:1B:81:ARG:NH2	2.24	0.71
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.73	0.71
20:1T:47:GLN:NE2	20:1T:67:ALA:O	2.24	0.71
20:1U:22:TYR:HE1	36:1k:43:PRO:HB2	1.56	0.71
4:1D:101:PRO:O	4:1D:105:ARG:NH1	2.23	0.71
5:1E:185:GLY:O	5:1E:187:ARG:NH2	2.24	0.71
7:1G:24:THR:HG23	7:1G:28:GLN:HB2	1.71	0.71
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.73	0.71
19:1S:30:GLN:NE2	19:1S:34:ASP:OD1	2.21	0.71
21:1V:27:TYR:HE2	21:1V:54:LYS:HB3	1.55	0.71
3:1C:61:LEU:HB3	3:1C:123:VAL:HG11	1.72	0.70
15:1O:165:PRO:HD2	15:1O:165:PRO:O	1.90	0.70
36:1k:38:ARG:HH21	36:1k:40:LEU:HG	1.56	0.70
20:1U:32:VAL:HG22	20:1U:74:GLN:HB2	1.73	0.70
39:1n:137:LYS:O	39:1n:137:LYS:NZ	2.24	0.70
36:1k:48:GLU:OE1	39:1n:33:ARG:NE	2.23	0.70
34:1i:107:ASP:OD2	40:1o:70:ARG:NH2	2.24	0.70
3:1C:183:VAL:O	22:1W:101:THR:OG1	2.07	0.70
18:1R:19:ASP:O	18:1R:25:ARG:NH2	2.25	0.70
34:1i:13:GLN:HE22	39:1n:156:ALA:HB3	1.55	0.70
4:1D:183:ARG:HE	4:1D:207:LEU:HD23	1.57	0.70
7:1G:11:VAL:HG23	7:1G:77:TRP:H	1.55	0.70
2:1B:57:VAL:HG13	4:1D:189:MET:HE1	1.73	0.70
16:1P:46:ILE:HG22	16:1P:48:PRO:HD3	1.74	0.70
37:1l:9:PHE:O	37:1l:26:LYS:NZ	2.24	0.70
43:1r:104:GLU:OE2	43:1r:104:GLU:N	2.22	0.70
3:1C:39:GLN:HB3	3:1C:51:PHE:HB2	1.71	0.70
12:1L:161:ARG:HG3	12:1L:164:ALA:H	1.57	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:317:VAL:HG13	16:1P:318:LEU:HD22	1.72	0.69
23:1X:129:LYS:HD3	27:1b:65:VAL:HG13	1.74	0.69
23:1X:72:GLN:OE1	23:1X:72:GLN:N	2.25	0.69
29:1d:46:ASN:HB3	29:1d:51:ARG:HB2	1.74	0.69
38:1m:112:GLU:OE1	38:1m:112:GLU:N	2.18	0.69
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.73	0.69
13:1M:307:TRP:NE1	38:1m:127:SER:OG	2.26	0.69
14:1N:44:LEU:HB3	14:1N:122:ILE:HG21	1.75	0.69
7:1G:43:HIS:HB3	7:1G:46:LEU:HB3	1.73	0.69
11:1K:47:ILE:HG12	14:1N:79:LEU:HD13	1.73	0.69
30:1e:88:GLU:HB3	30:1e:90:LYS:HE3	1.75	0.69
23:1X:124:LEU:HD21	25:1Z:70:ALA:HB2	1.74	0.69
5:1E:36:LYS:HD3	44:1s:62:ARG:HG3	1.74	0.69
14:1N:154:MET:HE1	14:1N:191:THR:HB	1.75	0.69
38:1m:2:PHE:CD1	38:1m:3:PRO:HD2	2.28	0.69
16:1P:243:GLN:N	16:1P:243:GLN:OE1	2.26	0.69
36:1k:31:VAL:HG21	39:1n:38:TYR:HB2	1.72	0.68
32:1g:113:PHE:H	41:1p:158:GLN:HE22	1.39	0.68
42:1q:122:GLN:OE1	42:1q:122:GLN:N	2.24	0.68
7:1G:365:ASN:HB3	7:1G:488:LYS:HZ3	1.57	0.68
19:1S:82:SER:OG	19:1S:84:ASP:OD1	2.12	0.68
4:1D:66:MET:HE1	4:1D:68:LEU:HD23	1.74	0.68
6:1F:299:PRO:HD3	6:1F:306:LEU:HA	1.76	0.68
6:1F:307:ILE:HD13	6:1F:312:CYS:HB3	1.76	0.68
13:1M:208:PRO:HG3	13:1M:216:LEU:HD22	1.73	0.68
4:1D:425:PHE:HA	4:1D:428:VAL:HG12	1.76	0.68
23:1X:69:PHE:HA	23:1X:72:GLN:HE22	1.58	0.68
4:1D:405:MET:HB3	4:1D:417:ILE:HG12	1.75	0.68
12:1L:142:ILE:HD13	13:1M:370:PRO:HB2	1.75	0.68
20:1U:34:SER:HB2	20:1U:40:LEU:HD21	1.75	0.68
38:1m:30:LYS:HD3	38:1m:30:LYS:N	2.09	0.68
3:1C:204:GLU:HA	17:1Q:50:ASN:HD22	1.57	0.68
9:1I:99:ARG:H	9:1I:104:ARG:HG2	1.57	0.68
13:1M:422:HIS:HD2	38:1m:59:ILE:H	1.40	0.68
14:1N:313:MET:HE2	14:1N:313:MET:N	2.08	0.68
7:1G:38:PRO:HG2	7:1G:90:ARG:HD3	1.74	0.68
25:1Z:90:ASN:ND2	25:1Z:123:GLU:O	2.26	0.68
1:1A:109:LYS:HD2	1:1A:110:GLY:N	2.08	0.68
2:1B:107:MET:O	2:1B:111:ARG:NH1	2.27	0.68
7:1G:276:ARG:HB2	7:1G:680:ALA:HB1	1.76	0.68
15:1O:312:VAL:HG11	28:1c:2:PHE:HB2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:43:ASP:OD1	20:1T:46:ASP:N	2.27	0.68
7:1G:352:ALA:HB1	7:1G:652:VAL:HG11	1.76	0.67
20:1T:54:MET:HE3	20:1T:76:ILE:HG21	1.76	0.67
20:1U:70:LEU:HD11	20:1U:79:TYR:HB3	1.75	0.67
26:1a:67:GLU:OE2	26:1a:67:GLU:N	2.24	0.67
42:1q:85:GLU:OE2	42:1q:85:GLU:N	2.25	0.67
43:1r:32:LYS:O	43:1r:35:GLN:NE2	2.27	0.67
8:1H:28:LEU:O	8:1H:32:GLN:HG3	1.94	0.67
8:1H:194:ASN:HB3	8:1H:201:THR:HG21	1.75	0.67
8:1H:253:GLU:HA	26:1a:21:MET:HE1	1.76	0.67
4:1D:228:MET:HB3	4:1D:229:LEU:HD22	1.77	0.67
9:1I:133:GLU:N	9:1I:133:GLU:OE1	2.26	0.67
19:1S:39:ARG:NH1	19:1S:83:ALA:O	2.27	0.67
1:1A:1:FME:HE2	25:1Z:134:LEU:HD11	1.76	0.67
10:1J:71:THR:OG1	11:1K:27:MET:SD	2.52	0.67
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.58	0.67
10:1J:57:PHE:HA	10:1J:61:LEU:HB2	1.77	0.67
14:1N:88:LYS:HG2	14:1N:148:SER:HB2	1.76	0.67
9:1I:14:MET:HE2	9:1I:14:MET:HA	1.77	0.67
12:1L:345:SER:O	12:1L:349:SER:OG	2.12	0.67
38:1m:3:PRO:HA	38:1m:4:LYS:HE2	1.77	0.67
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	1.77	0.66
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.77	0.66
2:1B:66:ARG:HD3	9:1I:48:ILE:HG12	1.78	0.66
4:1D:115:GLU:HB2	4:1D:194:ILE:HB	1.77	0.66
6:1F:363:THR:HG21	7:1G:97:LEU:HG	1.77	0.66
9:1I:97:GLU:OE2	9:1I:107:THR:HB	1.95	0.66
21:1V:64:VAL:HA	21:1V:67:LEU:HB2	1.76	0.66
39:1n:30:CYS:HB3	39:1n:35:LYS:HB3	1.78	0.66
3:1C:66:ASP:HB3	21:1V:85:ASN:HB3	1.75	0.66
12:1L:387:THR:OG1	12:1L:461:SER:O	2.13	0.66
13:1M:129:THR:HG21	13:1M:235:LEU:HD11	1.78	0.66
5:1E:195:PRO:HD3	6:1F:266:CYS:SG	2.35	0.66
10:1J:59:ILE:HD11	11:1K:64:LEU:HD21	1.78	0.66
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.77	0.66
9:1I:45:PRO:HB2	9:1I:47:THR:HG23	1.76	0.66
23:1X:34:GLN:N	23:1X:34:GLN:OE1	2.27	0.66
45:1L:701:3PE:H231	37:1l:88:ARG:HG2	1.77	0.66
22:1W:111:GLU:OE2	22:1W:111:GLU:N	2.27	0.66
3:1C:35:LYS:HE2	21:1V:98:PRO:HA	1.78	0.66
4:1D:239:THR:HG23	4:1D:293:CYS:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:194:LEU:HD23	14:1N:201:THR:HG21	1.77	0.66
33:1h:34:ILE:HG13	33:1h:35:PRO:HD3	1.78	0.66
39:1n:158:LYS:NZ	39:1n:159:GLU:O	2.23	0.66
8:1H:105:MET:HE3	8:1H:233:MET:HE1	1.78	0.66
15:1O:126:ARG:NH1	15:1O:206:TYR:OH	2.29	0.66
34:1i:24:ASP:OD2	39:1n:124:TRP:NE1	2.27	0.66
8:1H:31:MET:HE1	8:1H:272:TRP:CD1	2.31	0.66
8:1H:206:GLU:HG2	8:1H:207:LEU:HD23	1.78	0.66
13:1M:134:THR:HB	14:1N:302:LEU:HD12	1.76	0.66
14:1N:266:ILE:HG22	14:1N:270:MET:HE2	1.78	0.66
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.61	0.65
13:1M:191:SER:HB2	51:1M:501:PGT:H31	1.77	0.65
14:1N:88:LYS:NZ	14:1N:89:MET:O	2.29	0.65
16:1P:240:ASP:HA	16:1P:243:GLN:HE22	1.60	0.65
1:1A:107:THR:OG1	1:1A:108:GLN:OE1	2.15	0.65
12:1L:366:MET:HE3	12:1L:443:ILE:HD12	1.78	0.65
22:1W:48:HIS:O	22:1W:51:GLN:NE2	2.29	0.65
2:1B:125:TYR:HE1	9:1I:88:PRO:HB2	1.61	0.65
7:1G:534:ARG:NH1	7:1G:556:MET:O	2.30	0.65
33:1h:134:ASP:O	33:1h:138:LYS:NZ	2.30	0.65
20:1U:36:PHE:H	20:1U:71:MET:HE1	1.62	0.65
26:1a:57:VAL:HG13	26:1a:59:ARG:HG2	1.77	0.65
5:1E:171:GLU:HA	5:1E:174:ASP:HB2	1.79	0.65
14:1N:325:LEU:HD12	52:1N:402:CDL:H732	1.77	0.65
25:1Z:7:LYS:H	43:1r:39:LYS:HB3	1.62	0.65
38:1m:60:GLU:OE1	38:1m:60:GLU:N	2.19	0.65
8:1H:67:SER:HG	10:1J:28:TYR:HH	1.43	0.65
9:1I:7:MET:HA	9:1I:7:MET:HE3	1.78	0.65
16:1P:171:ILE:H	55:1P:501:NDP:H71N	1.43	0.65
23:1X:64:GLN:NE2	23:1X:68:ASP:OD2	2.29	0.65
13:1M:190:TRP:HA	13:1M:193:ILE:HD13	1.77	0.65
36:1k:40:LEU:HD11	39:1n:45:ALA:HB2	1.77	0.65
1:1A:3:ILE:O	1:1A:6:THR:OG1	2.14	0.65
12:1L:226:GLN:HG2	12:1L:314:MET:HE1	1.77	0.65
13:1M:178:ILE:HD13	41:1p:81:ILE:HD13	1.79	0.65
24:1Y:43:LYS:NZ	45:1Y:201:3PE:O11	2.29	0.65
32:1g:85:MET:H	32:1g:85:MET:HE2	1.61	0.65
22:1W:62:LYS:NZ	22:1W:106:PHE:O	2.29	0.65
37:1l:129:GLY:O	40:1o:97:ARG:NH2	2.30	0.65
5:1E:151:ALA:HB3	5:1E:163:ASP:HA	1.79	0.64
21:1V:57:MET:O	21:1V:61:GLU:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:18:THR:HG23	30:1e:19:ILE:HG23	1.79	0.64
2:1B:84:ASP:OD1	8:1H:58:LYS:NZ	2.29	0.64
6:1F:261:HIS:HB3	6:1F:288:ILE:HD11	1.79	0.64
7:1G:409:ILE:HG23	7:1G:422:LEU:HD13	1.79	0.64
10:1J:110:GLU:HG2	10:1J:112:GLU:H	1.63	0.64
12:1L:42:TYR:HH	34:1i:66:HIS:HD1	1.44	0.64
21:1V:54:LYS:NZ	21:1V:70:GLN:O	2.31	0.64
5:1E:163:ASP:HB2	5:1E:187:ARG:H	1.61	0.64
6:1F:297:VAL:HG22	6:1F:336:VAL:HA	1.79	0.64
22:1W:70:ASN:HD22	22:1W:82:LEU:HD11	1.63	0.64
25:1Z:48:TRP:O	25:1Z:52:LYS:NZ	2.29	0.64
35:1j:69:ASP:OD2	40:1o:113:ARG:NH1	2.31	0.64
4:1D:300:ARG:NH2	4:1D:422:ASP:OD1	2.31	0.64
6:1F:99:GLU:HG3	6:1F:104:THR:HB	1.79	0.64
7:1G:249:ARG:HE	7:1G:251:LEU:HD11	1.62	0.64
12:1L:577:VAL:HA	45:1Y:201:3PE:H331	1.78	0.64
22:1W:30:ARG:NH1	22:1W:30:ARG:O	2.30	0.64
4:1D:326:ASP:OD1	7:1G:127:ARG:NH2	2.31	0.64
17:1Q:69:LEU:HA	18:1R:27:ARG:HH12	1.63	0.64
22:1W:24:ASP:OD1	22:1W:25:MET:N	2.30	0.64
22:1W:36:TYR:OH	22:1W:64:ARG:NH1	2.31	0.64
15:1O:265:ASN:HD22	15:1O:268:GLU:H	1.44	0.64
30:1e:44:HIS:HD2	33:1h:129:ASP:HA	1.63	0.64
3:1C:210:ARG:NH2	7:1G:34:GLY:O	2.30	0.64
4:1D:55:HIS:NE2	8:1H:127:TYR:OH	2.30	0.64
6:1F:189:GLU:HG3	6:1F:222:VAL:HG21	1.79	0.64
7:1G:190:MET:HE2	7:1G:190:MET:HA	1.79	0.64
18:1R:37:GLU:CD	18:1R:37:GLU:H	2.06	0.64
22:1W:115:PRO:O	22:1W:121:LYS:NZ	2.30	0.64
2:1B:54:CYS:HB3	4:1D:108:TYR:HB2	1.80	0.64
6:1F:107:ASP:HA	6:1F:110:ILE:HG22	1.80	0.64
6:1F:256:PHE:HD1	6:1F:279:LEU:HD11	1.62	0.64
6:1F:266:CYS:SG	6:1F:268:VAL:HG23	2.38	0.64
3:1C:41:GLN:HE21	43:1r:65:PRO:HB2	1.63	0.63
6:1F:299:PRO:HG3	6:1F:307:ILE:HG13	1.79	0.63
13:1M:335:GLU:OE2	13:1M:335:GLU:N	2.22	0.63
42:1q:106:ARG:HB2	42:1q:109:ILE:HG13	1.78	0.63
4:1D:193:TYR:HE1	4:1D:201:GLN:H	1.47	0.63
7:1G:164:SER:OG	7:1G:165:GLU:OE1	2.15	0.63
8:1H:281:ARG:HB3	8:1H:284:GLN:HG3	1.80	0.63
9:1I:109:TYR:OH	46:1I:202:SF4:S1	2.56	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:146:LYS:O	15:1O:146:LYS:NZ	2.28	0.63
20:1T:75:GLU:OE1	20:1T:75:GLU:N	2.28	0.63
44:1s:58:LEU:HG	44:1s:62:ARG:HH12	1.61	0.63
7:1G:540:ASP:H	42:1q:145:LYS:HE3	1.63	0.63
9:1I:65:HIS:HD2	9:1I:113:MET:HE1	1.63	0.63
16:1P:115:HIS:HB2	16:1P:155:GLU:HG3	1.80	0.63
22:1W:30:ARG:NH1	22:1W:34:GLU:OE2	2.31	0.63
25:1Z:127:LEU:HD13	30:1e:97:HIS:CE1	2.32	0.63
34:1i:3:TYR:HB2	34:1i:8:LYS:HD2	1.81	0.63
3:1C:116:PRO:HD3	22:1W:20:ILE:HG22	1.80	0.63
17:1Q:18:ASP:HA	17:1Q:98:LYS:HA	1.80	0.63
1:1A:54:LYS:NZ	1:1A:115:GLU:O	2.29	0.63
4:1D:65:VAL:HG23	4:1D:77:ASP:HB3	1.80	0.63
7:1G:620:ARG:NH1	7:1G:633:TYR:OH	2.31	0.63
15:1O:83:TYR:HH	53:1O:401:GTP:HO3'	1.46	0.63
17:1Q:95:PHE:HA	17:1Q:98:LYS:HD3	1.80	0.63
32:1g:94:GLU:HB3	41:1p:8:VAL:HG21	1.79	0.63
43:1r:108:ASP:OD1	43:1r:109:GLN:N	2.32	0.63
4:1D:259:MET:HA	4:1D:259:MET:HE3	1.80	0.63
5:1E:143:GLU:HG3	6:1F:349:ARG:HH22	1.64	0.63
17:1Q:75:THR:HG22	17:1Q:77:ASP:H	1.64	0.63
6:1F:261:HIS:HE1	6:1F:337:MET:HG2	1.62	0.63
36:1k:18:TYR:HE1	36:1k:21:TRP:HB2	1.63	0.63
4:1D:375:GLY:O	4:1D:392:LYS:N	2.27	0.63
7:1G:274:LEU:HD11	7:1G:567:THR:HG21	1.81	0.63
13:1M:270:ILE:O	13:1M:274:SER:OG	2.16	0.63
12:1L:217:LEU:HD13	12:1L:277:THR:HG22	1.80	0.63
16:1P:113:ILE:HD12	16:1P:114:PRO:CD	2.26	0.63
17:1Q:57:MET:HE2	17:1Q:57:MET:HA	1.80	0.63
20:1U:36:PHE:HA	20:1U:40:LEU:HD23	1.81	0.63
22:1W:92:GLU:HA	22:1W:97:TRP:HE3	1.63	0.63
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.32	0.63
6:1F:166:ALA:HB3	6:1F:171:TYR:HB3	1.81	0.62
7:1G:121:MET:HA	7:1G:121:MET:HE3	1.81	0.62
7:1G:194:GLU:HG2	7:1G:195:LEU:HD22	1.80	0.62
8:1H:289:LEU:HA	8:1H:293:PHE:HB2	1.82	0.62
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.31	0.62
23:1X:46:ARG:NH1	25:1Z:76:GLN:OE1	2.32	0.62
27:1b:30:ILE:O	27:1b:33:SER:OG	2.17	0.62
33:1h:55:ILE:HD12	33:1h:56:PRO:HD2	1.81	0.62
3:1C:50:ILE:HB	3:1C:107:VAL:HG12	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:303:GLU:O	4:1D:307:SER:OG	2.15	0.62
23:1X:170:THR:OG1	23:1X:171:MET:SD	2.57	0.62
39:1n:83:GLU:CD	39:1n:83:GLU:H	2.07	0.62
6:1F:24:ASN:HB2	6:1F:29:HIS:CE1	2.34	0.62
7:1G:688:VAL:O	7:1G:692:THR:OG1	2.16	0.62
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.32	0.62
9:1I:128:VAL:HG12	18:1R:68:HIS:HB2	1.81	0.62
11:1K:91:GLN:OE1	11:1K:91:GLN:N	2.29	0.62
12:1L:314:MET:HA	12:1L:317:ILE:HG22	1.81	0.62
16:1P:10:LYS:NZ	17:1Q:63:GLU:OE1	2.29	0.62
41:1p:10:PRO:HD2	41:1p:108:ARG:HD2	1.81	0.62
2:1B:81:ARG:HE	8:1H:61:LEU:HD11	1.64	0.62
22:1W:89:GLU:OE1	22:1W:89:GLU:N	2.32	0.62
3:1C:49:GLU:HB3	3:1C:108:LYS:HZ2	1.64	0.62
7:1G:318:ILE:HG13	7:1G:522:LEU:HD11	1.81	0.62
23:1X:24:LEU:HB3	25:1Z:71:LEU:HD11	1.82	0.62
6:1F:179:ARG:HB3	44:1s:51:PHE:HE2	1.64	0.62
7:1G:199:ILE:HD13	7:1G:208:LEU:HD22	1.80	0.62
7:1G:695:ILE:HG13	7:1G:696:GLN:H	1.65	0.62
11:1K:5:TYR:HE1	11:1K:46:LEU:HB3	1.65	0.62
12:1L:294:THR:O	12:1L:524:ASN:ND2	2.32	0.62
13:1M:232:ALA:O	13:1M:237:LYS:NZ	2.32	0.62
16:1P:90:VAL:HG12	16:1P:128:LYS:HB2	1.80	0.62
21:1V:54:LYS:HA	21:1V:57:MET:HE1	1.82	0.62
26:1a:1:MET:N	26:1a:1:MET:SD	2.70	0.62
38:1m:4:LYS:HE2	38:1m:4:LYS:N	2.15	0.62
1:1A:8:LEU:O	1:1A:12:THR:HG23	1.99	0.62
16:1P:167:LYS:NZ	16:1P:228:PHE:O	2.28	0.62
2:1B:171:LYS:HB3	2:1B:174:ARG:HB3	1.82	0.62
4:1D:78:PRO:HG3	4:1D:402:LEU:HD12	1.80	0.62
7:1G:338:VAL:HB	7:1G:609:MET:HE1	1.81	0.62
1:1A:70:ALA:HB2	10:1J:59:ILE:HG21	1.81	0.61
11:1K:8:ILE:H	11:1K:8:ILE:HD12	1.65	0.61
16:1P:116:ALA:O	16:1P:119:GLN:NE2	2.33	0.61
23:1X:12:LEU:HD13	25:1Z:85:GLN:HB2	1.80	0.61
28:1c:23:THR:O	28:1c:27:LEU:N	2.29	0.61
13:1M:334:TYR:O	13:1M:338:HIS:N	2.32	0.61
16:1P:186:ARG:HG3	16:1P:187:TRP:HD1	1.64	0.61
38:1m:52:ASP:HB3	38:1m:55:ARG:HB2	1.81	0.61
6:1F:228:VAL:O	6:1F:231:SER:OG	2.18	0.61
12:1L:156:GLY:O	13:1M:416:ARG:NH2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:187:MET:HE2	14:1N:187:MET:HA	1.81	0.61
4:1D:261:ARG:NH1	4:1D:268:ASP:OD2	2.34	0.61
10:1J:4:TYR:HB2	10:1J:7:PHE:HB2	1.81	0.61
51:1M:501:PGT:O4P	51:1M:501:PGT:O6	2.18	0.61
14:1N:211:MET:HG2	14:1N:251:MET:HG3	1.82	0.61
3:1C:53:HIS:ND1	3:1C:55:ASP:OD2	2.34	0.61
8:1H:203:GLY:HA3	8:1H:207:LEU:HB2	1.81	0.61
9:1I:12:MET:HE2	9:1I:12:MET:HA	1.81	0.61
14:1N:207:ILE:HG22	14:1N:211:MET:HE1	1.83	0.61
23:1X:21:SER:HB2	26:1a:47:LEU:HD12	1.83	0.61
23:1X:72:GLN:HA	23:1X:75:ARG:HE	1.66	0.61
32:1g:23:THR:OG1	32:1g:24:ILE:N	2.33	0.61
32:1g:94:GLU:HA	32:1g:97:VAL:HG12	1.81	0.61
40:1o:61:TYR:HA	40:1o:64:GLN:HE22	1.65	0.61
6:1F:302:SER:HB3	6:1F:350:LEU:HD21	1.81	0.61
8:1H:170:GLU:OE1	23:1X:97:ARG:NH2	2.33	0.61
12:1L:364:LYS:NZ	36:1k:59:ASN:OD1	2.34	0.61
23:1X:129:LYS:NZ	27:1b:65:VAL:O	2.31	0.61
32:1g:116:ASN:OD1	32:1g:117:LYS:N	2.34	0.61
3:1C:40:VAL:HG23	43:1r:68:VAL:HG23	1.82	0.61
3:1C:96:LEU:HB2	3:1C:105:ILE:HB	1.82	0.61
4:1D:283:PHE:HA	4:1D:309:ARG:HH21	1.65	0.61
6:1F:133:ALA:HA	6:1F:174:ASP:H	1.66	0.61
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.81	0.61
20:1T:12:LYS:HE3	20:1T:16:LEU:HD11	1.83	0.61
39:1n:30:CYS:O	39:1n:32:HIS:N	2.33	0.61
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.17	0.61
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.34	0.61
17:1Q:58:GLU:OE1	17:1Q:58:GLU:N	2.19	0.61
29:1d:99:GLU:OE2	29:1d:99:GLU:N	2.21	0.61
37:1l:98:TRP:HA	37:1l:101:MET:HB2	1.82	0.61
4:1D:46:ASN:HB3	4:1D:67:GLU:HB3	1.81	0.61
4:1D:369:ALA:O	4:1D:372:GLY:N	2.34	0.61
7:1G:194:GLU:OE1	7:1G:385:ARG:NH2	2.34	0.61
13:1M:188:ASN:O	13:1M:188:ASN:ND2	2.24	0.61
15:1O:219:GLU:OE1	15:1O:219:GLU:N	2.30	0.61
19:1S:18:ILE:HG23	19:1S:52:ILE:HG23	1.82	0.61
21:1V:91:ARG:HH12	21:1V:95:ARG:HG2	1.65	0.61
6:1F:95:VAL:HG22	6:1F:228:VAL:HG11	1.83	0.61
7:1G:163:ALA:HA	7:1G:167:ALA:HB3	1.83	0.61
12:1L:573:MET:HA	12:1L:576:MET:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:12:LYS:HE2	20:1T:32:VAL:HG23	1.83	0.61
20:1U:72:CYS:O	20:1U:76:ILE:N	2.33	0.61
20:1U:35:HIS:CE1	20:1U:71:MET:HE2	2.36	0.60
22:1W:115:PRO:O	22:1W:115:PRO:HD2	2.01	0.60
6:1F:19:ASP:HA	6:1F:241:TRP:HZ2	1.66	0.60
7:1G:46:LEU:HD21	7:1G:161:ARG:HB2	1.83	0.60
9:1I:172:ASP:OD2	9:1I:176:ARG:NH2	2.34	0.60
12:1L:71:LEU:N	12:1L:74:VAL:O	2.30	0.60
16:1P:30:LEU:HA	16:1P:207:ILE:HD11	1.82	0.60
16:1P:134:HIS:HB2	16:1P:149:LYS:HE3	1.82	0.60
18:1R:59:CYS:O	18:1R:68:HIS:NE2	2.34	0.60
22:1W:44:PRO:HD3	22:1W:60:ARG:HH21	1.66	0.60
22:1W:91:GLU:OE1	22:1W:91:GLU:N	2.33	0.60
27:1b:12:TRP:HD1	27:1b:19:VAL:HG11	1.66	0.60
30:1e:85:LEU:HD11	30:1e:91:TYR:HB3	1.83	0.60
34:1i:103:ILE:HG22	41:1p:17:PRO:HB3	1.83	0.60
6:1F:91:LYS:HB3	6:1F:131:ALA:HA	1.82	0.60
5:1E:201:SER:OG	6:1F:26:TYR:OH	2.19	0.60
7:1G:36:GLN:HE22	17:1Q:49:VAL:HG13	1.67	0.60
8:1H:181:LEU:HA	8:1H:184:MET:HB2	1.84	0.60
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD21	1.83	0.60
39:1n:67:GLU:HA	39:1n:70:PHE:HB3	1.84	0.60
3:1C:58:ILE:H	3:1C:58:ILE:HD12	1.65	0.60
7:1G:12:PHE:HA	7:1G:17:SER:HA	1.83	0.60
7:1G:285:ARG:NH1	7:1G:289:GLY:O	2.34	0.60
33:1h:98:ALA:HB2	41:1p:81:ILE:HD11	1.82	0.60
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.35	0.60
9:1I:32:ARG:NH1	50:1I:204:PC1:O12	2.34	0.60
11:1K:2:PRO:HD3	30:1e:72:MET:HE1	1.82	0.60
13:1M:278:ARG:HB3	13:1M:278:ARG:HH11	1.66	0.60
16:1P:64:ASP:HB3	16:1P:67:GLN:HG2	1.84	0.60
16:1P:176:ASP:OD1	16:1P:180:ASN:ND2	2.34	0.60
25:1Z:27:ARG:NH1	25:1Z:28:ARG:O	2.35	0.60
26:1a:13:ALA:O	26:1a:17:PHE:HB2	2.00	0.60
6:1F:261:HIS:ND1	6:1F:337:MET:HA	2.16	0.60
7:1G:382:THR:HB	7:1G:454:GLY:HA3	1.82	0.60
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.32	0.60
12:1L:550:SER:HB3	13:1M:275:ILE:HG23	1.82	0.60
29:1d:106:LYS:HA	29:1d:106:LYS:HE3	1.84	0.60
4:1D:246:THR:HB	21:1V:12:GLY:HA3	1.84	0.60
7:1G:432:ILE:HD13	7:1G:437:HIS:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:65:HIS:ND1	9:1I:133:GLU:HG3	2.17	0.60
12:1L:324:LEU:HB3	12:1L:395:ILE:HD11	1.83	0.60
15:1O:307:GLY:O	15:1O:320:LYS:NZ	2.30	0.60
19:1S:74:LYS:NZ	19:1S:75:ASN:O	2.23	0.60
35:1j:61:ASP:HB3	35:1j:66:ILE:HB	1.83	0.60
37:1l:30:ARG:NH1	38:1m:34:GLU:OE2	2.34	0.60
2:1B:39:TRP:HA	2:1B:42:ARG:HH11	1.67	0.60
7:1G:575:ASN:HD21	7:1G:579:ARG:HG2	1.67	0.60
10:1J:125:TRP:HB2	25:1Z:137:THR:HG21	1.84	0.60
12:1L:306:THR:O	12:1L:310:LEU:HD12	2.01	0.60
12:1L:503:GLU:O	12:1L:507:THR:OG1	2.19	0.60
22:1W:62:LYS:HG2	22:1W:107:PHE:HE1	1.66	0.60
38:1m:44:ARG:HH21	39:1n:148:PRO:HB3	1.67	0.60
7:1G:534:ARG:NH2	7:1G:558:ASP:OD1	2.35	0.59
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.84	0.59
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.84	0.59
39:1n:139:LEU:O	39:1n:143:THR:OG1	2.18	0.59
1:1A:56:PHE:HZ	11:1K:75:LEU:HB3	1.67	0.59
6:1F:56:ILE:H	6:1F:56:ILE:HD12	1.67	0.59
6:1F:82:MET:HB3	6:1F:211:ALA:HB1	1.83	0.59
6:1F:99:GLU:OE1	6:1F:108:ARG:N	2.35	0.59
1:1A:90:MET:HE2	10:1J:154:VAL:HG13	1.84	0.59
6:1F:298:ILE:HB	6:1F:335:ILE:HB	1.84	0.59
14:1N:179:MET:HE3	14:1N:179:MET:HA	1.84	0.59
34:1i:123:PRO:HG2	34:1i:125:GLN:HE22	1.67	0.59
42:1q:13:GLN:HE21	42:1q:34:ARG:HA	1.68	0.59
2:1B:176:TRP:HA	2:1B:179:ARG:HE	1.68	0.59
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.84	0.59
13:1M:40:SER:O	33:1h:80:TYR:OH	2.18	0.59
14:1N:308:THR:HG22	14:1N:310:ASN:H	1.68	0.59
2:1B:59:MET:HB2	2:1B:116:MET:HE1	1.84	0.59
23:1X:68:ASP:OD1	23:1X:71:ARG:NH2	2.35	0.59
32:1g:112:CYS:SG	32:1g:113:PHE:N	2.76	0.59
5:1E:137:PHE:HE1	5:1E:176:LEU:HD23	1.67	0.59
7:1G:54:MET:HE1	7:1G:94:MET:HE2	1.84	0.59
13:1M:17:MET:HG2	31:1f:11:TRP:HZ2	1.68	0.59
18:1R:80:LYS:HZ1	18:1R:83:THR:HG22	1.68	0.59
19:1S:88:ARG:O	19:1S:88:ARG:NE	2.25	0.59
35:1j:69:ASP:OD1	40:1o:117:ARG:NH1	2.35	0.59
8:1H:81:LEU:HD21	8:1H:111:LEU:HB3	1.83	0.59
12:1L:401:MET:HE1	37:1l:126:GLN:HG2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:54:TYR:HA	16:1P:57:MET:HG2	1.84	0.59
21:1V:91:ARG:HH11	21:1V:91:ARG:C	2.10	0.59
4:1D:148:LEU:O	4:1D:174:ARG:NH1	2.35	0.59
7:1G:386:PHE:HB3	7:1G:671:PHE:HB2	1.84	0.59
12:1L:81:LYS:HD3	12:1L:83:ASP:HB2	1.83	0.59
23:1X:63:ASN:ND2	25:1Z:78:GLU:OE2	2.36	0.59
5:1E:41:GLY:HA3	44:1s:68:SER:HB3	1.85	0.59
7:1G:349:PHE:HE2	7:1G:362:TYR:HB3	1.67	0.59
12:1L:82:MET:HE1	12:1L:133:THR:HB	1.84	0.59
16:1P:235:ARG:NH2	16:1P:291:ASP:OD1	2.35	0.59
16:1P:270:PHE:HD2	16:1P:278:TRP:HB2	1.67	0.59
22:1W:25:MET:N	22:1W:25:MET:SD	2.75	0.59
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.36	0.59
3:1C:125:LYS:NZ	4:1D:252:ASN:OD1	2.35	0.59
7:1G:504:ASP:OD1	19:1S:55:ARG:NH2	2.33	0.59
12:1L:481:THR:HG22	40:1o:91:HIS:CD2	2.38	0.59
20:1T:84:LYS:HZ3	20:1T:86:VAL:HB	1.67	0.59
39:1n:69:GLU:O	39:1n:73:GLY:N	2.35	0.59
39:1n:176:ARG:HB3	39:1n:178:MET:HE1	1.84	0.59
7:1G:238:ILE:HG22	7:1G:252:PRO:HA	1.84	0.58
13:1M:422:HIS:O	38:1m:55:ARG:NH1	2.34	0.58
17:1Q:79:LEU:HD13	17:1Q:82:LEU:HD12	1.85	0.58
18:1R:32:GLN:NE2	42:1q:123:GLN:O	2.32	0.58
7:1G:99:ALA:O	7:1G:134:LYS:NZ	2.36	0.58
7:1G:407:ALA:HB1	7:1G:422:LEU:HD11	1.85	0.58
12:1L:153:LEU:HD21	13:1M:360:LEU:HD21	1.85	0.58
13:1M:425:ASN:HD22	38:1m:57:GLY:HA2	1.67	0.58
16:1P:29:PHE:HZ	16:1P:173:GLY:HA3	1.68	0.58
16:1P:181:TYR:O	16:1P:184:SER:OG	2.20	0.58
38:1m:51:ASN:O	39:1n:128:ARG:NH2	2.36	0.58
7:1G:359:ARG:NH2	7:1G:629:ASN:OD1	2.36	0.58
12:1L:8:THR:O	12:1L:11:THR:OG1	2.21	0.58
12:1L:129:MET:N	12:1L:129:MET:SD	2.77	0.58
13:1M:23:ILE:HD11	13:1M:92:LYS:HE2	1.84	0.58
17:1Q:93:VAL:HG12	17:1Q:103:PHE:HZ	1.69	0.58
20:1U:38:LYS:HD3	20:1U:38:LYS:N	2.18	0.58
21:1V:41:ALA:HB1	21:1V:99:TRP:CH2	2.37	0.58
29:1d:82:MET:HE2	29:1d:82:MET:HA	1.84	0.58
29:1d:111:GLU:OE1	32:1g:119:GLN:NE2	2.36	0.58
14:1N:217:MET:HA	14:1N:220:ILE:HB	1.84	0.58
19:1S:36:ILE:HA	19:1S:40:TYR:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:67:GLU:OE1	39:1n:67:GLU:N	2.36	0.58
39:1n:145:PRO:O	39:1n:149:ARG:NH2	2.36	0.58
1:1A:33:LYS:HA	2:1B:106:GLN:HA	1.86	0.58
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.37	0.58
6:1F:120:GLU:OE2	6:1F:236:ARG:NH1	2.37	0.58
7:1G:190:MET:SD	7:1G:192:MET:HE3	2.43	0.58
7:1G:365:ASN:HB2	7:1G:488:LYS:HB3	1.84	0.58
7:1G:451:VAL:HG12	7:1G:489:VAL:HG12	1.84	0.58
16:1P:108:ASP:HA	16:1P:112:LYS:HG3	1.85	0.58
4:1D:149:ASN:HD21	4:1D:371:LYS:HD3	1.67	0.58
7:1G:377:ILE:HA	7:1G:450:MET:HB3	1.86	0.58
13:1M:369:LEU:HD12	13:1M:370:PRO:HD2	1.86	0.58
16:1P:3:HIS:CD2	42:1q:132:LYS:HD2	2.37	0.58
16:1P:26:ALA:HB3	16:1P:47:VAL:HG23	1.84	0.58
18:1R:60:ASP:OD1	18:1R:62:GLY:N	2.36	0.58
22:1W:55:SER:HB3	22:1W:58:GLN:HG3	1.86	0.58
3:1C:110:TYR:HB3	21:1V:110:GLN:NE2	2.18	0.58
15:1O:192:MET:N	15:1O:192:MET:SD	2.76	0.58
22:1W:84:ILE:HA	22:1W:87:LYS:HB3	1.86	0.58
37:1l:135:TYR:OH	40:1o:40:ALA:O	2.20	0.58
7:1G:66:VAL:HB	7:1G:71:MET:HG3	1.84	0.58
8:1H:25:ARG:NH2	8:1H:51:ASP:OD2	2.36	0.58
9:1I:31:VAL:HG21	50:1I:204:PC1:H241	1.85	0.58
13:1M:78:MET:HA	13:1M:81:GLN:HE21	1.69	0.58
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.85	0.58
16:1P:81:ILE:HG12	16:1P:117:ILE:HG22	1.86	0.58
23:1X:52:PRO:HB3	25:1Z:80:ASP:OD1	2.03	0.58
4:1D:410:MET:HG3	8:1H:281:ARG:HD2	1.86	0.58
6:1F:109:GLU:O	6:1F:113:HIS:ND1	2.36	0.58
6:1F:258:ILE:HA	6:1F:334:VAL:HG13	1.86	0.58
9:1I:28:THR:O	9:1I:32:ARG:HG2	2.04	0.58
12:1L:560:THR:HA	12:1L:564:LYS:HB2	1.86	0.58
38:1m:125:ASN:O	41:1p:139:GLN:NE2	2.37	0.58
6:1F:245:PHE:O	6:1F:252:GLY:N	2.33	0.58
6:1F:258:ILE:N	6:1F:266:CYS:O	2.35	0.58
7:1G:276:ARG:NH1	7:1G:682:GLN:OE1	2.37	0.58
8:1H:90:PRO:HG3	8:1H:240:ILE:HG12	1.86	0.58
20:1U:28:GLU:OE2	20:1U:28:GLU:N	2.32	0.58
34:1i:105:PRO:HA	34:1i:116:ILE:HD11	1.86	0.58
38:1m:53:PRO:HG3	39:1n:128:ARG:HE	1.67	0.58
1:1A:44:MET:HB3	22:1W:96:VAL:HG11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:154:GLU:N	2:1B:154:GLU:OE2	2.37	0.57
15:1O:284:ILE:HG22	32:1g:27:GLN:HB2	1.84	0.57
21:1V:54:LYS:HD3	21:1V:57:MET:HE1	1.86	0.57
37:1l:4:VAL:HG23	37:1l:8:MET:HE2	1.85	0.57
40:1o:102:GLU:HA	40:1o:105:ARG:HB3	1.85	0.57
7:1G:422:LEU:H	7:1G:422:LEU:HD12	1.68	0.57
11:1K:1:FME:HG2	11:1K:2:PRO:HD2	1.85	0.57
12:1L:356:ILE:HD11	12:1L:430:ALA:HB2	1.86	0.57
39:1n:70:PHE:O	39:1n:74:GLN:N	2.37	0.57
2:1B:32:LYS:HA	2:1B:32:LYS:HE3	1.85	0.57
3:1C:133:GLU:HA	3:1C:136:ASP:HB2	1.87	0.57
6:1F:76:GLY:O	6:1F:80:SER:OG	2.21	0.57
7:1G:213:TYR:O	7:1G:216:THR:OG1	2.20	0.57
7:1G:534:ARG:HD2	7:1G:537:LEU:HD11	1.86	0.57
8:1H:140:ILE:HA	8:1H:143:GLU:HG2	1.86	0.57
8:1H:184:MET:HE1	8:1H:293:PHE:CD2	2.40	0.57
9:1I:35:GLY:HA3	50:1I:204:PC1:H331	1.85	0.57
12:1L:375:ILE:HD13	12:1L:458:LEU:HD21	1.86	0.57
13:1M:11:LEU:HD22	13:1M:100:ILE:HG21	1.84	0.57
19:1S:74:LYS:NZ	19:1S:75:ASN:H	2.03	0.57
4:1D:399:LEU:HD12	4:1D:428:VAL:HG21	1.85	0.57
5:1E:105:THR:HG23	5:1E:107:PRO:HD2	1.86	0.57
7:1G:521:VAL:HG13	7:1G:542:PHE:HB3	1.87	0.57
12:1L:42:TYR:OH	34:1i:66:HIS:ND1	2.30	0.57
12:1L:253:VAL:HG13	12:1L:310:LEU:HD21	1.86	0.57
13:1M:14:MET:HG3	31:1f:12:VAL:HB	1.86	0.57
13:1M:70:THR:HA	13:1M:103:GLN:HE21	1.68	0.57
15:1O:33:SER:HA	15:1O:182:ARG:HH21	1.68	0.57
19:1S:47:ASN:HB2	19:1S:50:LEU:HB3	1.87	0.57
39:1n:83:GLU:OE1	39:1n:83:GLU:N	2.33	0.57
3:1C:20:LYS:H	3:1C:20:LYS:HD2	1.68	0.57
13:1M:192:ASN:HA	13:1M:195:MET:HB3	1.86	0.57
15:1O:194:ILE:HD12	15:1O:194:ILE:H	1.70	0.57
18:1R:39:PHE:O	18:1R:43:LEU:HG	2.04	0.57
21:1V:8:THR:HG23	21:1V:15:VAL:HG22	1.85	0.57
21:1V:58:VAL:HG23	21:1V:67:LEU:HD11	1.87	0.57
30:1e:29:PRO:HB3	33:1h:138:LYS:HG2	1.86	0.57
37:1l:23:ALA:HA	37:1l:26:LYS:HB3	1.86	0.57
7:1G:396:ARG:HG2	7:1G:417:TYR:HD2	1.68	0.57
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.40	0.57
29:1d:31:LEU:HD21	29:1d:69:VAL:HG13	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:4:VAL:HG11	38:1m:65:ILE:HD13	1.86	0.57
6:1F:378:ARG:HB3	6:1F:383:ASP:HB3	1.87	0.57
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.86	0.57
16:1P:197:GLY:HA2	16:1P:288:HIS:HE1	1.69	0.57
4:1D:165:THR:O	4:1D:169:TRP:HB2	2.05	0.57
7:1G:384:PRO:HD2	7:1G:415:LEU:HD11	1.87	0.57
13:1M:14:MET:HE1	13:1M:30:HIS:CE1	2.39	0.57
13:1M:207:MET:HG2	13:1M:298:ILE:HD11	1.85	0.57
16:1P:157:ARG:NH1	16:1P:163:ALA:O	2.37	0.57
22:1W:98:LYS:HE3	22:1W:102:HIS:HB3	1.86	0.57
35:1j:10:ARG:HH22	35:1j:16:GLN:HB3	1.70	0.57
7:1G:196:SER:O	7:1G:199:ILE:HG13	2.04	0.57
14:1N:159:MET:HA	14:1N:159:MET:HE3	1.86	0.57
16:1P:200:THR:O	16:1P:238:LEU:N	2.35	0.57
4:1D:339:LYS:HB3	18:1R:69:PRO:HA	1.86	0.57
5:1E:149:VAL:HB	6:1F:257:ASN:HD21	1.70	0.57
13:1M:72:LEU:HD23	13:1M:75:LEU:HD12	1.86	0.57
18:1R:63:GLY:O	18:1R:67:GLY:N	2.38	0.57
24:1Y:93:GLY:HA3	24:1Y:118:GLY:HA2	1.87	0.57
38:1m:120:LEU:HB3	38:1m:122:GLN:HE22	1.69	0.57
42:1q:6:VAL:HG11	52:1r:201:CDL:HB31	1.87	0.57
3:1C:167:PRO:HA	17:1Q:82:LEU:HD21	1.86	0.56
4:1D:33:TRP:CG	15:1O:275:ILE:HD11	2.39	0.56
4:1D:95:THR:HA	4:1D:385:ARG:HG2	1.87	0.56
7:1G:58:GLU:OE2	7:1G:83:SER:OG	2.22	0.56
14:1N:170:LEU:HD23	14:1N:292:PHE:HD2	1.70	0.56
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.05	0.56
21:1V:94:LEU:HB3	21:1V:95:ARG:NH1	2.19	0.56
31:1f:1:MET:HE3	31:1f:2:ASN:HB3	1.87	0.56
33:1h:64:TRP:CE2	33:1h:77:ARG:HD3	2.40	0.56
2:1B:116:MET:HG2	2:1B:151:PRO:HG2	1.86	0.56
35:1j:64:LEU:HD22	40:1o:106:ARG:HD2	1.87	0.56
41:1p:162:MET:HA	41:1p:165:GLU:HB3	1.85	0.56
1:1A:108:GLN:O	1:1A:110:GLY:N	2.39	0.56
3:1C:13:PRO:HD3	4:1D:129:GLN:HG2	1.88	0.56
3:1C:206:PHE:CE1	4:1D:360:PRO:HD3	2.39	0.56
4:1D:241:ASP:OD2	4:1D:290:ARG:NH2	2.38	0.56
6:1F:29:HIS:HA	44:1s:39:ARG:HE	1.71	0.56
6:1F:98:ASP:OD2	6:1F:139:ARG:NH2	2.38	0.56
8:1H:14:LEU:HD21	8:1H:83:LEU:HD21	1.85	0.56
9:1I:111:ILE:HD11	9:1I:154:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:359:MET:HB2	12:1L:430:ALA:HA	1.87	0.56
12:1L:593:ILE:O	12:1L:597:ILE:HG22	2.05	0.56
14:1N:313:MET:HE1	15:1O:99:TRP:CZ3	2.40	0.56
17:1Q:90:GLU:HA	17:1Q:93:VAL:HG22	1.87	0.56
23:1X:34:GLN:HG2	23:1X:116:TRP:CE3	2.41	0.56
35:1j:54:PRO:HB2	35:1j:59:TRP:HZ2	1.70	0.56
43:1r:99:PRO:O	43:1r:101:LYS:NZ	2.28	0.56
3:1C:192:GLN:OE1	3:1C:195:ARG:NH1	2.38	0.56
4:1D:61:VAL:HG13	4:1D:425:PHE:CD2	2.41	0.56
5:1E:164:LEU:HB3	5:1E:169:ILE:HG23	1.86	0.56
7:1G:145:LEU:HD23	7:1G:145:LEU:H	1.69	0.56
13:1M:399:ASN:O	13:1M:403:THR:OG1	2.23	0.56
19:1S:56:GLU:N	19:1S:56:GLU:OE2	2.38	0.56
22:1W:34:GLU:HA	22:1W:37:ARG:HG3	1.88	0.56
34:1i:10:ARG:HB2	39:1n:155:PRO:HB3	1.87	0.56
38:1m:2:PHE:HD1	38:1m:3:PRO:CD	2.17	0.56
1:1A:48:ARG:HH12	10:1J:80:PRO:HD3	1.70	0.56
6:1F:54:ASP:N	6:1F:54:ASP:OD1	2.38	0.56
6:1F:294:LEU:HA	6:1F:338:ASP:HA	1.87	0.56
7:1G:60:GLU:OE1	7:1G:78:ASN:N	2.39	0.56
7:1G:665:GLN:NE2	7:1G:670:ASP:O	2.38	0.56
10:1J:42:GLY:O	10:1J:46:ASN:ND2	2.35	0.56
15:1O:214:MET:HE2	15:1O:214:MET:O	2.05	0.56
3:1C:205:ALA:HA	7:1G:122:MET:HE2	1.86	0.56
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	1.87	0.56
7:1G:350:PRO:HB3	7:1G:464:THR:HG22	1.86	0.56
15:1O:97:GLN:OE1	53:1O:401:GTP:N2	2.33	0.56
18:1R:78:GLU:OE1	18:1R:78:GLU:N	2.37	0.56
23:1X:146:ARG:NH2	30:1e:42:CYS:SG	2.76	0.56
25:1Z:120:MET:HG3	30:1e:68:ARG:HG2	1.87	0.56
36:1k:35:LEU:O	36:1k:39:GLY:N	2.35	0.56
40:1o:71:ASP:HB2	41:1p:22:GLN:H	1.71	0.56
4:1D:149:ASN:ND2	4:1D:370:PRO:HB2	2.14	0.56
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.37	0.56
5:1E:149:VAL:N	6:1F:105:CYS:SG	2.78	0.56
6:1F:404:ILE:HD11	7:1G:51:ASN:HA	1.87	0.56
7:1G:300:LEU:HA	7:1G:303:VAL:HG12	1.88	0.56
12:1L:61:MET:HE2	12:1L:61:MET:HA	1.87	0.56
13:1M:47:GLU:HB3	41:1p:92:ARG:HE	1.71	0.56
16:1P:92:ILE:HG13	16:1P:130:ILE:HB	1.87	0.56
3:1C:68:THR:HA	21:1V:82:GLN:HE21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:623:LEU:HD21	7:1G:630:LEU:HB3	1.88	0.56
37:1l:5:THR:OG1	37:1l:6:LYS:N	2.39	0.56
42:1q:49:TYR:HE2	42:1q:63:ILE:HG12	1.70	0.56
9:1I:99:ARG:HB2	9:1I:104:ARG:HA	1.88	0.56
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.33	0.56
16:1P:221:PRO:O	16:1P:224:LYS:NZ	2.28	0.56
4:1D:106:LEU:HD23	4:1D:427:GLU:HA	1.87	0.56
6:1F:312:CYS:HA	6:1F:315:VAL:HG12	1.88	0.56
12:1L:282:ALA:O	12:1L:285:THR:OG1	2.21	0.56
14:1N:1:FME:HE3	14:1N:46:LYS:HB2	1.87	0.56
37:1l:35:GLU:N	37:1l:35:GLU:OE2	2.39	0.56
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.37	0.56
2:1B:25:ARG:HG3	2:1B:27:GLU:H	1.71	0.55
2:1B:125:TYR:CE1	9:1I:88:PRO:HB2	2.41	0.55
8:1H:27:VAL:HG22	26:1a:5:ILE:HD13	1.87	0.55
10:1J:68:PHE:CZ	11:1K:75:LEU:HD21	2.41	0.55
15:1O:222:GLN:OE1	15:1O:222:GLN:N	2.39	0.55
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.39	0.55
38:1m:36:LEU:HD11	39:1n:7:ALA:HA	1.88	0.55
1:1A:32:GLU:OE1	1:1A:32:GLU:N	2.32	0.55
9:1I:83:CYS:SG	9:1I:109:TYR:OH	2.65	0.55
13:1M:269:MET:O	13:1M:273:SER:OG	2.24	0.55
14:1N:106:LEU:HD11	14:1N:139:LEU:HD13	1.88	0.55
19:1S:20:ILE:HA	19:1S:64:LEU:HA	1.88	0.55
19:1S:91:GLU:O	19:1S:95:SER:N	2.36	0.55
22:1W:62:LYS:O	22:1W:65:GLU:N	2.39	0.55
30:1e:9:LEU:HB2	30:1e:11:LEU:HD23	1.88	0.55
32:1g:79:TYR:HE2	33:1h:40:ILE:HD13	1.71	0.55
43:1r:106:SER:OG	43:1r:108:ASP:OD1	2.24	0.55
14:1N:284:MET:HE2	14:1N:284:MET:HA	1.89	0.55
22:1W:66:MET:HG3	22:1W:69:LYS:NZ	2.21	0.55
30:1e:93:PRO:HB3	30:1e:97:HIS:HD2	1.72	0.55
38:1m:51:ASN:HD22	39:1n:165:LEU:HD22	1.71	0.55
1:1A:94:LEU:HD21	10:1J:154:VAL:HG22	1.88	0.55
3:1C:93:VAL:HG22	3:1C:108:LYS:HG3	1.87	0.55
5:1E:116:ILE:HG13	5:1E:166:PRO:HA	1.89	0.55
7:1G:274:LEU:O	7:1G:278:ARG:NH2	2.40	0.55
9:1I:156:ASN:ND2	18:1R:34:GLU:OE2	2.37	0.55
13:1M:367:LEU:HD11	13:1M:408:LEU:HD21	1.88	0.55
15:1O:27:VAL:HG21	15:1O:39:ALA:HA	1.89	0.55
15:1O:248:TRP:HA	15:1O:251:GLN:HE22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:21:LEU:HD11	36:1k:47:ASN:HA	1.88	0.55
21:1V:46:TYR:CE1	43:1r:91:LYS:HD3	2.42	0.55
22:1W:75:ASP:OD2	22:1W:77:ARG:NH2	2.39	0.55
38:1m:19:PRO:HB3	39:1n:64:ARG:HH12	1.71	0.55
2:1B:30:VAL:HG22	2:1B:173:LEU:HB3	1.89	0.55
3:1C:87:GLN:HE22	21:1V:108:ALA:HB3	1.71	0.55
5:1E:35:VAL:O	5:1E:43:LYS:NZ	2.34	0.55
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.07	0.55
6:1F:89:ARG:NE	6:1F:217:GLY:O	2.40	0.55
7:1G:258:ILE:HD11	7:1G:579:ARG:HE	1.70	0.55
7:1G:508:LYS:HD3	7:1G:509:PRO:HD2	1.88	0.55
7:1G:601:ARG:NH1	7:1G:601:ARG:O	2.40	0.55
13:1M:277:LEU:HD21	13:1M:405:LEU:HB3	1.89	0.55
21:1V:18:THR:O	21:1V:18:THR:OG1	2.25	0.55
21:1V:99:TRP:CD1	21:1V:99:TRP:H	2.25	0.55
38:1m:105:LYS:O	38:1m:109:ASP:N	2.40	0.55
7:1G:673:MET:HA	7:1G:673:MET:HE3	1.88	0.55
17:1Q:112:LYS:HG2	17:1Q:113:PRO:HD3	1.89	0.55
39:1n:138:GLN:NE2	39:1n:155:PRO:O	2.38	0.55
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.25	0.55
4:1D:404:LYS:HE2	4:1D:404:LYS:HA	1.88	0.55
12:1L:216:LEU:HD22	12:1L:259:LEU:HD11	1.89	0.55
12:1L:291:CYS:O	12:1L:295:GLN:NE2	2.31	0.55
12:1L:501:ALA:O	12:1L:505:ASN:ND2	2.38	0.55
15:1O:139:TYR:HB2	15:1O:144:ILE:HD11	1.88	0.55
23:1X:121:LEU:HD13	25:1Z:62:ILE:HD11	1.89	0.55
30:1e:44:HIS:CG	33:1h:130:LYS:HG2	2.42	0.55
12:1L:516:PRO:HG3	39:1n:29:TRP:CZ2	2.42	0.55
15:1O:204:ASN:HB2	15:1O:208:LYS:HE3	1.89	0.55
25:1Z:38:VAL:O	25:1Z:42:THR:HG23	2.07	0.55
34:1i:110:LEU:HD23	34:1i:110:LEU:H	1.72	0.55
37:1l:13:TYR:CE2	37:1l:39:ASP:HB2	2.41	0.55
38:1m:51:ASN:OD1	39:1n:168:HIS:ND1	2.31	0.55
39:1n:123:GLN:O	39:1n:127:LEU:HD12	2.06	0.55
40:1o:61:TYR:HD1	40:1o:64:GLN:HE22	1.53	0.55
42:1q:78:ASP:OD1	42:1q:79:GLY:N	2.40	0.55
6:1F:261:HIS:CE1	6:1F:337:MET:HG2	2.42	0.55
12:1L:162:THR:HG1	37:1l:86:ARG:HH21	1.52	0.55
13:1M:14:MET:HE2	13:1M:26:ASN:HB3	1.88	0.55
17:1Q:55:TRP:HB2	17:1Q:86:PHE:HB2	1.89	0.55
23:1X:7:PRO:HD2	25:1Z:84:LEU:HD13	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:157:GLU:O	40:1o:33:ARG:NE	2.36	0.55
5:1E:116:ILE:HG23	5:1E:169:ILE:HG12	1.89	0.55
6:1F:63:SER:O	6:1F:251:SER:OG	2.23	0.55
10:1J:129:ASP:OD2	10:1J:130:THR:N	2.39	0.55
21:1V:57:MET:SD	21:1V:58:VAL:N	2.79	0.55
23:1X:20:SER:HG	26:1a:64:LYS:H	1.53	0.55
3:1C:63:PHE:HA	21:1V:89:LEU:HD21	1.88	0.54
5:1E:150:ASN:ND2	5:1E:163:ASP:OD2	2.22	0.54
9:1I:70:TYR:CE2	18:1R:87:CYS:HA	2.39	0.54
14:1N:218:LEU:HD23	14:1N:244:MET:HE2	1.89	0.54
20:1U:37:MET:HG2	20:1U:38:LYS:HD3	1.89	0.54
34:1i:54:ALA:HB3	34:1i:57:LYS:HZ3	1.72	0.54
3:1C:88:ASN:ND2	3:1C:112:ASP:OD1	2.35	0.54
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.89	0.54
11:1K:48:ILE:HD13	11:1K:56:ALA:HB1	1.90	0.54
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.38	0.54
17:1Q:112:LYS:HG2	17:1Q:113:PRO:CD	2.37	0.54
32:1g:35:GLU:N	32:1g:35:GLU:OE2	2.40	0.54
37:1l:60:PRO:HG3	37:1l:70:ARG:HH12	1.70	0.54
2:1B:34:ASP:HB3	2:1B:173:LEU:HB2	1.89	0.54
4:1D:163:ALA:N	8:1H:278:PRO:HA	2.18	0.54
5:1E:10:ARG:HH22	18:1R:77:LYS:HA	1.72	0.54
7:1G:243:ARG:NH1	7:1G:246:GLU:OE2	2.41	0.54
7:1G:375:ASP:OD2	7:1G:447:LYS:N	2.41	0.54
14:1N:25:HIS:HB2	30:1e:14:ASP:HB2	1.90	0.54
15:1O:146:LYS:HZ3	15:1O:149:VAL:HB	1.72	0.54
17:1Q:10:LEU:HD12	22:1W:16:SER:HB2	1.88	0.54
25:1Z:59:ARG:HD3	27:1b:81:LYS:HA	1.89	0.54
33:1h:61:PRO:HG2	33:1h:66:TYR:CZ	2.43	0.54
37:1l:16:THR:OG1	37:1l:19:GLU:OE2	2.26	0.54
5:1E:55:GLN:NE2	5:1E:89:MET:O	2.40	0.54
6:1F:253:THR:HA	6:1F:272:MET:HB2	1.88	0.54
7:1G:14:ASP:OD2	7:1G:81:THR:OG1	2.24	0.54
10:1J:150:GLY:HA3	11:1K:58:MET:HE1	1.90	0.54
12:1L:545:SER:O	12:1L:550:SER:OG	2.25	0.54
13:1M:396:MET:HE2	13:1M:396:MET:HA	1.90	0.54
15:1O:136:GLU:OE2	15:1O:140:ARG:NH1	2.40	0.54
15:1O:173:ASP:N	15:1O:223:TYR:O	2.32	0.54
15:1O:261:MET:HA	15:1O:261:MET:HE2	1.90	0.54
16:1P:215:ILE:HA	16:1P:218:ILE:HG12	1.90	0.54
42:1q:29:ARG:NH2	42:1q:65:THR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.89	0.54
7:1G:191:PHE:C	7:1G:192:MET:HE2	2.32	0.54
1:1A:65:PHE:O	1:1A:69:ILE:HG23	2.07	0.54
2:1B:86:MET:HE1	2:1B:100:LEU:HD11	1.90	0.54
6:1F:214:GLY:N	6:1F:218:CYS:O	2.40	0.54
6:1F:253:THR:HA	6:1F:272:MET:CB	2.36	0.54
9:1I:74:GLU:OE1	9:1I:75:GLU:N	2.41	0.54
14:1N:314:LYS:HZ2	15:1O:271:ASN:HA	1.71	0.54
15:1O:41:GLU:HA	15:1O:44:GLU:HG2	1.88	0.54
17:1Q:91:ASP:OD1	17:1Q:91:ASP:N	2.35	0.54
26:1a:32:GLY:O	26:1a:34:LYS:NZ	2.41	0.54
10:1J:105:TYR:O	10:1J:109:LYS:HG2	2.08	0.54
12:1L:81:LYS:C	12:1L:82:MET:HE2	2.33	0.54
14:1N:190:MET:HE1	14:1N:205:LEU:HA	1.88	0.54
15:1O:133:VAL:HG21	15:1O:206:TYR:HE1	1.71	0.54
16:1P:2:HIS:HB3	16:1P:5:LEU:HB2	1.90	0.54
16:1P:138:ASP:H	16:1P:146:LEU:HB3	1.73	0.54
2:1B:104:TYR:CE1	2:1B:111:ARG:HD2	2.43	0.54
3:1C:58:ILE:HD11	3:1C:118:GLU:HG3	1.88	0.54
13:1M:25:ILE:O	13:1M:29:VAL:HG23	2.07	0.54
15:1O:150:GLU:OE1	15:1O:150:GLU:N	2.30	0.54
40:1o:33:ARG:NH2	40:1o:100:GLU:OE2	2.37	0.54
2:1B:124:GLY:HA2	9:1I:115:LYS:HA	1.89	0.54
3:1C:113:GLU:OE1	3:1C:113:GLU:N	2.37	0.54
5:1E:143:GLU:HG2	6:1F:353:PHE:HD1	1.73	0.54
7:1G:681:SER:OG	7:1G:684:MET:HB2	2.07	0.54
9:1I:169:ILE:HD13	18:1R:66:LEU:HD11	1.88	0.54
12:1L:102:GLU:OE1	12:1L:456:ARG:NH1	2.41	0.54
12:1L:432:LEU:HD21	36:1k:65:ALA:HB2	1.90	0.54
12:1L:440:LEU:HD22	20:1U:14:ARG:HH12	1.73	0.54
15:1O:155:VAL:O	15:1O:159:THR:OG1	2.18	0.54
15:1O:224:SER:OG	15:1O:227:GLU:OE1	2.20	0.54
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.26	0.54
22:1W:34:GLU:OE2	22:1W:34:GLU:N	2.26	0.54
33:1h:14:SER:OG	39:1n:110:GLU:OE1	2.26	0.54
37:1l:54:SER:N	37:1l:57:GLU:OE1	2.40	0.54
40:1o:52:LEU:HA	40:1o:55:ARG:HD3	1.89	0.54
41:1p:84:MET:HE1	41:1p:152:ARG:HD2	1.90	0.54
41:1p:98:ASP:OD2	41:1p:141:ARG:NH1	2.41	0.54
6:1F:93:LEU:HD22	6:1F:94:VAL:H	1.73	0.54
6:1F:142:PHE:HB3	6:1F:145:GLU:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:93:LYS:O	13:1M:97:THR:OG1	2.25	0.54
15:1O:167:HIS:O	15:1O:218:CYS:HB2	2.08	0.54
15:1O:227:GLU:OE1	15:1O:227:GLU:N	2.41	0.54
17:1Q:127:ARG:HH22	44:1s:70:ARG:HH22	1.54	0.54
23:1X:43:MET:HE2	27:1b:52:TYR:CD2	2.43	0.54
1:1A:54:LYS:HB2	1:1A:113:TRP:HB2	1.90	0.53
2:1B:95:LYS:HE3	3:1C:155:TYR:CE1	2.42	0.53
5:1E:149:VAL:HG22	5:1E:190:ARG:HH22	1.72	0.53
6:1F:59:GLU:HG2	6:1F:235:CYS:HA	1.90	0.53
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	1.90	0.53
15:1O:270:LEU:O	15:1O:273:THR:OG1	2.25	0.53
25:1Z:43:LEU:O	25:1Z:46:GLY:N	2.41	0.53
37:1l:18:GLU:H	37:1l:18:GLU:CD	2.14	0.53
40:1o:28:TYR:O	40:1o:103:ARG:NH2	2.40	0.53
1:1A:105:GLU:O	1:1A:110:GLY:HA3	2.08	0.53
4:1D:33:TRP:NE1	15:1O:154:GLU:OE2	2.41	0.53
6:1F:262:VAL:HG23	6:1F:287:VAL:HG12	1.89	0.53
10:1J:129:ASP:HB2	30:1e:31:ARG:HD2	1.88	0.53
11:1K:37:MET:HE3	11:1K:67:ALA:HB3	1.90	0.53
11:1K:59:MET:HG3	14:1N:84:TRP:CH2	2.43	0.53
14:1N:179:MET:SD	14:1N:215:MET:HE2	2.48	0.53
16:1P:279:THR:HA	16:1P:283:LYS:HD2	1.91	0.53
35:1j:55:ASP:OD2	35:1j:57:SER:OG	2.27	0.53
37:1l:141:GLU:OE1	37:1l:141:GLU:N	2.41	0.53
43:1r:57:ASP:HB3	43:1r:60:ARG:HG3	1.89	0.53
6:1F:151:VAL:O	6:1F:155:GLU:HG2	2.08	0.53
9:1I:145:GLU:OE2	16:1P:66:GLY:N	2.38	0.53
12:1L:542:LEU:HD21	37:1l:88:ARG:HD3	1.91	0.53
17:1Q:90:GLU:CD	17:1Q:90:GLU:H	2.16	0.53
31:1f:51:ASN:OD1	31:1f:51:ASN:N	2.41	0.53
40:1o:87:ASP:HA	40:1o:90:GLU:HG3	1.90	0.53
4:1D:402:LEU:HD23	4:1D:421:GLN:HE21	1.73	0.53
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.91	0.53
7:1G:45:ARG:NH1	7:1G:261:GLU:OE1	2.41	0.53
7:1G:229:ASP:HB3	7:1G:236:SER:H	1.73	0.53
10:1J:71:THR:HG21	11:1K:75:LEU:HD12	1.91	0.53
12:1L:132:VAL:HG23	12:1L:258:PHE:CZ	2.43	0.53
15:1O:138:MET:HG3	15:1O:143:PHE:HB2	1.89	0.53
15:1O:145:ARG:HE	15:1O:147:GLN:HG2	1.73	0.53
16:1P:59:LEU:HA	16:1P:62:MET:HE1	1.89	0.53
16:1P:245:ILE:HA	16:1P:248:VAL:HG12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:315:ILE:H	16:1P:315:ILE:HD12	1.73	0.53
17:1Q:11:ILE:HG22	22:1W:23:ARG:HD2	1.90	0.53
23:1X:97:ARG:HB3	25:1Z:60:LEU:HD21	1.91	0.53
36:1k:18:TYR:CE1	36:1k:21:TRP:HB2	2.41	0.53
42:1q:97:PRO:HG2	42:1q:100:THR:HG23	1.91	0.53
1:1A:1:FME:O1	1:1A:2:ASN:N	2.42	0.53
4:1D:55:HIS:HE1	8:1H:206:GLU:HA	1.72	0.53
4:1D:295:ASP:OD1	9:1I:6:ASN:ND2	2.31	0.53
5:1E:148:CYS:N	6:1F:105:CYS:SG	2.82	0.53
6:1F:216:PHE:HA	17:1Q:129:ARG:NH2	2.24	0.53
6:1F:313:GLU:OE2	6:1F:314:THR:OG1	2.25	0.53
7:1G:349:PHE:HD1	7:1G:350:PRO:HD2	1.73	0.53
16:1P:97:ARG:NH1	55:1P:501:NDP:O3X	2.42	0.53
23:1X:162:HIS:NE2	33:1h:99:GLU:OE1	2.33	0.53
2:1B:93:THR:HG23	2:1B:96:MET:H	1.73	0.53
3:1C:33:LEU:HA	21:1V:98:PRO:HB2	1.90	0.53
4:1D:126:LEU:HD13	4:1D:330:VAL:HG21	1.91	0.53
7:1G:50:GLY:HA2	7:1G:69:CYS:SG	2.48	0.53
7:1G:80:LEU:HD22	7:1G:83:SER:HB2	1.91	0.53
7:1G:331:LEU:HD21	7:1G:525:LEU:HD22	1.90	0.53
8:1H:112:ALA:O	8:1H:115:SER:OG	2.27	0.53
11:1K:73:LEU:HD11	14:1N:38:LEU:HA	1.89	0.53
13:1M:428:ALA:N	39:1n:105:ASP:OD2	2.37	0.53
15:1O:25:ILE:O	15:1O:123:VAL:HA	2.09	0.53
15:1O:30:ASN:OD1	15:1O:31:ILE:N	2.41	0.53
16:1P:169:SER:HB3	16:1P:231:VAL:HG12	1.91	0.53
23:1X:76:HIS:O	23:1X:78:ALA:N	2.40	0.53
36:1k:38:ARG:HE	36:1k:40:LEU:HD12	1.74	0.53
3:1C:180:VAL:HG13	3:1C:182:ARG:HB3	1.90	0.53
5:1E:115:SER:HB2	5:1E:166:PRO:HB3	1.90	0.53
7:1G:26:VAL:HB	7:1G:68:ALA:HB1	1.90	0.53
16:1P:197:GLY:HA3	16:1P:238:LEU:HD22	1.91	0.53
18:1R:53:GLY:HA2	18:1R:93:GLN:HG2	1.90	0.53
42:1q:95:ASP:OD2	43:1r:33:ARG:N	2.40	0.53
43:1r:106:SER:HB3	43:1r:110:PRO:HA	1.90	0.53
1:1A:56:PHE:CZ	11:1K:75:LEU:HB3	2.44	0.53
7:1G:615:THR:OG1	7:1G:618:GLN:NE2	2.42	0.53
7:1G:640:ASN:OD1	7:1G:640:ASN:N	2.42	0.53
12:1L:295:GLN:O	12:1L:425:ARG:NH1	2.41	0.53
13:1M:168:GLN:NE2	33:1h:104:ARG:HD2	2.23	0.53
14:1N:262:PRO:O	14:1N:266:ILE:HG12	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:1b:15:GLU:OE2	27:1b:19:VAL:N	2.42	0.53
37:1l:30:ARG:NH1	38:1m:31:ALA:O	2.41	0.53
40:1o:61:TYR:HD2	40:1o:89:CYS:HB2	1.74	0.53
3:1C:10:THR:HG21	43:1r:56:ARG:HD2	1.90	0.53
3:1C:28:TYR:HE2	43:1r:94:VAL:H	1.57	0.53
3:1C:211:GLN:NE2	21:1V:114:PRO:O	2.41	0.53
7:1G:444:LYS:HA	7:1G:477:ILE:HD13	1.91	0.53
14:1N:147:GLN:HB3	33:1h:125:TYR:CZ	2.43	0.53
16:1P:268:ARG:HD3	16:1P:281:ARG:NH2	2.24	0.53
20:1U:61:GLU:OE1	39:1n:81:PHE:HB2	2.08	0.53
20:1U:81:ALA:HA	20:1U:86:VAL:HB	1.91	0.53
38:1m:94:ILE:HD11	38:1m:98:PHE:HD2	1.74	0.53
3:1C:180:VAL:HG21	3:1C:182:ARG:HH21	1.74	0.53
7:1G:366:THR:H	7:1G:491:ASN:HD21	1.57	0.53
7:1G:444:LYS:NZ	7:1G:476:ASN:O	2.40	0.53
9:1I:63:GLY:H	9:1I:133:GLU:HB3	1.74	0.53
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.90	0.53
16:1P:311:GLU:HG3	16:1P:336:PRO:HB3	1.91	0.53
20:1T:64:ASP:OD2	22:1W:30:ARG:NH1	2.42	0.53
21:1V:34:LEU:HD11	21:1V:44:ARG:HA	1.91	0.53
22:1W:101:THR:O	22:1W:105:ARG:NH1	2.42	0.53
26:1a:42:SER:O	26:1a:46:ASN:ND2	2.42	0.53
29:1d:105:ASP:HB3	29:1d:107:LYS:HZ2	1.74	0.53
37:1l:82:ASP:O	37:1l:88:ARG:HD2	2.09	0.53
40:1o:16:PRO:HB3	40:1o:104:GLU:HG2	1.91	0.53
3:1C:28:TYR:HD2	43:1r:94:VAL:HG22	1.73	0.52
3:1C:137:MET:HB3	3:1C:162:PHE:HB2	1.90	0.52
7:1G:161:ARG:NH2	17:1Q:133:LYS:O	2.42	0.52
8:1H:27:VAL:HB	8:1H:271:LEU:HD11	1.91	0.52
8:1H:271:LEU:HD23	8:1H:271:LEU:H	1.74	0.52
12:1L:355:ASP:OD1	12:1L:357:ARG:NE	2.41	0.52
13:1M:338:HIS:NE2	32:1g:34:ASP:OD2	2.42	0.52
14:1N:120:GLN:O	14:1N:176:ARG:NH2	2.40	0.52
14:1N:304:MET:HE1	15:1O:290:ASP:HB2	1.91	0.52
14:1N:321:LYS:HG2	14:1N:323:MET:H	1.74	0.52
21:1V:27:TYR:CE2	21:1V:54:LYS:HB3	2.39	0.52
23:1X:90:TYR:HA	26:1a:34:LYS:HG2	1.91	0.52
33:1h:94:LEU:HB3	41:1p:81:ILE:HD12	1.90	0.52
37:1l:13:TYR:HE2	37:1l:39:ASP:HB2	1.73	0.52
7:1G:192:MET:HG3	7:1G:691:VAL:HG12	1.90	0.52
12:1L:295:GLN:HB2	12:1L:301:ILE:HD12	1.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:1L:702:PC1:H271	13:1M:446:LEU:HD12	1.91	0.52
13:1M:47:GLU:OE1	13:1M:47:GLU:N	2.42	0.52
13:1M:243:MET:O	13:1M:247:THR:HG23	2.09	0.52
16:1P:322:ARG:NH1	16:1P:329:SER:O	2.42	0.52
31:1f:57:LYS:C	31:1f:57:LYS:HD3	2.33	0.52
35:1j:28:PHE:HA	35:1j:31:THR:HG22	1.89	0.52
39:1n:123:GLN:OE1	39:1n:126:ARG:NH2	2.38	0.52
4:1D:111:MET:N	4:1D:111:MET:SD	2.82	0.52
9:1L:48:ILE:HG23	9:1L:53:GLU:HG3	1.91	0.52
10:1J:115:ILE:O	10:1J:117:PHE:N	2.42	0.52
12:1L:135:ASN:ND2	12:1L:199:GLN:OE1	2.42	0.52
1:1A:106:TRP:CH2	27:1b:18:LEU:HD21	2.45	0.52
6:1F:212:ASP:OD1	6:1F:212:ASP:N	2.40	0.52
7:1G:449:PRO:O	7:1G:487:TRP:NE1	2.28	0.52
12:1L:407:TRP:CZ3	12:1L:410:LEU:HD22	2.44	0.52
14:1N:8:THR:O	14:1N:12:THR:HG23	2.09	0.52
14:1N:275:SER:OG	14:1N:278:MET:HB2	2.09	0.52
15:1O:24:VAL:O	15:1O:24:VAL:HG12	2.10	0.52
16:1P:29:PHE:CE2	16:1P:207:ILE:HD13	2.44	0.52
7:1G:332:LYS:HD3	7:1G:343:LEU:HD13	1.92	0.52
12:1L:55:MET:HG2	12:1L:471:ASN:HB3	1.92	0.52
13:1M:423:ILE:HG22	38:1m:58:VAL:HG12	1.90	0.52
16:1P:134:HIS:CE1	16:1P:286:ARG:HH12	2.27	0.52
27:1b:15:GLU:OE1	27:1b:18:LEU:N	2.42	0.52
44:1s:73:PRO:HG2	44:1s:74:ARG:HH12	1.75	0.52
3:1C:176:TYR:HA	3:1C:183:VAL:HA	1.92	0.52
6:1F:375:VAL:HA	6:1F:378:ARG:HD3	1.92	0.52
7:1G:550:GLY:HA2	7:1G:554:ALA:HB3	1.91	0.52
8:1H:70:MET:HA	8:1H:73:ILE:HG22	1.92	0.52
12:1L:62:ILE:HD12	41:1p:114:GLN:HB2	1.92	0.52
12:1L:444:ASN:ND2	35:1j:7:ILE:HG13	2.24	0.52
14:1N:163:LEU:O	14:1N:167:TRP:HB2	2.09	0.52
16:1P:57:MET:O	16:1P:60:ARG:HG2	2.08	0.52
16:1P:98:GLU:HA	16:1P:145:TYR:OH	2.10	0.52
17:1Q:27:GLU:H	17:1Q:27:GLU:CD	2.15	0.52
32:1g:66:PHE:O	32:1g:71:VAL:HG23	2.10	0.52
34:1i:74:VAL:C	34:1i:77:PRO:HD2	2.35	0.52
2:1B:65:PRO:HD3	4:1D:168:PHE:HB3	1.92	0.52
5:1E:7:PHE:HA	5:1E:92:ARG:HH12	1.75	0.52
5:1E:23:PHE:HB3	5:1E:27:ASN:HB2	1.91	0.52
6:1F:57:LEU:HD22	6:1F:80:SER:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:433:PHE:O	6:1F:437:HIS:ND1	2.43	0.52
7:1G:379:LEU:HD13	7:1G:408:LEU:HB2	1.92	0.52
8:1H:20:LEU:HA	8:1H:23:VAL:HG12	1.92	0.52
13:1M:54:LEU:HD13	33:1h:93:ILE:HG23	1.91	0.52
15:1O:13:ARG:H	15:1O:16:ARG:CZ	2.23	0.52
20:1T:37:MET:H	20:1T:37:MET:CE	2.22	0.52
21:1V:91:ARG:NH1	21:1V:95:ARG:HH11	2.07	0.52
30:1e:82:ARG:HD2	30:1e:86:ILE:HG12	1.91	0.52
32:1g:111:ASN:HA	41:1p:161:ARG:HH22	1.74	0.52
41:1p:58:ASN:N	41:1p:58:ASN:OD1	2.42	0.52
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.42	0.52
2:1B:57:VAL:CG1	4:1D:189:MET:HE1	2.40	0.52
2:1B:149:CYS:SG	9:1I:117:ILE:HG23	2.49	0.52
4:1D:202:ASP:OD1	4:1D:203:LEU:N	2.43	0.52
4:1D:221:ARG:HA	4:1D:224:GLU:HG2	1.92	0.52
6:1F:256:PHE:CD1	6:1F:270:GLU:HB3	2.45	0.52
7:1G:276:ARG:HA	42:1q:135:GLN:NE2	2.25	0.52
9:1I:116:CYS:SG	9:1I:117:ILE:N	2.82	0.52
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.75	0.52
16:1P:21:ALA:HB3	16:1P:45:VAL:HG12	1.92	0.52
16:1P:301:GLU:OE2	16:1P:301:GLU:N	2.23	0.52
20:1T:33:ASN:C	20:1T:33:ASN:HD22	2.18	0.52
21:1V:63:ASP:OD2	21:1V:66:LYS:N	2.39	0.52
32:1g:24:ILE:O	32:1g:26:LEU:N	2.42	0.52
1:1A:68:GLU:OE1	1:1A:98:LEU:HD22	2.09	0.52
6:1F:126:GLY:O	6:1F:171:TYR:OH	2.25	0.52
7:1G:227:SER:O	7:1G:253:ARG:NH2	2.43	0.52
8:1H:96:ILE:HG23	25:1Z:144:THR:HB	1.91	0.52
10:1J:163:ILE:HG13	14:1N:12:THR:HG21	1.92	0.52
13:1M:30:HIS:HA	13:1M:33:LEU:HB2	1.92	0.52
13:1M:307:TRP:NE1	38:1m:127:SER:HG	2.07	0.52
15:1O:197:ALA:O	15:1O:201:ASP:N	2.40	0.52
16:1P:132:ILE:HG22	16:1P:166:ILE:HB	1.91	0.52
16:1P:319:ARG:NH2	22:1W:53:ASP:OD1	2.41	0.52
21:1V:105:GLU:OE1	43:1r:72:GLN:NE2	2.43	0.52
1:1A:90:MET:HA	1:1A:90:MET:HE3	1.91	0.52
5:1E:99:HIS:HE1	5:1E:140:ILE:HD13	1.75	0.52
15:1O:35:LYS:HE2	15:1O:126:ARG:NH2	2.25	0.52
15:1O:140:ARG:CZ	15:1O:140:ARG:HA	2.40	0.52
18:1R:5:SER:OG	18:1R:9:GLU:HB3	2.10	0.52
32:1g:80:LEU:HD12	32:1g:81:PRO:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:18:LEU:HD13	39:1n:21:ARG:HH22	1.75	0.52
4:1D:125:LEU:HD11	4:1D:363:THR:HB	1.92	0.51
4:1D:407:LYS:HE3	4:1D:407:LYS:HA	1.92	0.51
5:1E:78:MET:HA	5:1E:81:TYR:CD2	2.46	0.51
7:1G:40:PHE:HZ	7:1G:116:LEU:HA	1.75	0.51
9:1I:156:ASN:OD1	18:1R:36:ASN:ND2	2.41	0.51
10:1J:7:PHE:O	10:1J:11:THR:OG1	2.23	0.51
13:1M:262:LEU:HD11	13:1M:302:MET:HB3	1.92	0.51
16:1P:335:LYS:HE3	16:1P:336:PRO:HD2	1.93	0.51
17:1Q:9:GLN:HE22	22:1W:23:ARG:HB2	1.75	0.51
17:1Q:66:GLU:OE1	17:1Q:66:GLU:N	2.43	0.51
20:1U:21:LEU:O	36:1k:46:ARG:NH1	2.43	0.51
32:1g:119:GLN:OE1	32:1g:119:GLN:N	2.43	0.51
34:1i:4:THR:OG1	34:1i:6:ASP:OD1	2.19	0.51
40:1o:7:ARG:NH2	40:1o:17:ASP:OD1	2.43	0.51
42:1q:86:TRP:CZ3	42:1q:98:PRO:HD2	2.45	0.51
44:1s:47:SER:N	44:1s:50:THR:OG1	2.43	0.51
1:1A:80:GLN:NE2	8:1H:314:ILE:HD13	2.25	0.51
2:1B:47:PRO:HD3	2:1B:74:VAL:HB	1.91	0.51
5:1E:97:LYS:HG2	5:1E:98:TYR:CD1	2.45	0.51
5:1E:103:CYS:HB3	5:1E:153:MET:HB2	1.91	0.51
6:1F:371:TRP:HH2	7:1G:129:ARG:HG3	1.75	0.51
7:1G:584:LYS:HG3	17:1Q:36:ARG:HH12	1.73	0.51
12:1L:19:ILE:HD11	12:1L:122:VAL:HB	1.92	0.51
15:1O:33:SER:OG	15:1O:35:LYS:NZ	2.42	0.51
16:1P:38:LEU:O	16:1P:43:SER:OG	2.24	0.51
20:1T:80:ILE:HA	20:1T:83:LYS:HG2	1.93	0.51
20:1U:26:ASP:OD1	20:1U:29:LYS:NZ	2.42	0.51
26:1a:4:GLU:OE1	26:1a:4:GLU:N	2.24	0.51
37:1l:30:ARG:HH22	38:1m:31:ALA:HB1	1.75	0.51
39:1n:25:HIS:CE1	39:1n:78:PRO:HB3	2.46	0.51
42:1q:6:VAL:HG12	52:1r:201:CDL:HA61	1.92	0.51
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.40	0.51
3:1C:129:TRP:HZ2	4:1D:78:PRO:HD2	1.75	0.51
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.41	0.51
12:1L:481:THR:O	12:1L:481:THR:OG1	2.29	0.51
13:1M:215:TRP:HZ3	13:1M:231:LEU:HD11	1.75	0.51
13:1M:237:LYS:HG2	13:1M:316:MET:HG3	1.93	0.51
14:1N:316:GLN:HA	15:1O:302:ARG:HH21	1.75	0.51
15:1O:279:LEU:HD12	15:1O:282:ILE:H	1.75	0.51
17:1Q:104:ASP:N	17:1Q:104:ASP:OD1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:90:LEU:O	22:1W:94:ILE:HG12	2.11	0.51
29:1d:26:LEU:HG	29:1d:27:THR:HG23	1.92	0.51
31:1f:43:LEU:HD22	31:1f:44:PHE:CE1	2.45	0.51
36:1k:20:GLN:HG2	36:1k:21:TRP:CD1	2.45	0.51
36:1k:20:GLN:N	36:1k:20:GLN:OE1	2.40	0.51
2:1B:81:ARG:HD3	8:1H:214:GLU:HA	1.91	0.51
4:1D:19:MET:SD	4:1D:19:MET:N	2.63	0.51
4:1D:209:ASP:OD1	25:1Z:16:TYR:OH	2.27	0.51
5:1E:122:LYS:HA	5:1E:122:LYS:HE3	1.92	0.51
6:1F:327:THR:OG1	6:1F:328:GLY:N	2.42	0.51
6:1F:432:GLN:O	6:1F:436:GLN:HG2	2.10	0.51
7:1G:537:LEU:HD22	7:1G:543:ILE:HD11	1.92	0.51
9:1I:97:GLU:O	9:1I:104:ARG:HB3	2.09	0.51
13:1M:243:MET:HB2	13:1M:301:ILE:HG12	1.92	0.51
42:1q:66:THR:HG23	42:1q:74:PHE:HB2	1.93	0.51
3:1C:167:PRO:HG3	17:1Q:79:LEU:HD22	1.93	0.51
3:1C:179:GLU:OE2	16:1P:40:ARG:NH2	2.44	0.51
5:1E:217:LEU:HD23	6:1F:44:LYS:HD2	1.91	0.51
7:1G:617:ASP:OD1	7:1G:617:ASP:N	2.43	0.51
7:1G:703:ILE:O	18:1R:85:GLY:HA2	2.11	0.51
12:1L:283:ILE:HD13	37:1I:112:MET:HG3	1.91	0.51
14:1N:275:SER:HB2	24:1Y:136:ALA:HB3	1.91	0.51
15:1O:70:ASP:O	15:1O:74:SER:N	2.43	0.51
19:1S:84:ASP:OD1	19:1S:84:ASP:N	2.40	0.51
21:1V:89:LEU:HD22	21:1V:93:MET:SD	2.51	0.51
35:1j:67:LEU:O	40:1o:110:ARG:NE	2.44	0.51
2:1B:165:ARG:NH1	42:1q:77:VAL:O	2.43	0.51
5:1E:30:ARG:HD3	44:1s:52:LEU:HB3	1.92	0.51
6:1F:214:GLY:HA3	6:1F:220:THR:HB	1.92	0.51
7:1G:584:LYS:HG3	17:1Q:36:ARG:NH1	2.25	0.51
9:1I:8:ARG:NE	9:1I:8:ARG:HA	2.26	0.51
12:1L:71:LEU:HB2	12:1L:74:VAL:HB	1.91	0.51
15:1O:164:LEU:HB2	15:1O:248:TRP:CZ3	2.46	0.51
17:1Q:55:TRP:NE1	17:1Q:108:ARG:HH22	2.09	0.51
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.10	0.51
40:1o:98:MET:N	40:1o:98:MET:SD	2.83	0.51
3:1C:28:TYR:O	3:1C:32:ILE:HD12	2.11	0.51
3:1C:94:TYR:HB2	3:1C:107:VAL:HG22	1.92	0.51
6:1F:255:LEU:HA	6:1F:269:GLU:HA	1.93	0.51
7:1G:661:LEU:H	7:1G:661:LEU:HD12	1.76	0.51
9:1I:141:THR:OG1	9:1I:146:GLU:OE1	2.29	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:7:LEU:HD21	12:1L:49:VAL:HG11	1.91	0.51
45:1L:701:3PE:H252	45:1L:701:3PE:O32	2.11	0.51
14:1N:37:LEU:HD21	14:1N:60:PHE:HD1	1.76	0.51
14:1N:200:MET:HA	14:1N:203:LEU:HB3	1.91	0.51
17:1Q:19:ILE:HG12	17:1Q:98:LYS:HB2	1.91	0.51
20:1U:69:LYS:NZ	34:1i:2:GLY:O	2.38	0.51
23:1X:102:GLN:H	23:1X:102:GLN:CD	2.15	0.51
35:1j:10:ARG:HH12	35:1j:16:GLN:HG2	1.76	0.51
4:1D:73:VAL:C	4:1D:74:ARG:HH11	2.19	0.51
8:1H:216:ALA:O	8:1H:219:PRO:HD2	2.10	0.51
12:1L:101:MET:HG3	12:1L:118:PHE:HE2	1.75	0.51
12:1L:576:MET:SD	45:1Y:201:3PE:H31	2.51	0.51
13:1M:181:TYR:O	41:1p:152:ARG:NH1	2.44	0.51
13:1M:294:MET:HA	13:1M:294:MET:HE3	1.92	0.51
15:1O:116:LEU:HD11	15:1O:256:PHE:HD1	1.75	0.51
16:1P:36:ASN:ND2	16:1P:40:ARG:HH22	2.08	0.51
20:1U:51:ILE:HD12	20:1U:52:MET:N	2.26	0.51
22:1W:51:GLN:O	22:1W:100:ARG:NH2	2.43	0.51
22:1W:64:ARG:O	22:1W:68:MET:HE2	2.10	0.51
4:1D:238:ARG:HD3	8:1H:281:ARG:HB2	1.93	0.51
4:1D:305:ARG:NH1	25:1Z:22:LYS:O	2.44	0.51
6:1F:60:VAL:HA	6:1F:63:SER:HB3	1.93	0.51
8:1H:28:LEU:HD13	8:1H:275:ALA:HB2	1.92	0.51
9:1I:92:ILE:HG12	9:1I:111:ILE:HG22	1.93	0.51
16:1P:294:LEU:HB2	16:1P:296:HIS:CD2	2.46	0.51
21:1V:1:ALA:N	21:1V:63:ASP:OD1	2.43	0.51
22:1W:100:ARG:O	22:1W:104:MET:HG2	2.11	0.51
6:1F:164:LYS:HB3	44:1s:63:MET:SD	2.51	0.51
7:1G:579:ARG:HD3	7:1G:634:ASP:HA	1.93	0.51
21:1V:45:LYS:HB3	43:1r:91:LYS:HE2	1.93	0.51
23:1X:9:LEU:HA	23:1X:12:LEU:HD12	1.93	0.51
2:1B:108:PRO:HB3	8:1H:61:LEU:HD23	1.93	0.50
5:1E:40:GLU:HA	5:1E:43:LYS:HE2	1.92	0.50
5:1E:151:ALA:HB1	5:1E:152:PRO:HD2	1.91	0.50
7:1G:41:CYS:HB3	7:1G:52:CYS:HB3	1.92	0.50
8:1H:299:ALA:HA	8:1H:302:MET:HE3	1.93	0.50
11:1K:55:LEU:O	11:1K:58:MET:HG3	2.11	0.50
15:1O:109:ALA:HB2	15:1O:269:VAL:HG21	1.94	0.50
16:1P:141:SER:OG	16:1P:146:LEU:HB2	2.10	0.50
19:1S:82:SER:OG	19:1S:85:GLN:OE1	2.26	0.50
20:1U:51:ILE:HD12	20:1U:52:MET:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:63:PHE:O	32:1g:68:ILE:HG12	2.11	0.50
41:1p:29:VAL:O	41:1p:33:THR:HG23	2.10	0.50
44:1s:63:MET:HE2	44:1s:63:MET:N	2.25	0.50
2:1B:127:HIS:CE1	9:1I:115:LYS:HE2	2.46	0.50
4:1D:357:GLN:HA	4:1D:384:SER:HA	1.93	0.50
6:1F:137:TYR:HE2	6:1F:186:CYS:HB3	1.75	0.50
6:1F:392:LEU:HG	6:1F:419:ILE:HD11	1.93	0.50
7:1G:601:ARG:HH12	7:1G:605:GLU:HB2	1.76	0.50
12:1L:205:ASN:ND2	12:1L:207:GLU:OE2	2.44	0.50
12:1L:349:SER:OG	12:1L:366:MET:HE1	2.11	0.50
12:1L:538:THR:HG22	45:1L:701:3PE:H272	1.93	0.50
16:1P:248:VAL:HG23	16:1P:334:VAL:HG21	1.94	0.50
20:1U:82:ASP:N	20:1U:82:ASP:OD1	2.44	0.50
23:1X:20:SER:OG	26:1a:64:LYS:N	2.36	0.50
26:1a:3:PHE:HA	26:1a:6:LEU:HD23	1.93	0.50
26:1a:28:LYS:HG2	26:1a:33:GLY:HA2	1.93	0.50
5:1E:201:SER:HG	6:1F:26:TYR:HH	1.58	0.50
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.47	0.50
9:1I:117:ILE:HB	9:1I:119:CYS:SG	2.52	0.50
12:1L:385:TYR:OH	35:1j:43:ASP:O	2.21	0.50
14:1N:272:LYS:HB3	24:1Y:140:VAL:HG21	1.93	0.50
15:1O:164:LEU:H	15:1O:164:LEU:HD12	1.76	0.50
18:1R:69:PRO:HG2	18:1R:86:TYR:CE2	2.47	0.50
20:1T:19:LEU:HD23	20:1T:25:ILE:HG21	1.92	0.50
20:1T:50:ILE:O	20:1T:54:MET:HG2	2.11	0.50
39:1n:142:GLU:OE2	39:1n:157:ARG:NH2	2.44	0.50
40:1o:82:GLU:OE1	40:1o:82:GLU:N	2.39	0.50
1:1A:106:TRP:CD2	45:1A:201:3PE:H231	2.46	0.50
2:1B:60:MET:HE3	4:1D:167:PHE:CZ	2.45	0.50
7:1G:248:MET:N	7:1G:248:MET:SD	2.85	0.50
7:1G:488:LYS:NZ	7:1G:639:ALA:O	2.25	0.50
10:1J:70:TYR:O	10:1J:74:MET:N	2.45	0.50
11:1K:34:GLU:HA	11:1K:37:MET:HG3	1.91	0.50
12:1L:86:SER:OG	12:1L:262:ARG:NH2	2.44	0.50
12:1L:129:MET:HA	12:1L:132:VAL:HG12	1.94	0.50
13:1M:1:FME:SD	13:1M:52:PHE:HB3	2.52	0.50
39:1n:153:LEU:HD21	39:1n:164:PRO:HB2	1.92	0.50
41:1p:139:GLN:O	41:1p:157:LYS:NZ	2.44	0.50
2:1B:162:GLN:OE1	42:1q:116:ASN:ND2	2.45	0.50
4:1D:71:GLU:HG3	4:1D:410:MET:HE1	1.94	0.50
7:1G:228:ILE:HG22	7:1G:583:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:379:LEU:HA	7:1G:452:VAL:HG13	1.94	0.50
14:1N:96:THR:HG22	14:1N:100:MET:HE1	1.92	0.50
17:1Q:26:PRO:HG2	17:1Q:29:HIS:HB2	1.94	0.50
23:1X:70:PHE:HB3	26:1a:69:ILE:HD13	1.93	0.50
34:1i:44:GLN:O	34:1i:48:LYS:HG2	2.11	0.50
34:1i:64:TYR:O	34:1i:68:ILE:HG13	2.12	0.50
35:1j:12:ARG:HH11	36:1k:50:TRP:CD1	2.29	0.50
2:1B:86:MET:HG2	2:1B:107:MET:SD	2.52	0.50
4:1D:200:HIS:NE2	9:1I:124:GLU:OE2	2.45	0.50
7:1G:350:PRO:HD2	7:1G:458:LEU:HD11	1.94	0.50
8:1H:215:TYR:CD1	8:1H:219:PRO:HB2	2.46	0.50
12:1L:302:VAL:O	12:1L:306:THR:HG23	2.12	0.50
19:1S:61:GLN:HE22	19:1S:63:LYS:HG3	1.74	0.50
34:1i:59:VAL:O	34:1i:63:THR:HG23	2.12	0.50
4:1D:362:ALA:HB1	4:1D:377:TYR:HE1	1.77	0.50
7:1G:218:ARG:N	7:1G:221:GLU:OE2	2.43	0.50
8:1H:178:SER:OG	8:1H:304:HIS:NE2	2.39	0.50
9:1I:8:ARG:HA	9:1I:8:ARG:CZ	2.41	0.50
33:1h:129:ASP:N	33:1h:129:ASP:OD1	2.43	0.50
38:1m:47:LEU:HA	38:1m:50:TYR:HB3	1.94	0.50
40:1o:34:LYS:NZ	40:1o:37:GLU:OE2	2.30	0.50
5:1E:6:LEU:O	5:1E:92:ARG:NH1	2.45	0.50
5:1E:86:PHE:HE1	7:1G:177:ARG:HG3	1.77	0.50
6:1F:123:LEU:HB3	6:1F:162:ILE:HD13	1.94	0.50
7:1G:10:GLU:H	7:1G:75:LYS:HZ3	1.60	0.50
9:1I:123:GLN:NE2	9:1I:133:GLU:OE1	2.44	0.50
13:1M:42:LEU:HD12	13:1M:67:VAL:HG11	1.93	0.50
15:1O:154:GLU:HA	15:1O:157:LYS:NZ	2.27	0.50
16:1P:119:GLN:NE2	16:1P:120:VAL:HG13	2.27	0.50
20:1T:20:LYS:HD2	20:1T:27:PRO:HB3	1.94	0.50
40:1o:47:ASP:OD1	40:1o:47:ASP:N	2.43	0.50
4:1D:2:ARG:HE	32:1g:31:ASP:HA	1.77	0.50
4:1D:51:PHE:HB3	4:1D:64:LEU:HB3	1.94	0.50
6:1F:254:LYS:HD3	6:1F:255:LEU:H	1.76	0.50
7:1G:25:THR:HG22	7:1G:28:GLN:HG3	1.94	0.50
10:1J:113:VAL:HG23	10:1J:119:PHE:HB2	1.93	0.50
12:1L:296:ASN:OD1	12:1L:357:ARG:NH1	2.45	0.50
12:1L:531:SER:HA	12:1L:535:ARG:HH21	1.76	0.50
22:1W:18:LYS:HD2	22:1W:19:PRO:HD2	1.94	0.50
25:1Z:95:ALA:HB2	25:1Z:106:VAL:HG11	1.93	0.50
25:1Z:121:MET:HE2	25:1Z:137:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:3:VAL:HA	31:1f:6:ILE:HG22	1.94	0.50
32:1g:61:VAL:HG13	32:1g:62:PHE:HD1	1.76	0.50
4:1D:62:LEU:HD12	4:1D:63:ARG:H	1.77	0.49
4:1D:63:ARG:O	4:1D:79:HIS:HB2	2.11	0.49
6:1F:384:ALA:O	6:1F:385:ARG:NH1	2.44	0.49
7:1G:138:GLU:HG2	18:1R:76:ASP:HB3	1.94	0.49
7:1G:174:THR:HA	7:1G:183:VAL:HA	1.92	0.49
7:1G:201:ASP:HA	17:1Q:45:MET:HB3	1.93	0.49
10:1J:55:MET:HA	10:1J:55:MET:HE3	1.92	0.49
19:1S:78:LEU:HD23	19:1S:78:LEU:H	1.77	0.49
21:1V:41:ALA:HB1	21:1V:99:TRP:CZ3	2.47	0.49
37:1l:156:TYR:CD2	40:1o:33:ARG:HB3	2.47	0.49
41:1p:70:VAL:O	41:1p:90:GLN:NE2	2.44	0.49
42:1q:32:ASP:OD1	42:1q:34:ARG:N	2.36	0.49
3:1C:203:TRP:CZ3	7:1G:36:GLN:HG2	2.47	0.49
4:1D:62:LEU:HD13	4:1D:425:PHE:CZ	2.47	0.49
4:1D:290:ARG:N	4:1D:295:ASP:OD2	2.42	0.49
6:1F:257:ASN:ND2	6:1F:267:THR:HG22	2.26	0.49
7:1G:632:ARG:NH2	19:1S:57:CYS:SG	2.84	0.49
8:1H:293:PHE:O	8:1H:297:THR:OG1	2.27	0.49
9:1I:98:PRO:HA	9:1I:104:ARG:HG2	1.93	0.49
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.46	0.49
12:1L:98:TRP:NE1	12:1L:102:GLU:OE2	2.45	0.49
12:1L:432:LEU:HD13	36:1k:62:PHE:HA	1.93	0.49
15:1O:133:VAL:HG21	15:1O:206:TYR:CE1	2.47	0.49
18:1R:20:ASP:O	18:1R:25:ARG:NH2	2.37	0.49
20:1T:35:HIS:CE1	20:1T:38:LYS:HZ1	2.30	0.49
23:1X:30:HIS:HA	23:1X:34:GLN:HE22	1.78	0.49
1:1A:48:ARG:HD2	10:1J:78:MET:HA	1.93	0.49
6:1F:139:ARG:NH1	6:1F:180:GLY:HA3	2.26	0.49
7:1G:141:ASN:OD1	7:1G:141:ASN:N	2.43	0.49
7:1G:231:MET:HB3	7:1G:266:LYS:HD2	1.94	0.49
7:1G:354:ALA:HB2	7:1G:648:LEU:HD12	1.95	0.49
7:1G:430:GLN:NE2	7:1G:431:ASP:OD1	2.45	0.49
8:1H:137:ALA:HB3	8:1H:282:TYR:OH	2.13	0.49
16:1P:27:THR:OG1	55:1P:501:NDP:O1X	2.30	0.49
16:1P:86:GLU:HB2	16:1P:87:HIS:CE1	2.48	0.49
4:1D:4:TRP:CG	13:1M:140:THR:HG1	2.30	0.49
4:1D:145:THR:HG1	4:1D:181:TYR:HH	1.60	0.49
6:1F:15:LEU:HB2	6:1F:271:GLU:N	2.27	0.49
6:1F:67:GLY:N	6:1F:73:PHE:O	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:105:CYS:N	6:1F:257:ASN:OD1	2.45	0.49
10:1J:99:MET:N	10:1J:99:MET:SD	2.85	0.49
12:1L:360:GLY:H	12:1L:362:LEU:HD23	1.77	0.49
12:1L:415:ALA:O	12:1L:419:THR:N	2.45	0.49
15:1O:144:ILE:HB	15:1O:148:CYS:SG	2.53	0.49
15:1O:174:VAL:HG21	15:1O:182:ARG:HH22	1.77	0.49
16:1P:30:LEU:HD12	16:1P:94:LEU:HD22	1.94	0.49
20:1T:37:MET:SD	20:1T:37:MET:N	2.78	0.49
34:1i:76:ILE:HD12	34:1i:77:PRO:CD	2.42	0.49
34:1i:100:LYS:NZ	41:1p:116:GLU:OE1	2.45	0.49
35:1j:12:ARG:HD2	36:1k:21:TRP:CZ3	2.48	0.49
35:1j:12:ARG:HD3	36:1k:50:TRP:CD1	2.48	0.49
38:1m:2:PHE:HD2	39:1n:72:TYR:CD1	2.30	0.49
43:1r:4:THR:H	43:1r:7:ILE:HD12	1.76	0.49
44:1s:49:TYR:O	44:1s:53:ASP:N	2.39	0.49
2:1B:96:MET:O	2:1B:96:MET:HE3	2.12	0.49
7:1G:110:GLN:HB3	7:1G:114:CYS:HB2	1.94	0.49
7:1G:157:THR:O	7:1G:161:ARG:HG2	2.12	0.49
7:1G:276:ARG:HE	42:1q:135:GLN:HE22	1.61	0.49
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	1.94	0.49
7:1G:595:GLU:HB2	7:1G:598:LYS:HG2	1.94	0.49
13:1M:193:ILE:H	13:1M:193:ILE:HD12	1.78	0.49
14:1N:80:TYR:HA	30:1e:67:LEU:HD21	1.94	0.49
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.39	0.49
20:1U:64:ASP:OD2	39:1n:17:ARG:NE	2.45	0.49
21:1V:43:TYR:HE1	21:1V:47:THR:HG21	1.78	0.49
40:1o:88:TYR:CZ	40:1o:92:LEU:HD11	2.46	0.49
2:1B:86:MET:O	2:1B:113:VAL:HA	2.13	0.49
4:1D:202:ASP:HB2	4:1D:323:ILE:HD13	1.94	0.49
6:1F:12:PHE:HZ	6:1F:245:PHE:HA	1.77	0.49
12:1L:496:MET:O	12:1L:500:LEU:HD12	2.12	0.49
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	1.93	0.49
13:1M:393:ILE:HA	13:1M:396:MET:HB2	1.94	0.49
13:1M:418:LYS:HD3	39:1n:94:GLU:OE2	2.12	0.49
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	1.94	0.49
17:1Q:28:GLU:O	17:1Q:32:THR:OG1	2.26	0.49
20:1T:31:SER:N	20:1T:34:SER:OG	2.35	0.49
22:1W:99:GLN:OE1	22:1W:99:GLN:HA	2.12	0.49
24:1Y:40:ILE:HD12	24:1Y:45:PRO:HG3	1.95	0.49
44:1s:73:PRO:HD2	44:1s:74:ARG:HH22	1.77	0.49
2:1B:70:ASP:OD2	8:1H:34:ARG:NH2	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:189:GLU:N	3:1C:189:GLU:OE1	2.45	0.49
4:1D:167:PHE:HD2	4:1D:168:PHE:CD1	2.31	0.49
6:1F:184:TYR:CE2	48:1F:501:FMN:H6	2.47	0.49
7:1G:319:ALA:HB3	7:1G:345:THR:HA	1.94	0.49
10:1J:36:SER:HA	10:1J:39:VAL:HG12	1.93	0.49
13:1M:73:LEU:HD21	13:1M:100:ILE:HG22	1.95	0.49
14:1N:25:HIS:NE2	30:1e:17:MET:SD	2.85	0.49
16:1P:248:VAL:HA	16:1P:334:VAL:HG11	1.94	0.49
27:1b:78:GLU:HA	27:1b:81:LYS:NZ	2.28	0.49
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.13	0.49
38:1m:109:ASP:HA	38:1m:112:GLU:OE2	2.12	0.49
40:1o:1:GLY:H3	40:1o:3:HIS:CD2	2.29	0.49
40:1o:27:ASP:N	40:1o:27:ASP:OD1	2.45	0.49
4:1D:37:ASP:CG	11:1K:95:LEU:HD11	2.38	0.49
6:1F:183:ALA:HB3	6:1F:186:CYS:SG	2.52	0.49
7:1G:275:LYS:HD2	42:1q:133:LYS:HG3	1.94	0.49
12:1L:72:GLN:OE1	13:1M:310:MET:HE1	2.13	0.49
13:1M:116:ILE:O	13:1M:120:ILE:HG12	2.12	0.49
14:1N:270:MET:HE1	14:1N:282:MET:SD	2.53	0.49
16:1P:36:ASN:ND2	16:1P:62:MET:HG2	2.28	0.49
20:1U:52:MET:HA	20:1U:55:GLU:HB2	1.94	0.49
21:1V:30:ILE:HA	21:1V:33:VAL:HG12	1.94	0.49
22:1W:68:MET:N	22:1W:68:MET:SD	2.85	0.49
33:1h:8:LEU:HD11	39:1n:174:ARG:CZ	2.43	0.49
38:1m:5:TYR:HE2	38:1m:14:PRO:HD3	1.76	0.49
4:1D:4:TRP:CD1	13:1M:140:THR:HA	2.48	0.49
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.95	0.49
6:1F:205:LEU:HB2	17:1Q:118:TYR:CZ	2.48	0.49
7:1G:348:VAL:HG12	7:1G:510:GLY:HA3	1.95	0.49
12:1L:81:LYS:HB2	12:1L:135:ASN:HD22	1.78	0.49
15:1O:319:LEU:HD12	28:1c:17:VAL:HG21	1.93	0.49
17:1Q:27:GLU:OE2	17:1Q:27:GLU:N	2.34	0.49
17:1Q:96:ALA:O	17:1Q:100:GLY:N	2.45	0.49
25:1Z:93:GLU:HG3	30:1e:97:HIS:NE2	2.28	0.49
34:1i:123:PRO:HG2	34:1i:125:GLN:NE2	2.28	0.49
37:1l:85:ILE:HG22	37:1l:88:ARG:HB2	1.95	0.49
4:1D:112:MET:HG3	4:1D:194:ILE:HG12	1.94	0.49
4:1D:180:PHE:CD2	4:1D:211:ILE:HG22	2.48	0.49
7:1G:271:TYR:O	7:1G:274:LEU:HB2	2.12	0.49
9:1I:99:ARG:NH2	9:1I:101:ASP:OD2	2.45	0.49
12:1L:407:TRP:CE3	37:1l:115:MET:HE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:30:HIS:CD2	31:1f:16:VAL:HB	2.47	0.49
19:1S:68:TYR:HB2	19:1S:72:GLN:HB3	1.94	0.49
19:1S:86:VAL:O	19:1S:89:THR:OG1	2.30	0.49
20:1T:26:ASP:N	20:1T:29:LYS:HE3	2.28	0.49
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.45	0.49
22:1W:90:LEU:HD12	22:1W:91:GLU:H	1.78	0.49
25:1Z:120:MET:HB2	30:1e:68:ARG:CZ	2.43	0.49
28:1c:28:TRP:O	28:1c:32:ILE:HD12	2.13	0.49
37:1l:12:PRO:O	37:1l:46:ASP:HB3	2.13	0.49
1:1A:48:ARG:HH22	10:1J:80:PRO:HD3	1.78	0.48
1:1A:80:GLN:HE22	8:1H:314:ILE:HD13	1.77	0.48
4:1D:233:ARG:NH2	9:1I:27:TRP:HA	2.28	0.48
4:1D:255:PHE:HZ	4:1D:401:GLY:HA3	1.78	0.48
5:1E:101:GLN:HB3	5:1E:142:VAL:HG11	1.95	0.48
6:1F:108:ARG:HG2	6:1F:112:ARG:HH12	1.78	0.48
7:1G:372:GLU:OE1	7:1G:372:GLU:N	2.42	0.48
7:1G:400:LEU:HD22	17:1Q:127:ARG:HG3	1.94	0.48
12:1L:129:MET:O	12:1L:133:THR:OG1	2.24	0.48
19:1S:47:ASN:HD22	19:1S:50:LEU:HB3	1.77	0.48
20:1T:32:VAL:O	20:1T:74:GLN:NE2	2.46	0.48
22:1W:65:GLU:OE1	22:1W:69:LYS:HD3	2.12	0.48
3:1C:49:GLU:HB3	3:1C:108:LYS:NZ	2.28	0.48
3:1C:68:THR:HA	21:1V:82:GLN:NE2	2.28	0.48
5:1E:148:CYS:HA	5:1E:153:MET:HE1	1.94	0.48
7:1G:27:LEU:O	7:1G:30:CYS:N	2.41	0.48
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.77	0.48
8:1H:70:MET:HE3	10:1J:28:TYR:CE1	2.48	0.48
8:1H:91:MET:O	8:1H:93:TYR:N	2.45	0.48
12:1L:56:HIS:ND1	41:1p:29:VAL:HG11	2.27	0.48
13:1M:29:VAL:O	13:1M:33:LEU:HD23	2.13	0.48
16:1P:48:PRO:HB2	16:1P:73:TRP:CD1	2.48	0.48
20:1U:23:ASP:N	20:1U:23:ASP:OD1	2.45	0.48
22:1W:75:ASP:HB3	22:1W:78:VAL:HG23	1.95	0.48
22:1W:90:LEU:HD12	22:1W:91:GLU:N	2.28	0.48
34:1i:54:ALA:HB3	34:1i:57:LYS:NZ	2.27	0.48
42:1q:46:ASN:OD1	42:1q:65:THR:N	2.46	0.48
1:1A:13:LEU:HG	8:1H:10:ILE:HD13	1.95	0.48
1:1A:93:PHE:HA	1:1A:96:ILE:HD11	1.95	0.48
2:1B:44:SER:OG	8:1H:51:ASP:OD1	2.28	0.48
3:1C:178:ASP:OD1	3:1C:181:LYS:NZ	2.35	0.48
5:1E:110:LEU:HD22	6:1F:261:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:215:VAL:HG22	6:1F:220:THR:OG1	2.13	0.48
7:1G:136:ALA:HB1	18:1R:74:ASN:HB2	1.95	0.48
7:1G:185:THR:O	7:1G:187:ILE:N	2.47	0.48
12:1L:10:THR:O	12:1L:13:ILE:HG22	2.14	0.48
12:1L:28:LYS:H	12:1L:28:LYS:CD	2.26	0.48
51:1M:501:PGT:H121	51:1M:501:PGT:H32	1.59	0.48
14:1N:14:MET:HA	14:1N:133:TRP:NE1	2.29	0.48
20:1T:72:CYS:HB3	20:1T:75:GLU:OE1	2.14	0.48
26:1a:43:TYR:HA	26:1a:46:ASN:HD21	1.78	0.48
42:1q:27:LEU:HD23	42:1q:33:VAL:HG13	1.94	0.48
42:1q:133:LYS:HE2	42:1q:133:LYS:HA	1.95	0.48
2:1B:132:VAL:O	2:1B:134:ARG:NH1	2.46	0.48
4:1D:322:GLU:CD	43:1r:44:PRO:HD3	2.38	0.48
5:1E:163:ASP:OD1	5:1E:190:ARG:HB3	2.13	0.48
7:1G:228:ILE:HD12	7:1G:237:ASN:HA	1.94	0.48
8:1H:26:LYS:NZ	26:1a:4:GLU:O	2.37	0.48
12:1L:76:LEU:HD21	12:1L:196:TRP:HE3	1.77	0.48
13:1M:278:ARG:HH12	38:1m:71:ARG:NH1	2.11	0.48
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.95	0.48
14:1N:199:THR:OG1	14:1N:347:ASN:OD1	2.31	0.48
30:1e:31:ARG:NH2	30:1e:68:ARG:HH21	2.10	0.48
3:1C:158:GLU:CD	17:1Q:24:GLY:HA3	2.39	0.48
6:1F:9:LYS:O	6:1F:12:PHE:HD2	1.97	0.48
7:1G:357:ASP:CG	19:1S:52:ILE:H	2.21	0.48
9:1I:161:TRP:O	9:1I:165:ILE:HG12	2.13	0.48
12:1L:7:LEU:HA	12:1L:10:THR:HG22	1.95	0.48
14:1N:167:TRP:HA	14:1N:288:LEU:HD13	1.94	0.48
14:1N:344:SER:O	29:1d:82:MET:HG3	2.12	0.48
33:1h:41:THR:O	33:1h:45:VAL:HG22	2.13	0.48
33:1h:49:GLU:OE2	33:1h:69:HIS:ND1	2.33	0.48
37:1l:63:ASP:OD1	37:1l:63:ASP:N	2.39	0.48
38:1m:26:PRO:C	38:1m:30:LYS:HZ3	2.21	0.48
1:1A:67:LEU:HD12	11:1K:65:VAL:HA	1.96	0.48
3:1C:47:GLU:OE2	3:1C:106:ARG:NH1	2.44	0.48
5:1E:202:LEU:HD22	6:1F:26:TYR:HD2	1.78	0.48
10:1J:119:PHE:HA	11:1K:1:FME:H	1.78	0.48
14:1N:338:PRO:O	23:1X:169:TRP:NE1	2.47	0.48
19:1S:47:ASN:OD1	19:1S:47:ASN:N	2.46	0.48
19:1S:74:LYS:HZ3	19:1S:75:ASN:H	1.60	0.48
20:1T:22:TYR:OH	20:1T:49:GLU:OE2	2.30	0.48
23:1X:95:LEU:HB3	23:1X:97:ARG:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:36:GLU:HB2	30:1e:62:PHE:CE1	2.49	0.48
43:1r:59:ARG:HG3	43:1r:60:ARG:HG2	1.95	0.48
1:1A:1:FME:H	1:1A:4:MET:HE1	1.78	0.48
2:1B:61:HIS:HE1	4:1D:174:ARG:HB3	1.79	0.48
2:1B:118:SER:N	46:1B:201:SF4:S1	2.87	0.48
6:1F:398:GLN:O	6:1F:402:HIS:ND1	2.47	0.48
9:1I:65:HIS:CD2	9:1I:113:MET:HE1	2.46	0.48
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.46	0.48
19:1S:55:ARG:H	19:1S:55:ARG:HD2	1.78	0.48
26:1a:9:ILE:HA	26:1a:12:MET:HG3	1.94	0.48
30:1e:46:ILE:HD12	30:1e:50:ARG:HH21	1.78	0.48
36:1k:13:MET:HE2	36:1k:13:MET:HA	1.95	0.48
1:1A:51:PHE:HB2	1:1A:55:PHE:CE2	2.48	0.48
1:1A:67:LEU:HD12	11:1K:65:VAL:HG12	1.94	0.48
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.39	0.48
2:1B:125:TYR:CD1	9:1I:117:ILE:HG13	2.49	0.48
2:1B:126:TYR:CD2	4:1D:85:ARG:HD2	2.48	0.48
3:1C:12:ARG:HA	4:1D:129:GLN:HG2	1.95	0.48
4:1D:266:GLN:HG3	43:1r:103:TRP:CZ3	2.49	0.48
6:1F:30:ASP:OD1	6:1F:35:GLY:N	2.46	0.48
7:1G:552:VAL:O	7:1G:555:PRO:HD2	2.13	0.48
7:1G:665:GLN:HA	7:1G:670:ASP:HB2	1.95	0.48
10:1J:152:TRP:CD1	30:1e:13:LEU:HB3	2.49	0.48
11:1K:67:ALA:HA	11:1K:70:GLU:OE2	2.14	0.48
11:1K:94:ASN:HD22	12:1L:583:LEU:HD11	1.79	0.48
13:1M:329:LEU:HA	13:1M:437:MET:HE1	1.96	0.48
19:1S:30:GLN:OE1	19:1S:33:ARG:NH1	2.43	0.48
23:1X:43:MET:HE2	27:1b:52:TYR:CE2	2.49	0.48
23:1X:142:HIS:ND1	25:1Z:114:THR:OG1	2.46	0.48
27:1b:40:TYR:O	27:1b:44:ILE:HG23	2.14	0.48
29:1d:51:ARG:O	29:1d:53:VAL:N	2.43	0.48
29:1d:91:PHE:HB3	29:1d:95:LYS:HZ1	1.78	0.48
4:1D:371:LYS:HD2	4:1D:422:ASP:HB2	1.94	0.48
5:1E:41:GLY:HA2	44:1s:71:GLN:HA	1.96	0.48
6:1F:256:PHE:CZ	6:1F:272:MET:HA	2.34	0.48
7:1G:336:ASN:OD1	19:1S:67:ARG:NH1	2.44	0.48
12:1L:54:PHE:O	12:1L:58:GLY:N	2.46	0.48
12:1L:444:ASN:ND2	12:1L:446:ASN:H	2.11	0.48
13:1M:121:LEU:HA	13:1M:124:ALA:HB3	1.95	0.48
20:1T:17:TYR:CD1	20:1T:17:TYR:C	2.90	0.48
28:1c:24:SER:HA	28:1c:27:LEU:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:24:GLU:O	8:1H:28:LEU:HB2	2.14	0.48
9:1I:26:LEU:O	9:1I:28:THR:N	2.47	0.48
10:1J:103:MET:SD	10:1J:104:VAL:N	2.87	0.48
10:1J:152:TRP:CE2	30:1e:13:LEU:HD13	2.48	0.48
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.14	0.48
12:1L:114:ILE:HD11	12:1L:118:PHE:HE1	1.78	0.48
12:1L:121:LEU:HD22	12:1L:246:LEU:HD23	1.96	0.48
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.49	0.48
14:1N:15:SER:O	14:1N:19:LEU:N	2.39	0.48
14:1N:250:SER:O	14:1N:259:GLY:HA3	2.14	0.48
15:1O:19:THR:OG1	15:1O:20:GLU:N	2.45	0.48
22:1W:70:ASN:OD1	22:1W:70:ASN:N	2.41	0.48
23:1X:43:MET:HE1	23:1X:47:TRP:CZ3	2.49	0.48
24:1Y:117:MET:HE3	24:1Y:117:MET:H	1.79	0.48
25:1Z:120:MET:HB3	25:1Z:123:GLU:OE1	2.13	0.48
28:1c:19:LEU:O	28:1c:23:THR:HG23	2.14	0.48
28:1c:28:TRP:NE1	29:1d:66:THR:HG22	2.29	0.48
4:1D:357:GLN:H	43:1r:59:ARG:HH22	1.60	0.47
5:1E:149:VAL:HA	6:1F:259:SER:OG	2.14	0.47
6:1F:111:ILE:HG23	6:1F:149:LEU:HD23	1.96	0.47
6:1F:137:TYR:HD2	6:1F:192:LEU:HG	1.79	0.47
6:1F:157:TYR:OH	6:1F:175:VAL:O	2.30	0.47
6:1F:412:ALA:HB1	6:1F:416:GLN:NE2	2.28	0.47
8:1H:273:ILE:HG23	8:1H:277:TYR:CD2	2.49	0.47
9:1I:72:SER:HB2	18:1R:47:GLN:HE21	1.77	0.47
13:1M:102:LEU:HD13	13:1M:128:PRO:HG2	1.96	0.47
13:1M:457:PRO:HA	32:1g:84:ARG:HH21	1.79	0.47
17:1Q:7:ASP:HA	17:1Q:10:LEU:HD23	1.95	0.47
17:1Q:81:ASN:O	17:1Q:82:LEU:HD23	2.14	0.47
18:1R:7:THR:O	18:1R:7:THR:HG22	2.14	0.47
20:1T:80:ILE:O	20:1T:84:LYS:HB3	2.14	0.47
21:1V:18:THR:OG1	21:1V:21:GLU:OE2	2.32	0.47
31:1f:11:TRP:O	31:1f:14:ILE:HG22	2.14	0.47
32:1g:85:MET:HE2	32:1g:85:MET:N	2.26	0.47
35:1j:33:TRP:O	35:1j:37:LEU:HD12	2.14	0.47
39:1n:178:MET:N	39:1n:178:MET:SD	2.87	0.47
4:1D:241:ASP:N	4:1D:292:ASP:OD2	2.35	0.47
4:1D:328:ALA:H	7:1G:126:ASP:HB2	1.79	0.47
4:1D:395:GLY:N	4:1D:427:GLU:OE2	2.35	0.47
6:1F:49:LEU:HD13	6:1F:127:ARG:HB2	1.96	0.47
6:1F:351:ILE:HD11	6:1F:372:MET:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:243:ARG:HD2	7:1G:244:THR:OG1	2.13	0.47
7:1G:283:MET:HG3	7:1G:291:LEU:HB3	1.95	0.47
7:1G:331:LEU:HA	7:1G:334:LEU:HB3	1.96	0.47
9:1I:9:GLU:N	9:1I:9:GLU:OE1	2.47	0.47
12:1L:49:VAL:HG22	41:1p:32:LEU:HG	1.96	0.47
14:1N:324:LYS:HA	14:1N:324:LYS:HD2	1.64	0.47
16:1P:90:VAL:HG11	16:1P:218:ILE:HG23	1.96	0.47
20:1T:65:ILE:HD12	20:1T:66:ASP:N	2.29	0.47
20:1U:71:MET:O	20:1U:71:MET:HE3	2.15	0.47
21:1V:47:THR:O	21:1V:51:THR:OG1	2.23	0.47
25:1Z:138:TYR:HB2	25:1Z:142:TRP:NE1	2.29	0.47
37:1l:80:ASP:CG	37:1l:83:MET:HE3	2.40	0.47
42:1q:96:ASP:OD2	42:1q:101:LYS:NZ	2.47	0.47
3:1C:155:TYR:HB2	22:1W:102:HIS:CE1	2.49	0.47
5:1E:36:LYS:HB3	5:1E:36:LYS:HE3	1.53	0.47
11:1K:37:MET:HG2	11:1K:67:ALA:HB1	1.96	0.47
12:1L:488:MET:HE1	35:1j:47:VAL:O	2.14	0.47
51:1M:501:PGT:H181	51:1M:501:PGT:H152	1.60	0.47
36:1k:17:ASP:OD1	36:1k:19:LYS:HG2	2.14	0.47
3:1C:7:THR:HG22	3:1C:8:ARG:HD3	1.96	0.47
3:1C:158:GLU:OE1	17:1Q:24:GLY:HA3	2.14	0.47
5:1E:201:SER:HB3	6:1F:20:ARG:NH2	2.29	0.47
6:1F:256:PHE:CD1	6:1F:279:LEU:HD11	2.47	0.47
7:1G:174:THR:O	7:1G:174:THR:OG1	2.28	0.47
7:1G:276:ARG:HA	42:1q:135:GLN:HE22	1.79	0.47
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	1.96	0.47
34:1i:52:ASP:HB2	34:1i:57:LYS:HE3	1.97	0.47
3:1C:175:ARG:NH1	16:1P:13:ARG:HE	2.13	0.47
7:1G:511:VAL:O	7:1G:514:ILE:HG22	2.14	0.47
9:1I:15:LYS:HE2	9:1I:15:LYS:HA	1.95	0.47
9:1I:81:LYS:N	46:1I:202:SF4:S4	2.78	0.47
10:1J:8:ILE:O	10:1J:12:ILE:HD12	2.14	0.47
10:1J:123:GLY:O	10:1J:126:VAL:HG22	2.15	0.47
10:1J:162:LEU:O	10:1J:166:VAL:HG23	2.14	0.47
12:1L:142:ILE:HD11	13:1M:371:PRO:HB3	1.95	0.47
12:1L:535:ARG:NH1	37:1l:90:ASP:OD2	2.48	0.47
45:1L:701:3PE:H112	45:1L:701:3PE:H11	1.96	0.47
14:1N:30:TRP:NE1	14:1N:34:GLU:OE2	2.48	0.47
14:1N:272:LYS:HG2	33:1h:108:LEU:HD21	1.97	0.47
16:1P:111:VAL:C	16:1P:114:PRO:HD2	2.39	0.47
20:1U:9:GLU:HA	20:1U:12:LYS:HE3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:84:LYS:HB2	20:1U:84:LYS:HE2	1.59	0.47
26:1a:6:LEU:HD13	26:1a:9:ILE:HD11	1.96	0.47
32:1g:36:ASN:O	32:1g:39:GLU:HG3	2.14	0.47
36:1k:18:TYR:OH	36:1k:46:ARG:O	2.33	0.47
3:1C:206:PHE:CZ	4:1D:359:PRO:HA	2.50	0.47
4:1D:293:CYS:SG	4:1D:420:THR:HG21	2.54	0.47
5:1E:119:ALA:HB3	5:1E:169:ILE:HD11	1.96	0.47
7:1G:36:GLN:HG3	7:1G:39:ARG:NH2	2.29	0.47
7:1G:54:MET:HA	7:1G:93:VAL:HG11	1.97	0.47
7:1G:56:LEU:HD12	7:1G:67:ALA:HA	1.97	0.47
7:1G:354:ALA:HB1	7:1G:358:LEU:HB2	1.96	0.47
14:1N:300:SER:OG	14:1N:301:SER:N	2.48	0.47
15:1O:57:HIS:ND1	15:1O:68:PRO:HB3	2.29	0.47
15:1O:221:LEU:HG	15:1O:223:TYR:HE1	1.80	0.47
18:1R:73:ILE:HG21	18:1R:84:CYS:HA	1.96	0.47
20:1U:11:ILE:HG22	20:1U:77:VAL:HG22	1.94	0.47
22:1W:46:THR:O	22:1W:50:PHE:HB2	2.15	0.47
22:1W:66:MET:HA	22:1W:69:LYS:HE2	1.96	0.47
22:1W:87:LYS:O	22:1W:87:LYS:HD3	2.15	0.47
37:1l:97:SER:HA	38:1m:5:TYR:CD1	2.49	0.47
42:1q:1:MET:HE2	42:1q:1:MET:HA	1.96	0.47
2:1B:91:THR:HG21	4:1D:85:ARG:HH11	1.80	0.47
4:1D:62:LEU:HD12	4:1D:63:ARG:N	2.30	0.47
5:1E:40:GLU:HG2	44:1s:67:SER:HA	1.95	0.47
5:1E:101:GLN:O	5:1E:154:VAL:HA	2.15	0.47
6:1F:134:ALA:HB3	6:1F:175:VAL:HA	1.96	0.47
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.80	0.47
7:1G:276:ARG:HE	42:1q:135:GLN:NE2	2.12	0.47
7:1G:335:LEU:HD23	7:1G:335:LEU:HA	1.76	0.47
7:1G:575:ASN:ND2	7:1G:579:ARG:HG2	2.28	0.47
7:1G:675:ASP:OD2	7:1G:677:ILE:N	2.47	0.47
8:1H:117:LEU:HD11	10:1J:69:GLY:HA3	1.97	0.47
8:1H:190:LEU:HD22	8:1H:198:PHE:HD1	1.80	0.47
12:1L:163:ASP:N	12:1L:163:ASP:OD1	2.48	0.47
12:1L:489:THR:O	12:1L:493:VAL:HG22	2.15	0.47
13:1M:17:MET:HG2	31:1f:11:TRP:CZ2	2.49	0.47
13:1M:30:HIS:O	13:1M:34:ILE:HG12	2.14	0.47
51:1M:501:PGT:H2	14:1N:276:ILE:HD12	1.95	0.47
15:1O:145:ARG:HE	15:1O:147:GLN:HB2	1.80	0.47
16:1P:197:GLY:HA2	16:1P:288:HIS:CE1	2.50	0.47
16:1P:311:GLU:OE1	16:1P:336:PRO:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:24:LYS:O	21:1V:28:THR:HG23	2.15	0.47
22:1W:55:SER:OG	22:1W:57:LYS:NZ	2.42	0.47
22:1W:63:VAL:O	22:1W:67:PHE:HD1	1.98	0.47
25:1Z:97:ILE:HD11	30:1e:82:ARG:HA	1.97	0.47
33:1h:21:PHE:CE2	33:1h:25:MET:HE1	2.49	0.47
37:1l:13:TYR:HD1	37:1l:14:PRO:HD2	1.80	0.47
38:1m:48:LEU:HD23	39:1n:165:LEU:HD21	1.97	0.47
39:1n:153:LEU:HD11	39:1n:165:LEU:HD12	1.97	0.47
4:1D:61:VAL:HG21	4:1D:83:LEU:HB2	1.96	0.47
5:1E:155:GLN:NE2	5:1E:160:TYR:HB3	2.29	0.47
7:1G:234:VAL:HG11	7:1G:390:LEU:HB2	1.96	0.47
10:1J:59:ILE:HD12	10:1J:60:TYR:N	2.30	0.47
12:1L:554:ASP:OD1	13:1M:288:TYR:OH	2.31	0.47
13:1M:163:ALA:O	13:1M:167:ILE:HG12	2.15	0.47
13:1M:176:PHE:CE1	13:1M:245:ARG:HB3	2.50	0.47
14:1N:109:SER:HB3	14:1N:157:MET:SD	2.55	0.47
15:1O:156:LYS:O	15:1O:160:ALA:N	2.46	0.47
16:1P:147:ARG:O	16:1P:151:VAL:HG22	2.15	0.47
25:1Z:68:ARG:HG3	26:1a:43:TYR:CE1	2.50	0.47
37:1l:7:ASP:N	37:1l:7:ASP:OD1	2.48	0.47
38:1m:44:ARG:HH22	39:1n:143:THR:HG23	1.80	0.47
40:1o:91:HIS:O	40:1o:95:VAL:HG12	2.15	0.47
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.41	0.47
6:1F:281:GLU:OE1	6:1F:286:GLY:HA2	2.14	0.47
14:1N:175:LEU:HD13	14:1N:219:LEU:HD11	1.97	0.47
16:1P:46:ILE:HG21	16:1P:84:VAL:HB	1.96	0.47
17:1Q:9:GLN:OE1	22:1W:19:PRO:HG3	2.13	0.47
19:1S:14:GLY:O	19:1S:69:ALA:N	2.47	0.47
21:1V:37:ILE:HD12	21:1V:38:PRO:CD	2.40	0.47
23:1X:157:LEU:HG	29:1d:21:LEU:HD21	1.96	0.47
34:1i:10:ARG:HH11	39:1n:163:PRO:HB2	1.80	0.47
36:1k:14:GLU:H	36:1k:14:GLU:CD	2.23	0.47
3:1C:90:PHE:CD2	3:1C:140:VAL:HB	2.50	0.47
5:1E:86:PHE:HD2	6:1F:200:GLN:HB2	1.80	0.47
6:1F:254:LYS:HD3	6:1F:255:LEU:N	2.30	0.47
7:1G:114:CYS:HB3	7:1G:117:GLN:HB2	1.96	0.47
7:1G:380:VAL:HA	7:1G:409:ILE:HD11	1.97	0.47
8:1H:127:TYR:HE1	8:1H:207:LEU:HD13	1.80	0.47
10:1J:86:ASN:ND2	10:1J:88:THR:OG1	2.46	0.47
12:1L:61:MET:HB2	12:1L:82:MET:HB2	1.96	0.47
14:1N:238:PRO:HB2	45:1N:401:3PE:C31	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:83:TYR:HD2	15:1O:190:HIS:HB3	1.80	0.47
17:1Q:108:ARG:NH1	17:1Q:108:ARG:HB2	2.29	0.47
20:1U:21:LEU:HD21	36:1k:47:ASN:N	2.30	0.47
20:1U:69:LYS:HZ2	34:1i:2:GLY:C	2.22	0.47
22:1W:40:TYR:CD2	22:1W:60:ARG:HD2	2.50	0.47
23:1X:51:ASP:HB3	23:1X:54:ARG:HG2	1.97	0.47
41:1p:116:GLU:OE2	41:1p:123:ASN:ND2	2.48	0.47
3:1C:34:PRO:O	21:1V:102:LEU:HD23	2.14	0.46
3:1C:198:ASP:OD1	3:1C:198:ASP:N	2.39	0.46
6:1F:66:ARG:HA	6:1F:74:PRO:HA	1.96	0.46
6:1F:82:MET:SD	6:1F:83:ASN:ND2	2.88	0.46
6:1F:93:LEU:O	6:1F:135:TYR:N	2.41	0.46
6:1F:101:GLU:OE2	6:1F:302:SER:N	2.46	0.46
8:1H:287:HIS:CE1	8:1H:291:LYS:HG3	2.49	0.46
12:1L:339:LEU:HD21	12:1L:376:GLY:HA3	1.96	0.46
12:1L:373:LEU:HD23	12:1L:431:PHE:CE2	2.50	0.46
13:1M:26:ASN:OD1	31:1f:13:HIS:HE1	1.98	0.46
13:1M:29:VAL:HG22	32:1g:60:VAL:HG11	1.97	0.46
15:1O:100:LEU:HD13	53:1O:401:GTP:C2	2.51	0.46
20:1T:37:MET:HG2	20:1T:38:LYS:HG3	1.96	0.46
20:1T:66:ASP:HB2	20:1T:69:LYS:HE3	1.97	0.46
27:1b:59:ASP:OD1	27:1b:59:ASP:N	2.37	0.46
27:1b:68:HIS:CE1	27:1b:70:GLN:HG3	2.50	0.46
35:1j:59:TRP:O	40:1o:106:ARG:NH1	2.30	0.46
38:1m:117:GLU:OE1	38:1m:117:GLU:N	2.48	0.46
1:1A:2:ASN:HB3	8:1H:2:PHE:CZ	2.50	0.46
2:1B:69:MET:HG2	2:1B:74:VAL:HG23	1.97	0.46
3:1C:101:PHE:HE1	43:1r:99:PRO:HG3	1.80	0.46
3:1C:182:ARG:HD2	22:1W:101:THR:HA	1.97	0.46
4:1D:309:ARG:HD2	25:1Z:21:TYR:CZ	2.50	0.46
6:1F:20:ARG:HG3	6:1F:269:GLU:HG3	1.98	0.46
6:1F:255:LEU:H	6:1F:255:LEU:HD12	1.80	0.46
6:1F:293:ASN:O	6:1F:339:ARG:HG2	2.15	0.46
7:1G:194:GLU:H	7:1G:194:GLU:CD	2.23	0.46
7:1G:199:ILE:HD12	7:1G:200:ILE:N	2.30	0.46
7:1G:380:VAL:HB	7:1G:453:LEU:HA	1.96	0.46
8:1H:288:LEU:HD11	50:1I:203:PC1:O22	2.15	0.46
12:1L:288:THR:HG21	12:1L:307:SER:HB2	1.97	0.46
12:1L:297:ASP:HB3	12:1L:300:LYS:HG2	1.96	0.46
13:1M:286:ILE:O	13:1M:289:SER:OG	2.29	0.46
14:1N:335:LEU:O	29:1d:37:LEU:HD21	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:1N:402:CDL:H751	52:1N:402:CDL:H611	1.97	0.46
18:1R:60:ASP:OD1	18:1R:60:ASP:C	2.59	0.46
33:1h:56:PRO:HG2	33:1h:59:TYR:HD2	1.79	0.46
36:1k:47:ASN:HB3	36:1k:48:GLU:OE2	2.15	0.46
44:1s:40:ASN:HD22	44:1s:43:HIS:HD2	1.62	0.46
1:1A:104:TYR:CE2	10:1J:166:VAL:HG22	2.50	0.46
2:1B:112:TYR:CZ	2:1B:167:ILE:HD11	2.50	0.46
3:1C:53:HIS:HD1	3:1C:55:ASP:H	1.62	0.46
3:1C:137:MET:HB3	3:1C:162:PHE:CG	2.51	0.46
3:1C:211:GLN:NE2	21:1V:115:ILE:O	2.48	0.46
4:1D:362:ALA:HB1	4:1D:377:TYR:CE1	2.51	0.46
7:1G:119:GLN:O	7:1G:123:PHE:N	2.47	0.46
7:1G:380:VAL:HG13	7:1G:409:ILE:HD11	1.96	0.46
7:1G:585:VAL:O	17:1Q:61:THR:OG1	2.32	0.46
12:1L:324:LEU:HD21	12:1L:476:THR:HG21	1.96	0.46
12:1L:539:TYR:HE2	38:1m:9:ARG:HH21	1.62	0.46
12:1L:573:MET:HB2	14:1N:167:TRP:CZ2	2.49	0.46
13:1M:357:THR:O	13:1M:361:MET:HG2	2.15	0.46
15:1O:139:TYR:HD2	15:1O:140:ARG:HH12	1.63	0.46
24:1Y:139:LYS:HE2	33:1h:112:ARG:HD2	1.96	0.46
25:1Z:140:PHE:HB2	26:1a:45:TRP:CG	2.51	0.46
1:1A:57:LEU:HD12	10:1J:172:THR:HG21	1.98	0.46
1:1A:80:GLN:OE1	8:1H:317:GLN:N	2.48	0.46
4:1D:180:PHE:O	4:1D:184:VAL:HG22	2.15	0.46
7:1G:94:MET:SD	7:1G:120:SER:OG	2.73	0.46
7:1G:145:LEU:HD21	7:1G:192:MET:HE1	1.96	0.46
7:1G:571:ALA:N	7:1G:583:THR:OG1	2.45	0.46
10:1J:95:SER:O	10:1J:99:MET:HE1	2.16	0.46
11:1K:97:GLN:OE1	11:1K:97:GLN:HA	2.16	0.46
12:1L:525:MET:HE3	12:1L:525:MET:HB3	1.73	0.46
13:1M:433:GLU:O	13:1M:437:MET:HG2	2.15	0.46
20:1T:34:SER:HB3	20:1T:40:LEU:HD21	1.96	0.46
20:1U:35:HIS:ND1	20:1U:71:MET:HE2	2.30	0.46
32:1g:56:TRP:O	32:1g:60:VAL:HG23	2.16	0.46
34:1i:68:ILE:O	34:1i:72:THR:HG23	2.15	0.46
37:1l:34:TYR:CD1	37:1l:48:PRO:HB3	2.50	0.46
44:1s:34:ASP:OD2	44:1s:39:ARG:NH2	2.48	0.46
2:1B:47:PRO:HA	2:1B:85:VAL:O	2.16	0.46
6:1F:242:PHE:CZ	6:1F:252:GLY:HA3	2.51	0.46
7:1G:27:LEU:HD23	7:1G:69:CYS:HA	1.96	0.46
7:1G:448:LYS:HA	7:1G:448:LYS:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:675:ASP:OD2	7:1G:675:ASP:C	2.59	0.46
8:1H:303:TRP:HE3	27:1b:28:ALA:HB2	1.79	0.46
13:1M:32:LEU:O	13:1M:35:SER:OG	2.30	0.46
13:1M:278:ARG:NH2	37:1l:82:ASP:OD1	2.48	0.46
14:1N:218:LEU:HD11	14:1N:330:ILE:HD11	1.97	0.46
16:1P:182:PHE:N	16:1P:182:PHE:CD1	2.81	0.46
23:1X:141:TYR:O	25:1Z:115:ARG:NH1	2.43	0.46
25:1Z:20:ASP:OD1	25:1Z:20:ASP:N	2.48	0.46
33:1h:34:ILE:CG1	33:1h:35:PRO:HD3	2.45	0.46
35:1j:14:PHE:HE1	35:1j:17:LEU:HD11	1.80	0.46
35:1j:45:ASP:HB2	35:1j:50:HIS:HB2	1.98	0.46
5:1E:48:LEU:O	5:1E:90:TYR:OH	2.34	0.46
6:1F:226:GLU:HG3	6:1F:254:LYS:NZ	2.29	0.46
7:1G:59:ILE:HG21	7:1G:77:TRP:NE1	2.31	0.46
7:1G:628:PRO:HD3	19:1S:21:HIS:CE1	2.50	0.46
12:1L:293:ILE:HD12	12:1L:294:THR:HG23	1.98	0.46
14:1N:244:MET:HE2	14:1N:244:MET:HA	1.96	0.46
14:1N:268:GLN:HG3	23:1X:167:PHE:HZ	1.80	0.46
15:1O:65:ASP:OD2	15:1O:67:LYS:NZ	2.48	0.46
20:1T:11:ILE:HD12	20:1T:81:ALA:HB2	1.96	0.46
20:1T:26:ASP:H	20:1T:29:LYS:HE3	1.80	0.46
20:1T:52:MET:SD	22:1W:41:ARG:NH2	2.89	0.46
24:1Y:49:LEU:HD23	24:1Y:49:LEU:H	1.81	0.46
30:1e:73:LYS:HA	30:1e:73:LYS:HD2	1.62	0.46
33:1h:62:GLU:OE1	33:1h:63:HIS:N	2.48	0.46
34:1i:7:GLU:HA	34:1i:10:ARG:HB3	1.97	0.46
35:1j:67:LEU:HG	40:1o:29:GLY:HA2	1.97	0.46
36:1k:23:ILE:HD11	36:1k:32:GLN:HB2	1.97	0.46
1:1A:1:FME:CN	1:1A:3:ILE:HG22	2.45	0.46
2:1B:48:MET:HE1	2:1B:80:PRO:HA	1.98	0.46
2:1B:117:GLY:O	2:1B:121:ASN:ND2	2.49	0.46
4:1D:76:CYS:SG	4:1D:403:ASP:HA	2.56	0.46
6:1F:144:ASN:HB2	44:1s:43:HIS:HB2	1.98	0.46
8:1H:183:MET:HE2	8:1H:183:MET:HB3	1.86	0.46
11:1K:25:HIS:ND1	11:1K:88:ASP:OD2	2.42	0.46
13:1M:302:MET:HE2	13:1M:302:MET:HB2	1.76	0.46
15:1O:104:ARG:HG3	15:1O:128:ILE:HG22	1.98	0.46
15:1O:308:TYR:CZ	29:1d:51:ARG:HD3	2.51	0.46
16:1P:278:TRP:CD1	16:1P:278:TRP:H	2.32	0.46
16:1P:283:LYS:HA	16:1P:286:ARG:HB2	1.98	0.46
17:1Q:62:ARG:HD3	17:1Q:62:ARG:HA	1.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:38:ASN:HB3	18:1R:43:LEU:HD11	1.97	0.46
37:1l:66:HIS:O	37:1l:70:ARG:N	2.49	0.46
1:1A:41:PHE:CE2	4:1D:63:ARG:HD3	2.50	0.46
2:1B:68:ASP:O	2:1B:68:ASP:OD2	2.33	0.46
3:1C:67:HIS:HB3	3:1C:70:ALA:HB3	1.98	0.46
3:1C:192:GLN:HE21	3:1C:192:GLN:HB3	1.59	0.46
4:1D:255:PHE:CZ	4:1D:401:GLY:HA3	2.51	0.46
6:1F:15:LEU:HD13	6:1F:271:GLU:HA	1.97	0.46
7:1G:487:TRP:HD1	7:1G:489:VAL:HG22	1.80	0.46
9:1I:43:ARG:CZ	43:1r:19:LEU:HG	2.46	0.46
10:1J:12:ILE:HB	10:1J:39:VAL:HG21	1.97	0.46
12:1L:14:ILE:HD12	34:1i:73:HIS:O	2.15	0.46
12:1L:338:MET:HE1	12:1L:461:SER:OG	2.16	0.46
14:1N:97:MET:HA	14:1N:97:MET:HE2	1.98	0.46
15:1O:179:ILE:O	15:1O:183:ILE:HG12	2.16	0.46
16:1P:185:MET:HA	16:1P:188:PHE:HD2	1.81	0.46
20:1U:11:ILE:HG12	20:1U:80:ILE:HG21	1.98	0.46
21:1V:17:GLU:HG2	21:1V:18:THR:HG23	1.98	0.46
22:1W:20:ILE:HG13	22:1W:21:PHE:N	2.30	0.46
33:1h:12:LYS:O	39:1n:106:TRP:NE1	2.47	0.46
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.96	0.46
40:1o:46:ASN:HA	40:1o:55:ARG:HH22	1.79	0.46
42:1q:73:THR:HG21	42:1q:81:MET:HE1	1.98	0.46
42:1q:86:TRP:CE3	42:1q:98:PRO:HD2	2.51	0.46
1:1A:66:ASP:OD2	10:1J:59:ILE:HG22	2.16	0.46
7:1G:61:LYS:HE3	7:1G:61:LYS:HB3	1.83	0.46
7:1G:181:MET:HE2	7:1G:181:MET:HA	1.97	0.46
7:1G:599:ILE:HG22	22:1W:122:PHE:HZ	1.81	0.46
11:1K:2:PRO:HG2	11:1K:5:TYR:CD2	2.50	0.46
12:1L:400:ASN:HA	12:1L:409:LEU:HD13	1.97	0.46
14:1N:118:VAL:O	14:1N:122:ILE:HG13	2.16	0.46
15:1O:33:SER:HA	15:1O:182:ARG:NH2	2.30	0.46
24:1Y:40:ILE:HG23	24:1Y:45:PRO:HG3	1.98	0.46
29:1d:105:ASP:O	29:1d:107:LYS:NZ	2.49	0.46
34:1i:47:ASN:O	34:1i:51:GLN:HG2	2.16	0.46
35:1j:70:ASP:OD1	35:1j:70:ASP:N	2.46	0.46
41:1p:23:THR:HB	41:1p:25:LEU:HD23	1.98	0.46
41:1p:72:ASP:OD1	41:1p:74:THR:HG22	2.15	0.46
43:1r:102:ARG:HE	43:1r:103:TRP:N	2.13	0.46
2:1B:61:HIS:CE1	4:1D:174:ARG:HB3	2.51	0.46
6:1F:106:LYS:HD3	6:1F:255:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:271:LYS:HA	12:1L:274:GLN:NE2	2.31	0.46
12:1L:560:THR:O	12:1L:565:THR:OG1	2.29	0.46
13:1M:22:MET:O	13:1M:26:ASN:ND2	2.49	0.46
23:1X:146:ARG:CZ	23:1X:146:ARG:HA	2.46	0.46
45:1Y:201:3PE:H2	45:1Y:201:3PE:H221	1.55	0.46
34:1i:58:ASN:OD1	34:1i:59:VAL:N	2.49	0.46
42:1q:141:SER:O	42:1q:142:THR:HB	2.16	0.46
6:1F:63:SER:HB2	6:1F:234:ILE:HD13	1.99	0.45
6:1F:361:GLN:O	7:1G:51:ASN:HB3	2.16	0.45
7:1G:185:THR:OG1	7:1G:187:ILE:O	2.27	0.45
10:1J:52:LEU:HD21	10:1J:143:ILE:HD11	1.98	0.45
12:1L:10:THR:O	12:1L:14:ILE:HG12	2.16	0.45
12:1L:160:GLY:HA3	39:1n:94:GLU:OE1	2.16	0.45
12:1L:482:MET:SD	12:1L:482:MET:N	2.89	0.45
13:1M:30:HIS:HD2	31:1f:16:VAL:HB	1.81	0.45
14:1N:55:ALA:HB2	14:1N:121:GLY:HA3	1.97	0.45
17:1Q:63:GLU:HG2	17:1Q:65:TRP:HE3	1.81	0.45
20:1U:63:PRO:HB2	20:1U:65:ILE:HG22	1.98	0.45
22:1W:21:PHE:HB3	22:1W:31:ARG:HH12	1.82	0.45
22:1W:76:PRO:HA	22:1W:79:VAL:HG12	1.98	0.45
25:1Z:76:GLN:O	25:1Z:80:ASP:HB2	2.16	0.45
25:1Z:97:ILE:HG23	25:1Z:98:MET:HE3	1.97	0.45
41:1p:35:ILE:O	41:1p:39:LEU:HB2	2.16	0.45
43:1r:45:SER:C	43:1r:51:ASN:HD21	2.24	0.45
3:1C:72:PHE:CE2	3:1C:105:ILE:HG12	2.51	0.45
4:1D:5:GLN:NE2	14:1N:304:MET:HB2	2.31	0.45
4:1D:23:LYS:HE3	4:1D:23:LYS:HB3	1.73	0.45
4:1D:357:GLN:OE1	43:1r:59:ARG:NH2	2.45	0.45
5:1E:86:PHE:O	7:1G:177:ARG:NH2	2.49	0.45
6:1F:28:ARG:HD3	44:1s:37:THR:O	2.17	0.45
6:1F:82:MET:HE3	6:1F:91:LYS:HZ3	1.81	0.45
6:1F:391:SER:O	6:1F:395:ILE:HG13	2.16	0.45
10:1J:167:VAL:O	10:1J:171:ILE:HG22	2.16	0.45
12:1L:88:MET:O	12:1L:91:PRO:HD2	2.16	0.45
12:1L:203:MET:HE3	12:1L:203:MET:HA	1.98	0.45
13:1M:193:ILE:HG23	13:1M:257:MET:SD	2.56	0.45
15:1O:111:ALA:HB1	15:1O:122:VAL:HG21	1.99	0.45
16:1P:41:MET:SD	16:1P:41:MET:N	2.78	0.45
17:1Q:53:LYS:C	17:1Q:54:LYS:HD2	2.40	0.45
18:1R:20:ASP:OD1	18:1R:21:GLY:N	2.44	0.45
20:1U:46:ASP:N	20:1U:46:ASP:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:40:VAL:HG12	3:1C:50:ILE:HD12	1.99	0.45
7:1G:104:ASP:O	7:1G:108:CYS:N	2.48	0.45
11:1K:93:LEU:HD21	14:1N:57:THR:HG21	1.97	0.45
12:1L:81:LYS:HD2	12:1L:81:LYS:O	2.15	0.45
15:1O:207:LYS:HA	15:1O:207:LYS:HE2	1.98	0.45
21:1V:23:LEU:HD22	21:1V:58:VAL:HG21	1.97	0.45
21:1V:88:SER:O	21:1V:92:LYS:HD3	2.16	0.45
32:1g:90:ARG:HA	32:1g:90:ARG:HD3	1.75	0.45
38:1m:45:GLU:OE1	38:1m:45:GLU:N	2.50	0.45
41:1p:48:ARG:O	41:1p:52:GLU:HG2	2.17	0.45
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.52	0.45
7:1G:226:GLU:HG3	17:1Q:38:PHE:CE2	2.51	0.45
9:1I:54:LYS:HG3	42:1q:91:HIS:NE2	2.32	0.45
12:1L:80:PHE:HB3	12:1L:82:MET:HE3	1.98	0.45
12:1L:240:PRO:HD2	12:1L:243:VAL:HG21	1.98	0.45
14:1N:274:GLU:HG3	14:1N:274:GLU:O	2.16	0.45
20:1U:28:GLU:H	20:1U:28:GLU:CD	2.23	0.45
22:1W:92:GLU:HG2	22:1W:98:LYS:CG	2.46	0.45
23:1X:12:LEU:HD21	25:1Z:84:LEU:HD11	1.97	0.45
35:1j:64:LEU:HD21	40:1o:102:GLU:CD	2.41	0.45
43:1r:47:LYS:HG2	43:1r:51:ASN:HD22	1.81	0.45
44:1s:68:SER:O	44:1s:68:SER:OG	2.22	0.45
1:1A:68:GLU:OE2	10:1J:161:LEU:HB3	2.17	0.45
4:1D:103:PHE:HB3	4:1D:114:ASN:HB3	1.98	0.45
6:1F:134:ALA:N	6:1F:174:ASP:O	2.49	0.45
6:1F:154:ARG:HH22	44:1s:58:LEU:HA	1.81	0.45
7:1G:45:ARG:HH22	7:1G:261:GLU:CG	2.27	0.45
7:1G:448:LYS:NZ	7:1G:484:THR:HG22	2.30	0.45
7:1G:603:LEU:HD12	7:1G:604:SER:N	2.32	0.45
8:1H:28:LEU:HD11	8:1H:274:ARG:HD3	1.98	0.45
8:1H:81:LEU:HA	8:1H:84:THR:HG22	1.99	0.45
8:1H:296:LEU:HD13	8:1H:300:LEU:HD23	1.99	0.45
12:1L:339:LEU:HD22	12:1L:373:LEU:HD12	1.98	0.45
13:1M:71:TRP:CZ3	32:1g:69:VAL:HG11	2.51	0.45
20:1U:17:TYR:OH	36:1k:16:PRO:O	2.15	0.45
21:1V:43:TYR:CE1	21:1V:47:THR:HG21	2.51	0.45
50:1f:101:PC1:H31	50:1f:101:PC1:H322	1.32	0.45
32:1g:75:THR:HG21	33:1h:36:VAL:HG11	1.99	0.45
33:1h:68:LYS:HB3	41:1p:62:TYR:CZ	2.52	0.45
34:1i:59:VAL:HG23	34:1i:60:ILE:HG23	1.98	0.45
35:1j:63:GLU:HG2	35:1j:64:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:1l:25:LYS:O	37:1l:25:LYS:HD3	2.16	0.45
39:1n:10:THR:N	39:1n:13:GLN:OE1	2.49	0.45
39:1n:106:TRP:CE3	39:1n:110:GLU:HB3	2.52	0.45
40:1o:34:LYS:HA	40:1o:34:LYS:HD2	1.80	0.45
40:1o:107:LEU:HD23	40:1o:107:LEU:HA	1.86	0.45
43:1r:8:GLN:HG2	43:1r:11:ARG:NH1	2.32	0.45
4:1D:413:ASP:OD1	8:1H:281:ARG:HD3	2.16	0.45
5:1E:146:GLY:HA3	6:1F:142:PHE:HZ	1.80	0.45
6:1F:276:LEU:HD23	6:1F:276:LEU:H	1.81	0.45
7:1G:88:LYS:HE3	7:1G:88:LYS:HB2	1.77	0.45
7:1G:333:ASP:HB3	7:1G:611:LEU:HD11	1.98	0.45
7:1G:655:GLN:HG3	7:1G:656:LEU:H	1.81	0.45
8:1H:132:ALA:O	8:1H:136:VAL:HG12	2.17	0.45
9:1I:30:LEU:HD12	50:1I:203:PC1:H231	1.99	0.45
12:1L:79:SER:HB2	12:1L:135:ASN:HB3	1.99	0.45
12:1L:108:MET:HB3	12:1L:114:ILE:HD13	1.97	0.45
13:1M:45:LEU:O	32:1g:84:ARG:NH1	2.49	0.45
14:1N:103:ALA:O	14:1N:107:GLY:N	2.41	0.45
16:1P:69:ILE:HD12	18:1R:26:VAL:HG13	1.97	0.45
16:1P:170:ASP:OD1	16:1P:170:ASP:N	2.49	0.45
16:1P:315:ILE:O	16:1P:319:ARG:HB2	2.17	0.45
21:1V:98:PRO:HD2	21:1V:99:TRP:CE2	2.52	0.45
22:1W:25:MET:HA	22:1W:28:ALA:HB3	1.97	0.45
30:1e:88:GLU:OE1	30:1e:88:GLU:N	2.50	0.45
42:1q:54:GLN:HB2	42:1q:59:HIS:HA	1.98	0.45
1:1A:3:ILE:HG23	1:1A:4:MET:H	1.81	0.45
4:1D:107:ASP:HB3	4:1D:114:ASN:HD21	1.80	0.45
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	1.98	0.45
6:1F:277:LYS:HE2	6:1F:277:LYS:HB2	1.64	0.45
7:1G:286:ASN:N	7:1G:290:LEU:O	2.47	0.45
8:1H:33:LEU:O	8:1H:33:LEU:HD23	2.17	0.45
9:1I:80:CYS:SG	9:1I:82:LEU:HB2	2.57	0.45
9:1I:175:TYR:CE1	43:1r:38:PRO:HG3	2.50	0.45
12:1L:144:TRP:CH2	12:1L:256:GLY:HA2	2.52	0.45
13:1M:201:MET:HG2	51:1M:501:PGT:H441	1.98	0.45
13:1M:360:LEU:O	13:1M:364:LEU:HG	2.17	0.45
16:1P:193:LEU:O	16:1P:257:PRO:HA	2.16	0.45
16:1P:301:GLU:H	16:1P:301:GLU:CD	2.15	0.45
19:1S:35:PHE:HB2	19:1S:86:VAL:HG21	1.98	0.45
21:1V:34:LEU:O	21:1V:44:ARG:NH2	2.50	0.45
22:1W:43:VAL:HG12	22:1W:56:VAL:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:55:ARG:O	25:1Z:59:ARG:HG3	2.17	0.45
29:1d:25:LYS:HE3	29:1d:25:LYS:HB3	1.87	0.45
36:1k:18:TYR:OH	36:1k:46:ARG:HB3	2.16	0.45
37:1l:50:LEU:HD12	37:1l:78:HIS:HA	1.98	0.45
40:1o:46:ASN:HA	40:1o:55:ARG:HH12	1.81	0.45
3:1C:16:ASP:HB3	3:1C:20:LYS:NZ	2.32	0.45
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	1.98	0.45
4:1D:132:PRO:HA	4:1D:135:GLN:HG3	1.99	0.45
5:1E:30:ARG:HB3	44:1s:52:LEU:HD12	1.98	0.45
5:1E:148:CYS:CB	47:1E:301:FES:S2	3.04	0.45
7:1G:528:ASP:OD2	7:1G:545:TYR:OH	2.17	0.45
9:1I:148:LEU:HD11	16:1P:65:LEU:HD22	1.99	0.45
10:1J:98:MET:HE2	10:1J:98:MET:HA	1.99	0.45
12:1L:533:MET:O	12:1L:533:MET:HE3	2.17	0.45
13:1M:244:MET:SD	13:1M:301:ILE:HD13	2.57	0.45
15:1O:45:LYS:HD3	15:1O:235:VAL:HG21	1.97	0.45
16:1P:119:GLN:HE22	16:1P:120:VAL:HG13	1.82	0.45
16:1P:210:VAL:O	16:1P:214:ILE:HG12	2.16	0.45
20:1T:51:ILE:HA	20:1T:54:MET:HB2	1.98	0.45
33:1h:91:MET:HE3	33:1h:91:MET:HB3	1.85	0.45
34:1i:120:LYS:HD2	40:1o:39:VAL:HG23	1.99	0.45
35:1j:34:PHE:CD1	35:1j:34:PHE:C	2.95	0.45
37:1l:115:MET:HA	37:1l:118:VAL:HG22	1.99	0.45
39:1n:120:LYS:HA	39:1n:123:GLN:HG2	1.98	0.45
41:1p:145:LEU:HD23	41:1p:145:LEU:HA	1.82	0.45
43:1r:50:ASN:OD1	43:1r:50:ASN:N	2.49	0.45
1:1A:44:MET:SD	1:1A:44:MET:N	2.75	0.45
1:1A:73:LEU:O	1:1A:76:PRO:HD2	2.17	0.45
3:1C:32:ILE:HG22	3:1C:33:LEU:HG	1.99	0.45
6:1F:268:VAL:HG12	6:1F:270:GLU:HB2	1.98	0.45
7:1G:296:TRP:HZ3	7:1G:561:LEU:HD22	1.82	0.45
8:1H:235:ASN:ND2	8:1H:266:LEU:HB3	2.31	0.45
9:1I:69:ARG:HD3	42:1q:108:TYR:CG	2.52	0.45
12:1L:557:TRP:O	12:1L:561:ILE:HG22	2.16	0.45
12:1L:564:LYS:HD3	12:1L:564:LYS:HA	1.73	0.45
13:1M:278:ARG:NE	37:1l:83:MET:HE2	2.31	0.45
13:1M:421:HIS:HB3	38:1m:50:TYR:OH	2.17	0.45
16:1P:22:THR:OG1	16:1P:88:SER:OG	2.34	0.45
16:1P:74:ASN:O	16:1P:80:SER:OG	2.30	0.45
19:1S:44:LYS:NZ	19:1S:48:PRO:HA	2.32	0.45
25:1Z:100:ASP:OD1	30:1e:81:GLN:NE2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:108:GLU:H	30:1e:74:ARG:HH22	1.65	0.45
34:1i:52:ASP:OD1	34:1i:52:ASP:N	2.49	0.45
34:1i:67:SER:O	34:1i:71:VAL:HG23	2.17	0.45
34:1i:68:ILE:HD12	34:1i:69:PHE:N	2.32	0.45
40:1o:61:TYR:HB3	40:1o:86:TRP:HA	1.99	0.45
2:1B:90:GLY:HA2	46:1B:201:SF4:S2	2.57	0.45
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.17	0.45
6:1F:18:GLU:HB2	6:1F:237:ARG:HH12	1.82	0.45
6:1F:208:PRO:HG3	17:1Q:119:GLY:HA2	1.99	0.45
6:1F:320:ASP:OD1	6:1F:320:ASP:N	2.50	0.45
6:1F:360:GLY:HA2	6:1F:366:ARG:HB2	1.99	0.45
6:1F:386:PRO:HD3	6:1F:430:MET:HE3	1.99	0.45
7:1G:195:LEU:HD12	7:1G:198:ASN:HD21	1.82	0.45
8:1H:183:MET:HB2	9:1I:27:TRP:CH2	2.52	0.45
11:1K:3:LEU:O	11:1K:6:MET:HE3	2.16	0.45
11:1K:34:GLU:H	11:1K:34:GLU:CD	2.25	0.45
12:1L:350:LEU:O	12:1L:350:LEU:HD23	2.17	0.45
15:1O:116:LEU:HD11	15:1O:256:PHE:CD1	2.52	0.45
16:1P:135:LEU:HD22	16:1P:169:SER:HB3	1.99	0.45
18:1R:60:ASP:OD1	18:1R:61:GLY:N	2.50	0.45
21:1V:7:THR:HG23	21:1V:9:GLY:H	1.82	0.45
25:1Z:143:TYR:CE1	26:1a:48:MET:HE1	2.52	0.45
39:1n:46:ARG:HA	39:1n:49:GLU:HG2	1.98	0.45
41:1p:72:ASP:HB3	41:1p:90:GLN:HE21	1.82	0.45
42:1q:56:PHE:HZ	43:1r:33:ARG:HH11	1.65	0.45
42:1q:69:ASN:OD1	42:1q:112:ASN:ND2	2.47	0.45
43:1r:3:ALA:HA	52:1r:201:CDL:HB22	1.99	0.45
43:1r:42:VAL:HB	43:1r:46:HIS:ND1	2.32	0.45
3:1C:87:GLN:H	3:1C:87:GLN:CD	2.25	0.44
4:1D:107:ASP:H	4:1D:114:ASN:ND2	2.15	0.44
4:1D:221:ARG:O	4:1D:224:GLU:HB2	2.17	0.44
5:1E:99:HIS:CE1	5:1E:140:ILE:HD13	2.53	0.44
7:1G:80:LEU:HD23	7:1G:80:LEU:HA	1.87	0.44
8:1H:43:TYR:CZ	52:1r:201:CDL:H141	2.52	0.44
10:1J:78:MET:O	10:1J:79:TYR:HD1	2.00	0.44
11:1K:93:LEU:HD12	14:1N:54:GLU:CD	2.41	0.44
12:1L:154:LEU:HB3	12:1L:243:VAL:CG1	2.47	0.44
12:1L:561:ILE:HG23	12:1L:562:LEU:H	1.81	0.44
13:1M:126:LEU:HD21	13:1M:153:THR:OG1	2.16	0.44
14:1N:309:ASN:ND2	14:1N:312:LYS:HE3	2.32	0.44
15:1O:240:TYR:O	15:1O:241:LEU:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:198:LYS:HA	16:1P:237:LEU:HD21	1.99	0.44
16:1P:206:TYR:CD2	16:1P:208:VAL:HG12	2.52	0.44
17:1Q:30:ILE:HD12	17:1Q:101:TRP:HD1	1.82	0.44
20:1U:8:LEU:HA	20:1U:11:ILE:HD12	1.99	0.44
26:1a:22:ALA:O	26:1a:26:ILE:HD12	2.15	0.44
26:1a:58:ASN:O	26:1a:58:ASN:ND2	2.49	0.44
27:1b:37:TYR:HD1	27:1b:40:TYR:HD2	1.65	0.44
33:1h:95:GLN:HB2	41:1p:82:LEU:HD21	1.99	0.44
36:1k:40:LEU:HD11	39:1n:45:ALA:CB	2.46	0.44
38:1m:91:LEU:O	38:1m:96:PRO:HD3	2.17	0.44
2:1B:45:LEU:HD23	2:1B:45:LEU:H	1.82	0.44
4:1D:184:VAL:HG23	4:1D:185:SER:H	1.82	0.44
5:1E:10:ARG:NH1	18:1R:78:GLU:OE1	2.51	0.44
7:1G:667:THR:OG1	7:1G:669:LYS:NZ	2.41	0.44
10:1J:38:GLY:HA2	10:1J:57:PHE:CE2	2.51	0.44
13:1M:95:TYR:HD1	13:1M:136:TRP:CD2	2.34	0.44
14:1N:267:ILE:HD12	14:1N:279:PRO:HB3	1.99	0.44
16:1P:20:VAL:HB	16:1P:89:ASN:H	1.82	0.44
20:1U:83:LYS:HD2	20:1U:83:LYS:HA	1.65	0.44
32:1g:105:LEU:HB2	32:1g:106:PRO:HD2	1.99	0.44
40:1o:71:ASP:O	41:1p:23:THR:OG1	2.27	0.44
43:1r:4:THR:O	43:1r:8:GLN:HG3	2.16	0.44
2:1B:145:TYR:CZ	9:1I:144:HIS:HB2	2.53	0.44
4:1D:150:HIS:O	4:1D:154:VAL:HG23	2.17	0.44
5:1E:27:ASN:HD22	5:1E:30:ARG:HE	1.65	0.44
5:1E:48:LEU:HB3	5:1E:49:PRO:HD3	1.99	0.44
6:1F:121:GLY:HA2	6:1F:124:VAL:HG22	1.99	0.44
7:1G:87:LYS:HB2	7:1G:87:LYS:HE3	1.77	0.44
7:1G:272:ASP:OD1	7:1G:681:SER:HB2	2.17	0.44
7:1G:357:ASP:O	19:1S:55:ARG:NH1	2.50	0.44
8:1H:157:ASN:ND2	8:1H:165:LEU:HD22	2.32	0.44
12:1L:15:LEU:HD22	12:1L:125:LEU:HD22	1.99	0.44
12:1L:250:SER:HB2	12:1L:333:ALA:HA	1.99	0.44
12:1L:363:TYR:CD2	12:1L:370:THR:HG21	2.52	0.44
12:1L:529:TYR:HB3	12:1L:530:PRO:HD3	2.00	0.44
12:1L:564:LYS:HG3	38:1m:76:TYR:CE2	2.52	0.44
15:1O:188:ASN:O	15:1O:191:GLU:HG3	2.18	0.44
16:1P:29:PHE:CD1	16:1P:175:GLU:HG2	2.52	0.44
16:1P:54:TYR:O	16:1P:57:MET:HB2	2.18	0.44
20:1T:58:PHE:HB2	20:1T:60:PHE:HE2	1.82	0.44
20:1U:37:MET:SD	20:1U:37:MET:N	2.73	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:34:GLU:H	22:1W:34:GLU:CD	2.20	0.44
23:1X:47:TRP:CZ3	33:1h:141:PRO:HG3	2.52	0.44
23:1X:106:PHE:O	23:1X:110:VAL:HG22	2.17	0.44
25:1Z:98:MET:HA	25:1Z:101:VAL:HG23	1.98	0.44
32:1g:59:ARG:O	32:1g:63:PHE:HB2	2.17	0.44
32:1g:100:ARG:HG2	32:1g:107:LEU:O	2.17	0.44
37:1l:127:PRO:HD3	40:1o:1:GLY:H1	1.82	0.44
37:1l:132:GLN:OE1	37:1l:155:HIS:ND1	2.50	0.44
41:1p:2:ASP:HB3	41:1p:6:LYS:NZ	2.33	0.44
41:1p:7:ASP:OD1	41:1p:7:ASP:N	2.49	0.44
41:1p:39:LEU:HD23	41:1p:39:LEU:HA	1.85	0.44
41:1p:81:ILE:HA	41:1p:84:MET:HB2	1.99	0.44
2:1B:82:GLN:HE21	8:1H:216:ALA:HA	1.83	0.44
4:1D:68:LEU:HB2	4:1D:70:GLY:O	2.16	0.44
5:1E:9:HIS:NE2	5:1E:63:ILE:HB	2.32	0.44
6:1F:249:ARG:HA	6:1F:249:ARG:CZ	2.48	0.44
6:1F:355:LYS:HE3	6:1F:355:LYS:HB3	1.71	0.44
7:1G:216:THR:O	7:1G:243:ARG:NH2	2.51	0.44
7:1G:475:GLN:NE2	7:1G:646:ASN:OD1	2.30	0.44
7:1G:494:HIS:HB2	7:1G:576:THR:HB	1.99	0.44
8:1H:20:LEU:HD11	8:1H:232:ILE:HD11	1.98	0.44
8:1H:35:LYS:HG3	9:1I:47:THR:OG1	2.18	0.44
12:1L:28:LYS:H	12:1L:28:LYS:HD3	1.81	0.44
13:1M:29:VAL:HG22	32:1g:60:VAL:CG1	2.47	0.44
14:1N:207:ILE:O	14:1N:210:THR:OG1	2.30	0.44
15:1O:223:TYR:HD2	15:1O:227:GLU:HB3	1.82	0.44
16:1P:267:GLY:HA2	16:1P:279:THR:HG23	1.99	0.44
19:1S:68:TYR:N	19:1S:72:GLN:O	2.46	0.44
20:1T:6:LEU:HD23	20:1T:84:LYS:HE2	1.98	0.44
23:1X:141:TYR:HA	25:1Z:115:ARG:HD3	1.99	0.44
3:1C:50:ILE:O	3:1C:107:VAL:HA	2.17	0.44
4:1D:63:ARG:HA	4:1D:63:ARG:HD2	1.86	0.44
4:1D:332:PRO:HB3	4:1D:352:TYR:HE1	1.82	0.44
7:1G:283:MET:SD	7:1G:291:LEU:HB3	2.58	0.44
7:1G:444:LYS:HA	7:1G:444:LYS:HD3	1.83	0.44
8:1H:195:ARG:HH21	8:1H:274:ARG:NH1	2.16	0.44
9:1I:14:MET:HG3	25:1Z:33:TYR:OH	2.17	0.44
9:1I:146:GLU:HG2	42:1q:124:TYR:O	2.16	0.44
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.82	0.44
12:1L:319:ILE:O	12:1L:321:GLN:HG2	2.17	0.44
15:1O:22:SER:OG	15:1O:119:GLY:O	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:97:ARG:HH21	55:1P:501:NDP:H51A	1.83	0.44
16:1P:139:ILE:H	16:1P:139:ILE:HD12	1.82	0.44
20:1T:18:VAL:HG11	20:1T:57:GLU:HG2	1.99	0.44
22:1W:27:GLU:OE1	22:1W:27:GLU:N	2.43	0.44
25:1Z:93:GLU:O	25:1Z:96:ILE:HG22	2.17	0.44
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.53	0.44
27:1b:31:LEU:O	27:1b:35:SER:N	2.51	0.44
29:1d:17:GLU:N	29:1d:17:GLU:OE2	2.51	0.44
32:1g:72:LEU:H	32:1g:72:LEU:HD12	1.82	0.44
40:1o:26:PRO:O	40:1o:30:PHE:HB2	2.18	0.44
1:1A:111:LEU:HD22	1:1A:111:LEU:H	1.81	0.44
2:1B:102:LYS:HB3	2:1B:102:LYS:HE3	1.77	0.44
2:1B:129:SER:OG	2:1B:132:VAL:HG12	2.18	0.44
3:1C:84:PRO:HB3	17:1Q:95:PHE:CE2	2.52	0.44
6:1F:134:ALA:HB2	6:1F:173:PHE:CZ	2.52	0.44
7:1G:125:SER:OG	7:1G:126:ASP:N	2.51	0.44
8:1H:222:MET:N	8:1H:222:MET:HE2	2.33	0.44
8:1H:227:GLU:O	8:1H:231:ILE:HG12	2.18	0.44
9:1I:34:LEU:HD11	50:1I:203:PC1:H2B1	1.99	0.44
12:1L:97:THR:HG21	12:1L:125:LEU:HD11	2.00	0.44
13:1M:47:GLU:OE2	41:1p:93:ARG:HG2	2.18	0.44
13:1M:278:ARG:NH2	37:1l:80:ASP:OD1	2.50	0.44
13:1M:389:SER:O	13:1M:392:THR:HG22	2.18	0.44
51:1M:501:PGT:H131	51:1M:501:PGT:H361	1.99	0.44
14:1N:58:LYS:O	14:1N:62:THR:HG22	2.17	0.44
16:1P:79:ASP:OD1	16:1P:82:ARG:NH1	2.50	0.44
16:1P:313:LYS:HA	16:1P:313:LYS:HE3	1.99	0.44
19:1S:49:ASP:N	19:1S:49:ASP:OD1	2.44	0.44
33:1h:94:LEU:HD23	33:1h:94:LEU:HA	1.83	0.44
34:1i:4:THR:O	34:1i:8:LYS:HG2	2.17	0.44
34:1i:76:ILE:HD12	34:1i:77:PRO:N	2.31	0.44
37:1l:111:PHE:O	37:1l:115:MET:HG3	2.18	0.44
38:1m:120:LEU:HB3	38:1m:122:GLN:NE2	2.31	0.44
40:1o:3:HIS:CD2	40:1o:4:LEU:HD22	2.53	0.44
43:1r:47:LYS:HG2	43:1r:51:ASN:ND2	2.33	0.44
1:1A:74:PRO:HB3	10:1J:143:ILE:HG22	2.00	0.44
3:1C:129:TRP:CZ3	4:1D:399:LEU:HB3	2.53	0.44
4:1D:34:ASN:ND2	15:1O:158:VAL:HA	2.33	0.44
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.36	0.44
4:1D:173:GLU:HA	4:1D:176:LYS:HG3	1.99	0.44
5:1E:195:PRO:HG2	5:1E:199:LEU:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:112:ARG:O	6:1F:148:ASN:ND2	2.35	0.44
10:1J:103:MET:O	10:1J:107:ALA:N	2.48	0.44
12:1L:331:MET:HA	12:1L:331:MET:HE3	1.99	0.44
12:1L:559:GLU:HA	12:1L:563:PRO:HG2	1.99	0.44
13:1M:139:GLN:HG3	13:1M:340:ARG:HH12	1.83	0.44
13:1M:237:LYS:CG	13:1M:316:MET:HG3	2.47	0.44
15:1O:300:PRO:O	28:1c:2:PHE:HE2	2.00	0.44
16:1P:81:ILE:HG21	16:1P:117:ILE:HG22	2.00	0.44
21:1V:52:ASN:N	21:1V:52:ASN:OD1	2.49	0.44
25:1Z:105:LYS:C	25:1Z:105:LYS:HD3	2.43	0.44
38:1m:14:PRO:HB2	38:1m:16:THR:HG22	1.99	0.44
38:1m:106:THR:HA	38:1m:109:ASP:HB2	1.99	0.44
3:1C:11:ILE:HA	4:1D:128:ILE:HD13	1.99	0.44
4:1D:270:ARG:HG2	4:1D:278:TYR:CE1	2.53	0.44
12:1L:119:LYS:HB3	12:1L:119:LYS:HE2	1.80	0.44
13:1M:1:FME:HG3	13:1M:2:LEU:HD22	1.99	0.44
13:1M:122:PHE:CE2	13:1M:206:LYS:HD2	2.53	0.44
13:1M:388:TRP:CE2	38:1m:108:ARG:HD2	2.53	0.44
14:1N:14:MET:HA	14:1N:133:TRP:HE1	1.83	0.44
15:1O:265:ASN:HB3	15:1O:268:GLU:HB3	2.00	0.44
19:1S:81:PHE:CE1	19:1S:85:GLN:HB2	2.39	0.44
20:1T:58:PHE:HB2	20:1T:60:PHE:CE2	2.53	0.44
22:1W:28:ALA:O	22:1W:32:VAL:HG13	2.18	0.44
22:1W:39:TRP:CE2	22:1W:90:LEU:HB3	2.52	0.44
23:1X:102:GLN:OE1	23:1X:102:GLN:N	2.36	0.44
31:1f:7:VAL:O	31:1f:11:TRP:HB3	2.18	0.44
32:1g:47:TYR:OH	32:1g:61:VAL:HG11	2.18	0.44
32:1g:117:LYS:NZ	41:1p:74:THR:OG1	2.47	0.44
33:1h:42:LEU:HD23	33:1h:42:LEU:HA	1.83	0.44
37:1l:58:ARG:HH12	37:1l:71:LEU:HD23	1.83	0.44
39:1n:158:LYS:NZ	39:1n:159:GLU:OE2	2.46	0.44
40:1o:57:TYR:O	40:1o:60:HIS:ND1	2.51	0.44
42:1q:48:TYR:HE2	42:1q:86:TRP:CG	2.36	0.44
43:1r:40:LEU:H	43:1r:40:LEU:HD22	1.83	0.44
4:1D:283:PHE:HB3	4:1D:310:ILE:HD11	1.99	0.44
6:1F:385:ARG:H	6:1F:388:GLU:CD	2.26	0.44
9:1I:98:PRO:HB3	9:1I:104:ARG:CZ	2.48	0.44
12:1L:122:VAL:O	12:1L:126:ILE:HG12	2.18	0.44
13:1M:154:LEU:HB3	14:1N:287:LEU:HD11	2.00	0.44
14:1N:88:LYS:HE2	30:1e:52:GLU:OE1	2.17	0.44
15:1O:41:GLU:OE2	15:1O:41:GLU:N	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:40:ALA:O	18:1R:44:ILE:HG22	2.18	0.44
19:1S:68:TYR:HD1	19:1S:72:GLN:HG3	1.81	0.44
23:1X:46:ARG:NH1	25:1Z:80:ASP:OD2	2.50	0.44
23:1X:120:ASP:OD1	23:1X:121:LEU:N	2.45	0.44
30:1e:84:LYS:HE3	30:1e:84:LYS:HB3	1.85	0.44
30:1e:93:PRO:HB3	30:1e:97:HIS:CD2	2.52	0.44
37:1l:91:THR:HG22	37:1l:91:THR:O	2.18	0.44
38:1m:32:GLN:OE1	38:1m:32:GLN:O	2.35	0.44
38:1m:44:ARG:NH2	39:1n:148:PRO:HB3	2.31	0.44
41:1p:26:PRO:HB2	41:1p:31:TYR:HE2	1.83	0.44
3:1C:130:TYR:OH	4:1D:390:LYS:NZ	2.50	0.43
3:1C:185:ALA:HB2	22:1W:105:ARG:HE	1.82	0.43
4:1D:266:GLN:HG3	43:1r:103:TRP:HZ3	1.83	0.43
4:1D:346:ILE:HG23	7:1G:117:GLN:HG3	1.99	0.43
6:1F:223:ALA:HA	48:1F:501:FMN:O1P	2.18	0.43
12:1L:90:ILE:HB	12:1L:91:PRO:HD3	2.00	0.43
45:1L:701:3PE:H231	37:1l:88:ARG:HA	2.00	0.43
14:1N:320:THR:HG21	15:1O:265:ASN:HA	2.00	0.43
15:1O:214:MET:HE2	15:1O:214:MET:C	2.43	0.43
15:1O:224:SER:O	15:1O:228:ALA:N	2.48	0.43
16:1P:39:GLY:HA3	16:1P:62:MET:O	2.17	0.43
16:1P:50:ARG:HH21	55:1P:501:NDP:C4A	2.31	0.43
17:1Q:29:HIS:ND1	17:1Q:33:ARG:HD3	2.32	0.43
20:1T:37:MET:SD	20:1T:38:LYS:NZ	2.91	0.43
20:1T:79:TYR:CZ	20:1T:83:LYS:HD2	2.52	0.43
21:1V:91:ARG:NH1	21:1V:95:ARG:HG2	2.29	0.43
24:1Y:89:TYR:O	24:1Y:93:GLY:N	2.44	0.43
27:1b:31:LEU:H	27:1b:31:LEU:HD12	1.83	0.43
34:1i:63:THR:O	34:1i:67:SER:N	2.50	0.43
37:1l:27:TYR:CE2	37:1l:48:PRO:HD3	2.53	0.43
39:1n:135:GLU:HB2	39:1n:164:PRO:HA	2.00	0.43
42:1q:48:TYR:CD1	42:1q:62:VAL:HG23	2.53	0.43
2:1B:75:VAL:HG11	8:1H:25:ARG:HD3	2.00	0.43
3:1C:18:VAL:HG13	3:1C:22:LEU:HD23	2.00	0.43
3:1C:136:ASP:OD2	3:1C:150:ARG:HA	2.18	0.43
4:1D:141:PHE:CZ	4:1D:184:VAL:HG21	2.54	0.43
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.19	0.43
5:1E:154:VAL:HG22	5:1E:156:ILE:HD12	1.99	0.43
6:1F:41:ASP:OD1	6:1F:42:TRP:N	2.50	0.43
6:1F:224:ASN:ND2	6:1F:225:VAL:H	2.16	0.43
6:1F:392:LEU:HD12	6:1F:395:ILE:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:53:ARG:N	47:1G:804:FES:S1	2.88	0.43
8:1H:190:LEU:HD11	8:1H:273:ILE:HG21	2.00	0.43
10:1J:99:MET:H	10:1J:99:MET:CE	2.29	0.43
12:1L:226:GLN:O	12:1L:230:HIS:N	2.51	0.43
12:1L:234:PRO:O	12:1L:237:MET:HG2	2.18	0.43
14:1N:162:ILE:HA	14:1N:185:ALA:HA	2.00	0.43
15:1O:85:ASP:OD1	15:1O:85:ASP:N	2.50	0.43
16:1P:242:VAL:HG12	16:1P:253:PHE:HE1	1.82	0.43
16:1P:315:ILE:HG23	16:1P:322:ARG:HH22	1.82	0.43
17:1Q:49:VAL:C	17:1Q:51:ASN:H	2.27	0.43
18:1R:75:LEU:HA	18:1R:75:LEU:HD23	1.68	0.43
34:1i:98:GLU:HG2	34:1i:99:ARG:O	2.18	0.43
35:1j:34:PHE:O	35:1j:38:TRP:HB3	2.17	0.43
1:1A:1:FME:CN	25:1Z:142:TRP:HB3	2.49	0.43
2:1B:107:MET:HG2	2:1B:111:ARG:HB3	2.00	0.43
3:1C:97:LEU:HD12	3:1C:104:GLN:HE21	1.81	0.43
5:1E:88:THR:OG1	5:1E:89:MET:N	2.50	0.43
6:1F:194:GLU:HG2	17:1Q:133:LYS:HD3	2.00	0.43
7:1G:36:GLN:OE1	17:1Q:49:VAL:HG22	2.19	0.43
7:1G:196:SER:HB3	7:1G:265:ASP:OD2	2.19	0.43
7:1G:237:ASN:CG	7:1G:253:ARG:HE	2.26	0.43
7:1G:336:ASN:OD1	19:1S:67:ARG:HD2	2.18	0.43
7:1G:349:PHE:CE2	7:1G:362:TYR:HB3	2.51	0.43
8:1H:77:LEU:HD22	8:1H:81:LEU:HD13	2.01	0.43
8:1H:222:MET:HE2	8:1H:222:MET:H	1.84	0.43
12:1L:11:THR:HG22	12:1L:46:LEU:HB3	2.00	0.43
12:1L:184:LEU:HD23	13:1M:393:ILE:HG12	2.00	0.43
12:1L:483:PRO:HG3	35:1j:53:TYR:CZ	2.53	0.43
13:1M:225:ILE:HD13	13:1M:331:ASN:HB2	2.00	0.43
14:1N:88:LYS:HE3	14:1N:88:LYS:HB3	1.77	0.43
14:1N:175:LEU:HD21	14:1N:227:THR:HA	2.00	0.43
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	2.00	0.43
16:1P:20:VAL:O	16:1P:88:SER:OG	2.34	0.43
55:1P:501:NDP:H2N	55:1P:501:NDP:H2D	1.77	0.43
21:1V:67:LEU:HD23	21:1V:67:LEU:HA	1.84	0.43
45:1Y:201:3PE:H371	45:1Y:201:3PE:H231	1.99	0.43
29:1d:74:TYR:HD1	29:1d:77:LYS:HD3	1.82	0.43
33:1h:127:THR:OG1	33:1h:128:ILE:N	2.51	0.43
35:1j:67:LEU:HB3	35:1j:71:GLU:OE2	2.17	0.43
37:1l:18:GLU:CD	37:1l:18:GLU:N	2.76	0.43
1:1A:103:ALA:O	1:1A:107:THR:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:1E:32:GLU:HA	5:1E:35:VAL:HG12	1.99	0.43
6:1F:34:LYS:HE2	6:1F:34:LYS:HB2	1.78	0.43
7:1G:546:GLN:HG3	7:1G:599:ILE:HD11	2.00	0.43
8:1H:111:LEU:HD12	8:1H:111:LEU:HA	1.90	0.43
8:1H:162:LEU:HD21	8:1H:237:PHE:HE1	1.83	0.43
8:1H:309:ILE:HG22	27:1b:38:THR:HG22	2.00	0.43
10:1J:4:TYR:O	10:1J:7:PHE:HB2	2.18	0.43
10:1J:84:VAL:HA	10:1J:90:PHE:CE2	2.53	0.43
12:1L:8:THR:HG21	12:1L:82:MET:HG3	2.00	0.43
12:1L:316:THR:OG1	12:1L:325:ALA:HB2	2.18	0.43
13:1M:107:ILE:O	13:1M:111:THR:OG1	2.28	0.43
16:1P:36:ASN:O	16:1P:40:ARG:NH1	2.51	0.43
18:1R:30:ASP:C	18:1R:31:ARG:HD3	2.43	0.43
19:1S:70:PHE:O	19:1S:70:PHE:CG	2.72	0.43
21:1V:51:THR:O	21:1V:55:LEU:N	2.44	0.43
23:1X:139:ASN:OD1	23:1X:139:ASN:N	2.50	0.43
35:1j:6:HIS:C	35:1j:7:ILE:HD13	2.42	0.43
4:1D:217:ASN:CG	43:1r:22:LYS:HB2	2.44	0.43
7:1G:113:GLU:OE1	17:1Q:43:ASN:ND2	2.42	0.43
7:1G:415:LEU:HB3	7:1G:417:TYR:CE1	2.52	0.43
7:1G:622:ARG:O	7:1G:625:GLU:HG2	2.17	0.43
9:1I:43:ARG:NH1	43:1r:19:LEU:HG	2.33	0.43
10:1J:109:LYS:N	10:1J:109:LYS:HE2	2.33	0.43
12:1L:37:LYS:HE2	12:1L:37:LYS:HB3	1.76	0.43
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.53	0.43
13:1M:332:THR:HG21	13:1M:437:MET:HE2	2.00	0.43
14:1N:22:ILE:HB	30:1e:5:VAL:HG12	2.00	0.43
15:1O:41:GLU:H	15:1O:41:GLU:CD	2.25	0.43
16:1P:87:HIS:HB3	18:1R:23:TYR:HA	2.00	0.43
16:1P:134:HIS:NE2	16:1P:169:SER:O	2.49	0.43
20:1T:66:ASP:O	20:1T:69:LYS:HG3	2.19	0.43
25:1Z:30:LEU:HB3	25:1Z:34:SER:OG	2.19	0.43
29:1d:73:TYR:O	29:1d:77:LYS:HG3	2.19	0.43
33:1h:69:HIS:CG	33:1h:70:PRO:HD2	2.54	0.43
34:1i:31:GLU:OE1	39:1n:115:PRO:HD2	2.18	0.43
34:1i:55:PRO:O	34:1i:59:VAL:HG22	2.18	0.43
35:1j:51:PHE:HB3	40:1o:91:HIS:CD2	2.54	0.43
37:1l:126:GLN:NE2	58:1l:201:MYR:O1	2.51	0.43
40:1o:98:MET:HA	40:1o:101:PHE:HB3	2.01	0.43
41:1p:28:PRO:O	41:1p:32:LEU:HD22	2.18	0.43
41:1p:79:LYS:HE2	41:1p:79:LYS:HB3	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:347:HIS:O	4:1D:351:LEU:HB2	2.18	0.43
6:1F:65:LEU:HB3	6:1F:75:THR:OG1	2.18	0.43
6:1F:188:GLU:OE2	6:1F:405:CYS:HB2	2.18	0.43
7:1G:194:GLU:HG3	7:1G:389:PRO:HB3	2.01	0.43
7:1G:297:GLU:O	7:1G:301:SER:OG	2.31	0.43
8:1H:127:TYR:OH	8:1H:206:GLU:O	2.36	0.43
8:1H:142:TYR:CD1	8:1H:289:LEU:HD22	2.53	0.43
12:1L:13:ILE:HD12	12:1L:13:ILE:HA	1.81	0.43
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.54	0.43
16:1P:83:LYS:HA	16:1P:86:GLU:OE2	2.18	0.43
17:1Q:7:ASP:HA	17:1Q:10:LEU:CD2	2.48	0.43
20:1U:11:ILE:O	20:1U:15:VAL:N	2.50	0.43
26:1a:6:LEU:HB3	52:1r:201:CDL:H191	2.01	0.43
29:1d:2:MET:HA	29:1d:2:MET:HE3	2.00	0.43
3:1C:57:VAL:HG23	3:1C:58:ILE:HD12	2.00	0.43
3:1C:57:VAL:O	3:1C:61:LEU:HB2	2.19	0.43
6:1F:26:TYR:OH	6:1F:268:VAL:HG22	2.19	0.43
6:1F:48:ILE:HD11	6:1F:56:ILE:HG13	2.01	0.43
6:1F:300:GLY:HA3	6:1F:329:LEU:O	2.19	0.43
48:1F:501:FMN:H4'	48:1F:501:FMN:H1'2	1.86	0.43
7:1G:585:VAL:HG23	17:1Q:61:THR:OG1	2.19	0.43
10:1J:45:LEU:HD23	10:1J:50:SER:HA	2.00	0.43
10:1J:86:ASN:OD1	10:1J:87:LYS:N	2.51	0.43
12:1L:111:ASP:OD2	39:1n:96:TYR:OH	2.33	0.43
12:1L:270:ASN:OD1	12:1L:272:LEU:N	2.52	0.43
13:1M:310:MET:HE3	13:1M:459:TYR:HA	2.00	0.43
14:1N:62:THR:HG21	14:1N:114:TRP:CG	2.54	0.43
15:1O:157:LYS:HB2	15:1O:157:LYS:HE2	1.73	0.43
15:1O:214:MET:HE1	15:1O:220:VAL:HG22	2.00	0.43
21:1V:68:GLU:OE1	21:1V:75:GLN:HA	2.19	0.43
25:1Z:51:MET:O	25:1Z:55:ARG:HG3	2.19	0.43
36:1k:12:LYS:HD3	36:1k:12:LYS:HA	1.72	0.43
36:1k:44:TRP:HB2	39:1n:37:ARG:HD2	2.00	0.43
39:1n:21:ARG:CZ	39:1n:21:ARG:HB3	2.48	0.43
43:1r:7:ILE:H	43:1r:7:ILE:HG13	1.63	0.43
1:1A:15:SER:HA	8:1H:76:ILE:HD11	2.00	0.43
3:1C:177:ASP:OD1	16:1P:40:ARG:NH2	2.52	0.43
4:1D:347:HIS:NE2	7:1G:125:SER:O	2.52	0.43
6:1F:295:LEU:H	6:1F:338:ASP:HA	1.84	0.43
7:1G:503:LEU:HD21	7:1G:509:PRO:HB3	2.00	0.43
8:1H:141:SER:O	8:1H:289:LEU:HD21	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.17	0.43
12:1L:149:ILE:HG12	13:1M:364:LEU:HD22	2.01	0.43
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.44	0.43
16:1P:322:ARG:HD3	16:1P:326:TRP:O	2.19	0.43
19:1S:19:ARG:N	19:1S:65:TRP:O	2.45	0.43
20:1U:12:LYS:O	20:1U:16:LEU:HG	2.19	0.43
21:1V:64:VAL:HB	21:1V:76:ILE:HG13	2.01	0.43
24:1Y:117:MET:HE3	24:1Y:117:MET:N	2.33	0.43
42:1q:134:ILE:HD13	42:1q:134:ILE:HA	1.89	0.43
44:1s:73:PRO:HD2	44:1s:74:ARG:NH2	2.33	0.43
1:1A:12:THR:HA	1:1A:15:SER:OG	2.19	0.43
3:1C:83:VAL:HB	3:1C:86:ARG:HD2	2.01	0.43
3:1C:209:TYR:CG	4:1D:360:PRO:HD2	2.53	0.43
4:1D:3:GLN:NE2	4:1D:5:GLN:OE1	2.41	0.43
4:1D:145:THR:OG1	4:1D:181:TYR:OH	2.30	0.43
4:1D:165:THR:HG22	8:1H:32:GLN:CD	2.44	0.43
6:1F:291:TRP:CE3	6:1F:294:LEU:HD21	2.54	0.43
7:1G:139:ASP:OD1	7:1G:139:ASP:N	2.51	0.43
7:1G:690:ALA:HB2	7:1G:698:VAL:HG11	2.00	0.43
12:1L:47:SER:HB2	12:1L:90:ILE:HG22	2.01	0.43
12:1L:370:THR:HG23	12:1L:431:PHE:CD2	2.53	0.43
14:1N:309:ASN:HD21	14:1N:312:LYS:HE3	1.84	0.43
16:1P:116:ALA:HA	16:1P:119:GLN:HE21	1.84	0.43
20:1U:70:LEU:HD21	20:1U:79:TYR:CG	2.53	0.43
22:1W:75:ASP:OD1	22:1W:76:PRO:HD2	2.19	0.43
23:1X:56:LEU:HD21	25:1Z:84:LEU:HD21	2.00	0.43
25:1Z:89:GLU:OE2	30:1e:96:HIS:ND1	2.51	0.43
40:1o:13:SER:C	40:1o:14:LYS:HD2	2.44	0.43
42:1q:13:GLN:NE2	42:1q:34:ARG:HA	2.34	0.43
42:1q:83:PRO:HB2	42:1q:85:GLU:OE2	2.18	0.43
3:1C:132:ARG:HH21	3:1C:149:ARG:HB2	1.83	0.43
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	2.01	0.43
5:1E:88:THR:HG23	6:1F:182:GLY:O	2.19	0.43
5:1E:124:LEU:HG	5:1E:126:ILE:HG12	2.00	0.43
6:1F:301:GLY:HA2	6:1F:333:ALA:HB3	2.01	0.43
7:1G:418:ARG:CZ	7:1G:418:ARG:HB2	2.49	0.43
8:1H:173:TRP:HB3	8:1H:175:ILE:HG22	2.00	0.43
9:1I:114:THR:HG21	9:1I:144:HIS:CE1	2.53	0.43
12:1L:131:LEU:HD12	12:1L:143:GLY:C	2.44	0.43
14:1N:66:ALA:HB2	14:1N:104:MET:HG2	2.01	0.43
14:1N:238:PRO:HB2	45:1N:401:3PE:O32	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:241:LEU:HD12	16:1P:242:VAL:N	2.34	0.43
20:1T:37:MET:H	20:1T:37:MET:HE3	1.83	0.43
24:1Y:80:ARG:HB3	24:1Y:82:LYS:HZ2	1.84	0.43
33:1h:119:ASP:OD1	33:1h:119:ASP:N	2.48	0.43
37:1l:77:ILE:HD11	38:1m:67:TRP:CG	2.54	0.43
39:1n:67:GLU:O	39:1n:71:TRP:N	2.35	0.43
1:1A:106:TRP:CH2	8:1H:291:LYS:HD2	2.53	0.42
2:1B:101:ARG:O	2:1B:104:TYR:HB3	2.19	0.42
4:1D:88:GLU:HA	4:1D:91:ILE:HD12	2.00	0.42
7:1G:59:ILE:HG12	7:1G:77:TRP:CD1	2.54	0.42
7:1G:381:GLY:O	7:1G:456:SER:OG	2.37	0.42
7:1G:403:ASP:OD1	17:1Q:127:ARG:NH2	2.52	0.42
7:1G:469:ALA:O	7:1G:473:ILE:HG12	2.19	0.42
12:1L:250:SER:CB	12:1L:333:ALA:HA	2.49	0.42
12:1L:370:THR:HA	12:1L:431:PHE:CE2	2.53	0.42
13:1M:6:ILE:HD12	31:1f:23:GLY:HA2	2.01	0.42
14:1N:270:MET:HB2	14:1N:279:PRO:HG3	2.02	0.42
15:1O:57:HIS:CG	15:1O:68:PRO:HB3	2.54	0.42
16:1P:327:LEU:HD12	16:1P:328:THR:N	2.34	0.42
17:1Q:26:PRO:HB2	17:1Q:28:GLU:OE1	2.19	0.42
19:1S:20:ILE:HD12	19:1S:20:ILE:C	2.44	0.42
19:1S:72:GLN:OE1	19:1S:73:GLU:N	2.52	0.42
20:1U:66:ASP:HA	20:1U:69:LYS:HB2	1.99	0.42
32:1g:87:GLU:OE1	32:1g:87:GLU:N	2.51	0.42
37:1l:26:LYS:HE2	37:1l:26:LYS:HB2	1.82	0.42
39:1n:25:HIS:O	39:1n:28:SER:OG	2.34	0.42
40:1o:18:PRO:HA	40:1o:21:MET:SD	2.58	0.42
41:1p:139:GLN:O	41:1p:143:SER:OG	2.34	0.42
42:1q:13:GLN:NE2	42:1q:35:VAL:HG12	2.34	0.42
1:1A:54:LYS:HD3	1:1A:114:ALA:O	2.19	0.42
4:1D:202:ASP:OD2	25:1Z:8:GLN:NE2	2.51	0.42
4:1D:267:TRP:CE3	4:1D:272:THR:HG21	2.54	0.42
4:1D:328:ALA:HA	4:1D:331:SER:O	2.19	0.42
5:1E:101:GLN:OE1	5:1E:101:GLN:HA	2.19	0.42
6:1F:21:ILE:H	6:1F:21:ILE:HD12	1.84	0.42
7:1G:198:ASN:ND2	7:1G:262:TRP:HB3	2.34	0.42
8:1H:59:GLU:HA	8:1H:60:PRO:HD3	1.84	0.42
8:1H:105:MET:HE2	8:1H:105:MET:HB3	1.77	0.42
8:1H:137:ALA:O	8:1H:141:SER:OG	2.23	0.42
8:1H:215:TYR:HD1	8:1H:219:PRO:HB2	1.83	0.42
9:1I:65:HIS:HA	9:1I:133:GLU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:70:TYR:CD1	9:1I:76:ARG:HG2	2.54	0.42
10:1J:77:GLU:HB3	11:1K:25:HIS:CE1	2.54	0.42
12:1L:304:PHE:HZ	12:1L:526:LEU:HG	1.84	0.42
13:1M:122:PHE:CZ	13:1M:206:LYS:HD2	2.54	0.42
13:1M:450:ASN:OD1	13:1M:452:LYS:NZ	2.52	0.42
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.55	0.42
14:1N:304:MET:HE3	14:1N:304:MET:HB3	1.77	0.42
21:1V:15:VAL:HA	21:1V:77:GLU:HG2	2.01	0.42
23:1X:136:LEU:HD12	23:1X:137:PRO:HD2	2.01	0.42
34:1i:52:ASP:HB2	34:1i:57:LYS:CE	2.49	0.42
35:1j:56:PRO:HA	35:1j:59:TRP:CD2	2.54	0.42
36:1k:33:GLU:O	36:1k:37:ALA:N	2.41	0.42
41:1p:35:ILE:HD12	41:1p:36:PHE:N	2.34	0.42
41:1p:119:SER:O	41:1p:123:ASN:HB2	2.19	0.42
1:1A:93:PHE:CD1	1:1A:93:PHE:C	2.96	0.42
3:1C:127:ALA:O	3:1C:131:GLU:HG2	2.19	0.42
4:1D:34:ASN:HD22	15:1O:158:VAL:HA	1.83	0.42
4:1D:209:ASP:OD1	4:1D:209:ASP:N	2.52	0.42
7:1G:38:PRO:HG3	7:1G:123:PHE:CE2	2.54	0.42
7:1G:255:HIS:CE1	7:1G:258:ILE:HG12	2.54	0.42
7:1G:329:VAL:HG23	7:1G:505:LEU:HD21	2.00	0.42
7:1G:333:ASP:O	7:1G:337:ARG:N	2.45	0.42
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.54	0.42
12:1L:161:ARG:NH1	39:1n:88:THR:O	2.45	0.42
12:1L:444:ASN:HB2	35:1j:7:ILE:HG21	2.01	0.42
15:1O:65:ASP:OD1	28:1c:2:PHE:HA	2.20	0.42
15:1O:198:TYR:O	15:1O:202:ILE:HG12	2.19	0.42
16:1P:196:LEU:HD12	16:1P:196:LEU:HA	1.92	0.42
19:1S:32:VAL:HG22	19:1S:62:PRO:HB3	2.01	0.42
27:1b:79:TRP:CD1	27:1b:79:TRP:H	2.37	0.42
31:1f:35:THR:HG23	31:1f:38:ARG:HB2	2.01	0.42
34:1i:9:LEU:O	34:1i:13:GLN:HG3	2.18	0.42
39:1n:82:PRO:HA	39:1n:87:GLY:HA3	2.01	0.42
40:1o:68:CYS:O	40:1o:72:SER:HB3	2.19	0.42
1:1A:54:LYS:HD2	4:1D:71:GLU:OE1	2.20	0.42
2:1B:88:VAL:HG11	2:1B:136:CYS:SG	2.59	0.42
3:1C:53:HIS:CG	3:1C:54:PRO:HD2	2.54	0.42
3:1C:92:ILE:HD11	3:1C:140:VAL:HG11	2.00	0.42
4:1D:202:ASP:OD1	4:1D:203:LEU:HD12	2.20	0.42
4:1D:241:ASP:O	4:1D:242:ILE:HD13	2.19	0.42
5:1E:163:ASP:CG	5:1E:186:PRO:HB3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:256:PHE:O	6:1F:267:THR:HA	2.18	0.42
6:1F:274:VAL:O	6:1F:317:MET:HG2	2.20	0.42
7:1G:159:CYS:HB3	46:1G:802:SF4:S3	2.59	0.42
7:1G:218:ARG:HD2	7:1G:219:PRO:HD2	2.01	0.42
8:1H:11:ILE:H	8:1H:11:ILE:HD12	1.84	0.42
9:1I:92:ILE:HA	9:1I:111:ILE:HG22	2.00	0.42
9:1I:120:GLY:O	9:1I:124:GLU:HG3	2.18	0.42
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.54	0.42
13:1M:12:LEU:HB3	13:1M:13:PRO:HD3	1.99	0.42
13:1M:53:SER:HA	31:1f:34:LEU:HD21	2.02	0.42
13:1M:114:GLU:OE2	13:1M:174:LEU:HB2	2.19	0.42
14:1N:89:MET:HE2	14:1N:89:MET:HB3	1.74	0.42
15:1O:285:GLY:HA3	32:1g:28:GLU:HG2	2.00	0.42
21:1V:27:TYR:HB2	21:1V:55:LEU:HD13	2.01	0.42
22:1W:17:VAL:HG22	22:1W:18:LYS:N	2.34	0.42
23:1X:171:MET:SD	23:1X:171:MET:N	2.92	0.42
27:1b:62:MET:SD	27:1b:62:MET:N	2.92	0.42
29:1d:91:PHE:O	29:1d:95:LYS:HG2	2.19	0.42
2:1B:114:VAL:HG13	2:1B:144:ILE:HG22	2.01	0.42
4:1D:62:LEU:HD13	4:1D:425:PHE:HZ	1.83	0.42
4:1D:74:ARG:N	4:1D:74:ARG:HD2	2.34	0.42
4:1D:107:ASP:CB	4:1D:114:ASN:HD21	2.33	0.42
4:1D:183:ARG:NE	4:1D:207:LEU:HD23	2.30	0.42
4:1D:289:SER:N	4:1D:295:ASP:OD2	2.52	0.42
4:1D:411:LEU:HD23	4:1D:411:LEU:H	1.84	0.42
4:1D:411:LEU:HA	4:1D:414:VAL:HG23	2.02	0.42
6:1F:65:LEU:HD12	6:1F:65:LEU:HA	1.93	0.42
6:1F:277:LYS:O	6:1F:281:GLU:HG2	2.20	0.42
6:1F:296:ALA:HA	6:1F:308:PRO:HA	2.00	0.42
6:1F:398:GLN:HG2	7:1G:92:GLY:HA3	2.02	0.42
7:1G:59:ILE:HD12	7:1G:79:ILE:HA	2.02	0.42
7:1G:323:VAL:H	7:1G:498:SER:HB3	1.85	0.42
7:1G:453:LEU:O	7:1G:493:LEU:N	2.53	0.42
8:1H:68:ILE:O	8:1H:72:ILE:HG12	2.19	0.42
8:1H:192:GLU:OE1	8:1H:192:GLU:HA	2.19	0.42
9:1I:138:GLU:OE1	9:1I:138:GLU:N	2.50	0.42
11:1K:4:VAL:O	11:1K:8:ILE:HD12	2.19	0.42
12:1L:67:HIS:HA	12:1L:77:SER:OG	2.19	0.42
12:1L:161:ARG:HD3	39:1n:90:TYR:O	2.20	0.42
12:1L:446:ASN:HD22	35:1j:7:ILE:HD11	1.84	0.42
14:1N:156:THR:O	14:1N:160:LEU:HD23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:206:TYR:HA	15:1O:210:PHE:HB3	2.01	0.42
15:1O:308:TYR:OH	29:1d:51:ARG:NH1	2.51	0.42
16:1P:56:THR:HB	16:1P:70:PHE:HE2	1.83	0.42
16:1P:310:LEU:O	16:1P:310:LEU:HD22	2.20	0.42
19:1S:63:LYS:HZ2	19:1S:65:TRP:NE1	2.17	0.42
19:1S:77:SER:OG	19:1S:79:ASN:OD1	2.26	0.42
28:1c:27:LEU:HD13	29:1d:70:PHE:HD1	1.84	0.42
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.37	0.42
40:1o:7:ARG:HD3	40:1o:15:GLU:HB2	2.00	0.42
40:1o:34:LYS:NZ	40:1o:35:GLU:O	2.41	0.42
1:1A:92:LEU:HD13	8:1H:302:MET:HG2	2.00	0.42
2:1B:81:ARG:HD3	8:1H:214:GLU:HG2	2.01	0.42
3:1C:196:LYS:HZ2	7:1G:223:ARG:HE	1.66	0.42
4:1D:66:MET:C	4:1D:66:MET:HE2	2.44	0.42
4:1D:87:THR:OG1	4:1D:88:GLU:OE1	2.35	0.42
4:1D:169:TRP:CZ3	9:1I:40:TYR:CZ	3.08	0.42
6:1F:189:GLU:HB2	6:1F:222:VAL:HG11	2.00	0.42
7:1G:153:CYS:SG	7:1G:155:GLN:N	2.81	0.42
7:1G:229:ASP:HB3	7:1G:236:SER:N	2.35	0.42
7:1G:318:ILE:HD11	7:1G:514:ILE:HG12	2.02	0.42
12:1L:331:MET:HE1	12:1L:468:ILE:HD12	2.02	0.42
12:1L:511:LEU:O	12:1L:511:LEU:HD13	2.19	0.42
13:1M:51:ASN:O	33:1h:89:LYS:NZ	2.43	0.42
13:1M:312:ALA:O	13:1M:316:MET:HB2	2.20	0.42
14:1N:150:ASN:OD1	14:1N:153:LEU:N	2.46	0.42
14:1N:236:LYS:HG3	14:1N:237:MET:HG2	2.01	0.42
15:1O:95:ARG:NH1	15:1O:281:GLU:O	2.43	0.42
15:1O:104:ARG:HE	15:1O:104:ARG:HB3	1.60	0.42
15:1O:204:ASN:O	15:1O:208:LYS:HG2	2.20	0.42
15:1O:282:ILE:HD12	15:1O:282:ILE:HA	1.88	0.42
18:1R:84:CYS:HB3	18:1R:87:CYS:HB2	2.02	0.42
20:1U:45:LEU:HB2	57:1n:201:EHZ:C20	2.50	0.42
21:1V:59:LYS:HE2	21:1V:59:LYS:HB2	1.68	0.42
22:1W:56:VAL:O	22:1W:60:ARG:HG2	2.20	0.42
23:1X:38:PRO:HG3	23:1X:65:CYS:SG	2.59	0.42
23:1X:94:GLN:NE2	26:1a:37:ARG:HE	2.06	0.42
24:1Y:140:VAL:HG12	33:1h:112:ARG:HB2	2.02	0.42
28:1c:33:LYS:O	28:1c:37:GLU:HG3	2.20	0.42
38:1m:34:GLU:CD	38:1m:34:GLU:H	2.28	0.42
4:1D:71:GLU:OE1	4:1D:71:GLU:N	2.41	0.42
5:1E:46:ALA:HB3	5:1E:73:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:189:GLU:HA	6:1F:192:LEU:HB3	2.02	0.42
6:1F:416:GLN:HB3	6:1F:420:ARG:NH2	2.34	0.42
7:1G:102:PRO:HG3	7:1G:151:THR:HG23	2.00	0.42
7:1G:379:LEU:H	7:1G:379:LEU:HD12	1.84	0.42
7:1G:447:LYS:HD3	7:1G:447:LYS:HA	1.69	0.42
7:1G:487:TRP:CD1	7:1G:489:VAL:HG22	2.54	0.42
8:1H:201:THR:O	8:1H:210:GLY:HA3	2.20	0.42
8:1H:236:ALA:O	8:1H:240:ILE:HG22	2.20	0.42
11:1K:31:LEU:HA	11:1K:34:GLU:OE1	2.19	0.42
12:1L:75:GLU:OE1	12:1L:75:GLU:N	2.53	0.42
12:1L:285:THR:HB	12:1L:415:ALA:HB2	2.02	0.42
12:1L:287:PHE:HD1	37:1l:108:PHE:HE2	1.67	0.42
13:1M:47:GLU:HG2	41:1p:92:ARG:HB3	2.01	0.42
14:1N:251:MET:HB3	14:1N:293:TYR:CE1	2.55	0.42
15:1O:3:TYR:HB2	15:1O:260:ARG:NH2	2.35	0.42
18:1R:19:ASP:OD1	18:1R:19:ASP:C	2.62	0.42
19:1S:19:ARG:HA	19:1S:53:LEU:O	2.19	0.42
20:1T:17:TYR:HA	20:1T:20:LYS:NZ	2.35	0.42
21:1V:31:LEU:HG	21:1V:51:THR:HG21	2.00	0.42
21:1V:54:LYS:HE3	21:1V:71:LEU:HD23	2.00	0.42
31:1f:38:ARG:NH1	31:1f:56:TRP:O	2.53	0.42
39:1n:51:LYS:HA	39:1n:51:LYS:HD3	1.80	0.42
3:1C:78:LEU:HD12	3:1C:94:TYR:CE2	2.54	0.42
3:1C:118:GLU:HA	3:1C:143:ALA:HB3	2.01	0.42
6:1F:15:LEU:N	6:1F:271:GLU:HB2	2.34	0.42
6:1F:37:GLN:HA	6:1F:41:ASP:O	2.20	0.42
6:1F:105:CYS:O	6:1F:109:GLU:HG2	2.19	0.42
10:1J:6:ALA:HB3	10:1J:124:ASP:CG	2.45	0.42
12:1L:69:MET:SD	12:1L:71:LEU:HG	2.60	0.42
14:1N:222:SER:HB2	14:1N:233:THR:HG21	2.02	0.42
14:1N:258:SER:OG	14:1N:333:SER:O	2.35	0.42
16:1P:271:GLU:HG2	16:1P:280:THR:HG22	2.02	0.42
23:1X:43:MET:HE1	23:1X:47:TRP:HZ3	1.84	0.42
23:1X:112:ASP:OD2	23:1X:113:LYS:N	2.52	0.42
28:1c:28:TRP:O	28:1c:31:LEU:N	2.52	0.42
40:1o:62:LEU:HB2	40:1o:86:TRP:NE1	2.35	0.42
40:1o:69:LYS:HE3	40:1o:69:LYS:HB3	1.75	0.42
42:1q:44:TYR:HB3	42:1q:68:MET:HE1	2.00	0.42
1:1A:106:TRP:CZ3	27:1b:18:LEU:HD21	2.54	0.42
7:1G:55:CYS:HB3	47:1G:804:FES:S2	2.59	0.42
7:1G:365:ASN:N	7:1G:491:ASN:OD1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:183:MET:HB2	9:1I:27:TRP:CZ3	2.55	0.42
12:1L:21:MET:O	12:1L:21:MET:HE3	2.19	0.42
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.55	0.42
12:1L:125:LEU:O	12:1L:129:MET:HG2	2.20	0.42
12:1L:240:PRO:HB2	12:1L:243:VAL:HG23	2.02	0.42
12:1L:546:GLN:HB2	13:1M:278:ARG:HD3	2.02	0.42
13:1M:13:PRO:HB3	45:1N:401:3PE:H2C1	2.02	0.42
13:1M:318:ALA:HB1	13:1M:374:ASN:ND2	2.35	0.42
51:1M:501:PGT:H212	14:1N:281:LEU:HD13	2.02	0.42
15:1O:245:LYS:HB2	15:1O:245:LYS:HE2	1.81	0.42
16:1P:171:ILE:HG21	16:1P:207:ILE:HD12	2.01	0.42
18:1R:59:CYS:SG	18:1R:84:CYS:HB3	2.54	0.42
20:1U:13:ASP:O	20:1U:17:TYR:HB2	2.19	0.42
20:1U:32:VAL:O	20:1U:74:GLN:N	2.52	0.42
23:1X:43:MET:HE3	23:1X:43:MET:HB3	1.75	0.42
23:1X:76:HIS:ND1	23:1X:113:LYS:HE2	2.33	0.42
23:1X:82:THR:OG1	23:1X:83:GLU:N	2.53	0.42
36:1k:35:LEU:HB3	36:1k:40:LEU:HB2	2.02	0.42
2:1B:38:ASN:OD1	2:1B:168:LYS:HA	2.20	0.42
5:1E:87:TYR:CD2	6:1F:181:ALA:HB3	2.55	0.42
5:1E:116:ILE:HD13	5:1E:152:PRO:HB2	2.01	0.42
5:1E:167:LYS:O	5:1E:170:GLU:HB2	2.20	0.42
6:1F:29:HIS:CD2	6:1F:29:HIS:H	2.37	0.42
7:1G:255:HIS:O	7:1G:260:GLU:N	2.50	0.42
7:1G:672:TYR:HA	7:1G:684:MET:HE1	2.02	0.42
8:1H:186:PHE:CD2	50:1I:203:PC1:H2E1	2.54	0.42
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.20	0.42
11:1K:43:MET:O	11:1K:47:ILE:HD12	2.20	0.42
12:1L:15:LEU:HD12	12:1L:15:LEU:H	1.85	0.42
12:1L:90:ILE:O	12:1L:94:LEU:HG	2.20	0.42
13:1M:115:LEU:HD23	13:1M:115:LEU:HA	1.87	0.42
13:1M:152:TYR:C	13:1M:205:VAL:HG11	2.45	0.42
13:1M:318:ALA:HB2	13:1M:373:ILE:CG2	2.47	0.42
13:1M:434:ASN:HB3	33:1h:21:PHE:CE2	2.55	0.42
14:1N:215:MET:HE1	14:1N:219:LEU:HD22	2.01	0.42
14:1N:341:PRO:HB2	29:1d:79:GLN:NE2	2.34	0.42
15:1O:50:HIS:HA	15:1O:123:VAL:HG13	2.02	0.42
17:1Q:43:ASN:C	17:1Q:43:ASN:OD1	2.62	0.42
17:1Q:120:ALA:O	17:1Q:128:THR:OG1	2.31	0.42
20:1U:33:ASN:HA	20:1U:72:CYS:SG	2.60	0.42
22:1W:50:PHE:HB3	22:1W:52:LEU:CD1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:21:TYR:CD1	25:1Z:21:TYR:C	2.97	0.42
31:1f:2:ASN:ND2	31:1f:5:GLN:HB3	2.35	0.42
42:1q:76:ASP:OD2	42:1q:76:ASP:C	2.63	0.42
3:1C:56:GLY:O	3:1C:60:VAL:HG22	2.21	0.41
4:1D:90:LEU:H	4:1D:90:LEU:HD12	1.85	0.41
4:1D:203:LEU:HD12	4:1D:203:LEU:H	1.84	0.41
4:1D:282:GLU:HG2	4:1D:309:ARG:HH22	1.85	0.41
4:1D:412:ALA:HB3	8:1H:281:ARG:HG3	2.01	0.41
5:1E:190:ARG:HD2	5:1E:193:CYS:HA	2.02	0.41
5:1E:196:ALA:HB3	6:1F:264:HIS:ND1	2.36	0.41
6:1F:140:GLY:O	6:1F:179:ARG:NH2	2.50	0.41
7:1G:45:ARG:CZ	7:1G:260:GLU:HB3	2.50	0.41
7:1G:447:LYS:O	7:1G:448:LYS:HD2	2.20	0.41
7:1G:628:PRO:HG2	19:1S:57:CYS:HB3	2.01	0.41
8:1H:199:ASP:HB3	8:1H:279:ARG:NH2	2.35	0.41
12:1L:132:VAL:HG13	12:1L:133:THR:HG23	2.02	0.41
12:1L:248:HIS:CE1	12:1L:252:MET:HE3	2.55	0.41
12:1L:279:CYS:O	12:1L:283:ILE:HG22	2.20	0.41
12:1L:346:ILE:O	12:1L:350:LEU:HB3	2.19	0.41
12:1L:420:ALA:O	12:1L:424:THR:HG23	2.19	0.41
12:1L:514:LYS:HE2	12:1L:514:LYS:HB3	1.89	0.41
14:1N:135:LYS:NZ	14:1N:187:MET:SD	2.93	0.41
15:1O:183:ILE:HA	15:1O:186:LYS:HG2	2.02	0.41
16:1P:10:LYS:HD3	16:1P:10:LYS:HA	1.74	0.41
20:1T:24:LYS:C	20:1T:25:ILE:HD13	2.45	0.41
25:1Z:43:LEU:O	25:1Z:47:TYR:HD1	2.03	0.41
37:1l:145:ASP:OD2	37:1l:147:THR:OG1	2.27	0.41
39:1n:48:ASP:OD2	39:1n:48:ASP:N	2.49	0.41
41:1p:136:LYS:HE2	41:1p:136:LYS:HB3	1.80	0.41
2:1B:60:MET:HE3	4:1D:167:PHE:HZ	1.84	0.41
3:1C:41:GLN:OE1	43:1r:67:ILE:HA	2.21	0.41
3:1C:94:TYR:HB2	3:1C:107:VAL:CG2	2.50	0.41
3:1C:152:LEU:HD21	4:1D:430:ARG:NH2	2.36	0.41
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.19	0.41
5:1E:39:PRO:HB3	44:1s:66:PRO:HD2	2.02	0.41
6:1F:12:PHE:HZ	6:1F:246:GLY:N	2.18	0.41
6:1F:247:ARG:HB3	6:1F:250:ASN:HD22	1.84	0.41
6:1F:295:LEU:HB2	6:1F:339:ARG:HD2	2.01	0.41
6:1F:298:ILE:O	6:1F:334:VAL:HA	2.19	0.41
7:1G:190:MET:HE3	7:1G:695:ILE:HG22	2.01	0.41
9:1I:101:ASP:OD1	9:1I:102:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:50:SER:N	10:1J:139:GLU:OE1	2.53	0.41
10:1J:168:ILE:HD13	10:1J:168:ILE:HA	1.84	0.41
12:1L:273:VAL:O	12:1L:277:THR:HG23	2.20	0.41
13:1M:100:ILE:HD12	13:1M:101:LEU:N	2.35	0.41
13:1M:165:VAL:HG23	14:1N:271:THR:HG21	2.02	0.41
13:1M:277:LEU:HD23	13:1M:277:LEU:HA	1.82	0.41
13:1M:432:ARG:NH1	32:1g:46:GLY:O	2.52	0.41
15:1O:78:SER:HB3	15:1O:81:LYS:HB2	2.02	0.41
15:1O:182:ARG:O	15:1O:186:LYS:HE3	2.19	0.41
15:1O:275:ILE:HG23	15:1O:277:VAL:HG22	2.02	0.41
15:1O:281:GLU:H	15:1O:281:GLU:CD	2.27	0.41
16:1P:71:MET:HE1	18:1R:29:SER:OG	2.20	0.41
17:1Q:93:VAL:HG12	17:1Q:103:PHE:CZ	2.52	0.41
21:1V:23:LEU:HD22	21:1V:58:VAL:HG11	2.01	0.41
32:1g:63:PHE:CE1	32:1g:68:ILE:HD11	2.55	0.41
36:1k:44:TRP:CE3	36:1k:47:ASN:ND2	2.88	0.41
42:1q:55:PHE:CZ	42:1q:58:ARG:HD3	2.54	0.41
1:1A:52:SER:C	1:1A:53:MET:HE2	2.45	0.41
1:1A:69:ILE:HD12	8:1H:147:ALA:HB3	2.01	0.41
4:1D:270:ARG:HD3	4:1D:368:GLU:HB3	2.03	0.41
6:1F:257:ASN:HB3	6:1F:333:ALA:HA	2.02	0.41
7:1G:28:GLN:HA	7:1G:31:GLU:OE2	2.21	0.41
7:1G:377:ILE:HD12	7:1G:450:MET:HG2	2.02	0.41
7:1G:478:ARG:NE	7:1G:478:ARG:O	2.53	0.41
8:1H:115:SER:O	8:1H:119:SER:HB2	2.19	0.41
8:1H:281:ARG:NE	8:1H:283:ASP:OD1	2.52	0.41
10:1J:56:VAL:HB	11:1K:41:PHE:HE2	1.84	0.41
12:1L:64:SER:HB2	34:1i:95:THR:HA	2.01	0.41
12:1L:292:ALA:HB2	12:1L:304:PHE:HB3	2.01	0.41
15:1O:38:LEU:HD13	15:1O:172:VAL:HG22	2.01	0.41
15:1O:154:GLU:HA	15:1O:157:LYS:HZ1	1.85	0.41
21:1V:72:GLN:N	21:1V:72:GLN:OE1	2.54	0.41
21:1V:94:LEU:HG	21:1V:95:ARG:HH22	1.85	0.41
36:1k:74:PHE:O	36:1k:78:VAL:HG23	2.20	0.41
40:1o:50:LEU:HD21	40:1o:59:ALA:HB1	2.01	0.41
40:1o:64:GLN:OE1	40:1o:64:GLN:N	2.50	0.41
42:1q:78:ASP:O	42:1q:81:MET:HG3	2.20	0.41
2:1B:69:MET:H	2:1B:69:MET:CE	2.22	0.41
3:1C:39:GLN:HB3	3:1C:51:PHE:CB	2.47	0.41
4:1D:130:PRO:HA	4:1D:325:VAL:HG12	2.03	0.41
4:1D:151:ILE:HD11	4:1D:218:PHE:HZ	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:344:VAL:HG12	6:1F:380:VAL:HG22	2.02	0.41
7:1G:11:VAL:HG21	7:1G:73:VAL:HG21	2.01	0.41
7:1G:460:ARG:NH2	7:1G:462:ASP:OD2	2.53	0.41
7:1G:522:LEU:HD12	7:1G:523:PHE:H	1.86	0.41
8:1H:62:ARG:H	8:1H:62:ARG:HG2	1.71	0.41
12:1L:368:PHE:HE1	35:1j:28:PHE:HD2	1.67	0.41
12:1L:433:GLY:C	12:1L:434:LYS:HD2	2.46	0.41
12:1L:541:ASN:OD1	45:1L:701:3PE:H2C1	2.20	0.41
15:1O:89:ASN:OD1	32:1g:24:ILE:HG23	2.21	0.41
16:1P:19:ILE:O	16:1P:19:ILE:HG13	2.19	0.41
21:1V:76:ILE:O	21:1V:80:ILE:HG12	2.20	0.41
23:1X:4:VAL:HG12	25:1Z:107:GLY:O	2.20	0.41
25:1Z:51:MET:SD	25:1Z:55:ARG:NH1	2.94	0.41
31:1f:44:PHE:CD2	33:1h:84:GLU:HB3	2.55	0.41
33:1h:89:LYS:HB3	33:1h:89:LYS:HE3	1.82	0.41
35:1j:45:ASP:HB2	35:1j:50:HIS:CB	2.51	0.41
40:1o:6:ARG:NE	40:1o:105:ARG:HH21	2.19	0.41
3:1C:38:GLN:OE1	3:1C:110:TYR:OH	2.30	0.41
4:1D:348:HIS:HE1	9:1I:125:ALA:O	2.04	0.41
5:1E:86:PHE:CE1	7:1G:177:ARG:HG3	2.55	0.41
6:1F:29:HIS:CE1	6:1F:39:ARG:HH11	2.37	0.41
6:1F:208:PRO:HD2	17:1Q:118:TYR:HD1	1.84	0.41
7:1G:347:GLU:O	7:1G:510:GLY:N	2.54	0.41
7:1G:454:GLY:HA2	7:1G:493:LEU:HB3	2.01	0.41
7:1G:564:ALA:HB1	7:1G:568:GLU:HG2	2.02	0.41
8:1H:19:PHE:HB3	26:1a:12:MET:HE2	2.02	0.41
9:1I:18:THR:HA	27:1b:12:TRP:CH2	2.54	0.41
12:1L:71:LEU:HD11	13:1M:380:PHE:CZ	2.55	0.41
12:1L:184:LEU:HD23	13:1M:393:ILE:HG21	2.02	0.41
12:1L:298:ILE:H	12:1L:298:ILE:HD12	1.86	0.41
13:1M:14:MET:HE1	13:1M:30:HIS:ND1	2.36	0.41
13:1M:209:LEU:HD12	13:1M:210:TYR:O	2.21	0.41
13:1M:263:MET:HE1	38:1m:104:PHE:CD2	2.55	0.41
13:1M:388:TRP:O	38:1m:108:ARG:NH1	2.53	0.41
16:1P:84:VAL:HG23	16:1P:85:VAL:HG13	2.02	0.41
20:1T:36:PHE:HA	20:1T:40:LEU:HB2	2.02	0.41
23:1X:58:GLU:OE1	23:1X:58:GLU:N	2.43	0.41
24:1Y:130:GLU:HG2	24:1Y:132:TRP:HE1	1.85	0.41
27:1b:78:GLU:HA	27:1b:81:LYS:HZ3	1.84	0.41
32:1g:48:ASP:OD2	32:1g:48:ASP:C	2.63	0.41
36:1k:26:THR:O	36:1k:28:LEU:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:57:ASP:O	43:1r:61:GLU:N	2.42	0.41
3:1C:79:THR:HG21	4:1D:377:TYR:CD2	2.56	0.41
3:1C:175:ARG:NE	3:1C:186:GLU:OE1	2.50	0.41
6:1F:95:VAL:H	6:1F:136:ILE:HA	1.84	0.41
6:1F:262:VAL:HA	6:1F:287:VAL:HA	2.02	0.41
6:1F:347:ILE:HG12	6:1F:418:LEU:HG	2.02	0.41
6:1F:417:GLY:HA2	6:1F:420:ARG:HE	1.86	0.41
7:1G:39:ARG:HB2	47:1G:804:FES:S2	2.61	0.41
7:1G:288:LYS:HB3	7:1G:288:LYS:HE3	1.77	0.41
7:1G:545:TYR:HB3	7:1G:560:ILE:HD13	2.03	0.41
8:1H:307:LEU:HB3	8:1H:308:PRO:HD3	2.02	0.41
9:1I:64:GLU:O	9:1I:134:GLY:N	2.48	0.41
10:1J:28:TYR:N	10:1J:28:TYR:CD1	2.88	0.41
10:1J:136:PHE:CE1	30:1e:28:ILE:HG21	2.56	0.41
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	2.03	0.41
13:1M:137:GLY:HA2	13:1M:224:PRO:HD3	2.03	0.41
13:1M:457:PRO:HA	32:1g:84:ARG:NH2	2.35	0.41
14:1N:109:SER:C	14:1N:112:HIS:HD1	2.25	0.41
15:1O:216:GLU:H	15:1O:216:GLU:HG3	1.67	0.41
17:1Q:113:PRO:O	17:1Q:113:PRO:HD2	2.20	0.41
18:1R:80:LYS:HD2	18:1R:81:THR:O	2.21	0.41
19:1S:16:ARG:HH21	19:1S:69:ALA:HA	1.85	0.41
19:1S:67:ARG:HA	19:1S:73:GLU:HG2	2.02	0.41
20:1T:13:ASP:OD2	20:1T:14:ARG:N	2.53	0.41
20:1U:47:GLN:O	20:1U:50:ILE:HG13	2.21	0.41
20:1U:78:ASP:HB3	34:1i:15:ARG:NE	2.36	0.41
20:1U:79:TYR:CZ	20:1U:83:LYS:HG2	2.56	0.41
22:1W:92:GLU:O	22:1W:98:LYS:HG3	2.20	0.41
25:1Z:68:ARG:HG3	26:1a:43:TYR:CZ	2.55	0.41
26:1a:39:ALA:HA	26:1a:44:GLN:HB2	2.02	0.41
32:1g:70:LEU:HD12	32:1g:70:LEU:HA	1.91	0.41
33:1h:115:ARG:HB2	33:1h:123:TYR:CE2	2.55	0.41
34:1i:106:GLY:HA2	34:1i:118:LEU:HD22	2.03	0.41
35:1j:68:PRO:O	40:1o:110:ARG:NH2	2.40	0.41
38:1m:30:LYS:N	38:1m:30:LYS:CD	2.77	0.41
39:1n:23:LEU:HD23	39:1n:23:LEU:HA	1.83	0.41
40:1o:62:LEU:HD22	40:1o:86:TRP:CZ2	2.56	0.41
41:1p:104:ILE:O	41:1p:108:ARG:HG3	2.20	0.41
44:1s:40:ASN:HD22	44:1s:43:HIS:CD2	2.39	0.41
1:1A:1:FME:HCN	25:1Z:142:TRP:CE3	2.55	0.41
2:1B:92:LEU:HB3	2:1B:133:VAL:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:197:PHE:HA	7:1G:220:TRP:O	2.21	0.41
4:1D:329:LYS:HA	7:1G:121:MET:HE1	2.02	0.41
6:1F:16:LYS:HE2	6:1F:16:LYS:HB2	1.89	0.41
6:1F:122:CYS:O	6:1F:126:GLY:N	2.41	0.41
7:1G:84:GLU:OE2	7:1G:88:LYS:NZ	2.30	0.41
7:1G:364:LEU:HD12	7:1G:576:THR:C	2.46	0.41
7:1G:646:ASN:HB3	7:1G:650:LYS:NZ	2.35	0.41
8:1H:28:LEU:HD12	8:1H:32:GLN:NE2	2.35	0.41
12:1L:237:MET:SD	12:1L:303:ALA:HB2	2.61	0.41
13:1M:168:GLN:HB2	13:1M:174:LEU:HD11	2.02	0.41
14:1N:236:LYS:HB2	14:1N:311:MET:SD	2.61	0.41
15:1O:164:LEU:HD23	15:1O:247:PRO:HB2	2.03	0.41
15:1O:204:ASN:OD1	15:1O:204:ASN:N	2.44	0.41
19:1S:53:LEU:HB3	19:1S:55:ARG:HD3	2.03	0.41
29:1d:39:TYR:O	29:1d:42:GLY:N	2.53	0.41
35:1j:34:PHE:C	35:1j:34:PHE:HD1	2.29	0.41
1:1A:22:PHE:HB3	1:1A:23:TRP:HE3	1.85	0.41
4:1D:402:LEU:HD23	4:1D:421:GLN:NE2	2.34	0.41
6:1F:15:LEU:HB2	6:1F:271:GLU:HB2	2.02	0.41
8:1H:127:TYR:CE1	8:1H:207:LEU:HD13	2.55	0.41
12:1L:295:GLN:HE22	12:1L:524:ASN:HA	1.85	0.41
12:1L:351:ASN:C	12:1L:352:ASP:OD1	2.64	0.41
13:1M:197:LEU:HD23	13:1M:197:LEU:HA	1.87	0.41
14:1N:40:MET:O	14:1N:40:MET:HE3	2.20	0.41
15:1O:318:TRP:O	29:1d:58:LEU:N	2.42	0.41
17:1Q:33:ARG:HE	17:1Q:33:ARG:HB3	1.69	0.41
19:1S:74:LYS:HA	19:1S:74:LYS:HD2	1.80	0.41
21:1V:93:MET:HA	21:1V:96:TRP:CD1	2.56	0.41
22:1W:21:PHE:HB2	22:1W:80:ASP:OD2	2.21	0.41
24:1Y:35:VAL:HG21	45:1Y:202:3PE:H252	2.03	0.41
34:1i:120:LYS:C	34:1i:120:LYS:HD3	2.45	0.41
37:1l:130:PRO:O	40:1o:97:ARG:NE	2.54	0.41
1:1A:22:PHE:HB3	1:1A:23:TRP:CE3	2.55	0.41
1:1A:66:ASP:OD2	1:1A:66:ASP:C	2.64	0.41
1:1A:104:TYR:HE2	10:1J:166:VAL:HA	1.85	0.41
2:1B:81:ARG:HH22	2:1B:106:GLN:HB2	1.86	0.41
2:1B:109:GLU:HG2	2:1B:111:ARG:NH1	2.36	0.41
2:1B:171:LYS:H	16:1P:52:GLU:CD	2.29	0.41
3:1C:85:THR:OG1	17:1Q:91:ASP:OD2	2.32	0.41
3:1C:86:ARG:NH1	3:1C:91:GLU:OE1	2.54	0.41
4:1D:224:GLU:CD	9:1I:36:MET:HE1	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:354:GLU:HG2	4:1D:355:GLY:O	2.20	0.41
5:1E:86:PHE:CD2	6:1F:200:GLN:HB2	2.56	0.41
6:1F:12:PHE:CZ	6:1F:246:GLY:N	2.89	0.41
6:1F:295:LEU:N	6:1F:337:MET:O	2.54	0.41
7:1G:42:TYR:HE1	17:1Q:116:LYS:HG3	1.86	0.41
7:1G:439:PHE:HD1	7:1G:442:ILE:HD13	1.85	0.41
7:1G:458:LEU:HD12	7:1G:458:LEU:O	2.21	0.41
8:1H:106:LEU:HA	8:1H:106:LEU:HD23	1.78	0.41
9:1I:31:VAL:HG11	50:1I:204:PC1:H241	2.03	0.41
9:1I:64:GLU:HB2	9:1I:139:PHE:CD1	2.56	0.41
11:1K:51:THR:HG23	11:1K:53:PHE:HB2	2.01	0.41
12:1L:88:MET:C	12:1L:91:PRO:HD2	2.45	0.41
12:1L:145:GLU:O	12:1L:149:ILE:HG22	2.21	0.41
12:1L:226:GLN:HE21	12:1L:284:THR:HG21	1.85	0.41
12:1L:532:ILE:HG12	37:1L:101:MET:HE2	2.03	0.41
12:1L:589:LEU:HD12	12:1L:589:LEU:HA	1.91	0.41
13:1M:176:PHE:HA	13:1M:179:ILE:HG22	2.03	0.41
13:1M:207:MET:HE1	13:1M:240:GLY:HA2	2.02	0.41
13:1M:419:TYR:CE1	39:1n:99:PRO:HD3	2.56	0.41
13:1M:431:THR:HG21	32:1g:58:MET:HE1	2.03	0.41
13:1M:442:LEU:HD12	13:1M:442:LEU:HA	1.81	0.41
14:1N:236:LYS:NZ	14:1N:314:LYS:O	2.50	0.41
14:1N:320:THR:OG1	15:1O:265:ASN:OD1	2.27	0.41
15:1O:24:VAL:O	15:1O:166:PRO:HB3	2.19	0.41
15:1O:188:ASN:N	15:1O:191:GLU:OE2	2.54	0.41
16:1P:26:ALA:HA	16:1P:31:GLY:HA3	2.03	0.41
16:1P:144:ARG:HD2	16:1P:147:ARG:HD2	2.03	0.41
16:1P:208:VAL:O	16:1P:212:LYS:NZ	2.48	0.41
17:1Q:9:GLN:OE1	17:1Q:9:GLN:O	2.38	0.41
19:1S:54:ILE:O	19:1S:54:ILE:HD12	2.20	0.41
20:1T:29:LYS:HZ2	20:1T:40:LEU:HD22	1.86	0.41
21:1V:24:LYS:HE3	21:1V:59:LYS:HA	2.02	0.41
26:1a:28:LYS:HE3	26:1a:28:LYS:HB3	1.61	0.41
32:1g:40:LYS:C	32:1g:40:LYS:HD3	2.46	0.41
32:1g:50:ASP:OD1	32:1g:50:ASP:C	2.63	0.41
32:1g:112:CYS:HB3	41:1p:141:ARG:HD3	2.03	0.41
34:1i:28:SER:HB3	34:1i:31:GLU:CG	2.51	0.41
36:1k:14:GLU:CD	36:1k:14:GLU:N	2.79	0.41
37:1l:97:SER:HA	38:1m:5:TYR:CE1	2.56	0.41
41:1p:5:ASP:OD2	41:1p:8:VAL:HG23	2.21	0.41
1:1A:97:LEU:HD12	1:1A:97:LEU:HA	1.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:56:GLY:C	3:1C:59:PRO:HD2	2.46	0.41
5:1E:144:CYS:SG	5:1E:146:GLY:N	2.94	0.41
5:1E:147:ALA:O	5:1E:149:VAL:N	2.54	0.41
6:1F:247:ARG:NH1	6:1F:318:ASP:OD2	2.51	0.41
7:1G:126:ASP:N	7:1G:126:ASP:OD1	2.54	0.41
7:1G:396:ARG:HH11	7:1G:399:TRP:CD1	2.39	0.41
7:1G:405:LYS:HA	7:1G:405:LYS:HD3	1.83	0.41
7:1G:562:PRO:HB2	7:1G:593:ALA:HB2	2.03	0.41
7:1G:682:GLN:O	7:1G:686:LYS:HG2	2.21	0.41
10:1J:23:LYS:HA	10:1J:23:LYS:HD2	1.98	0.41
11:1K:6:MET:SD	11:1K:6:MET:C	3.04	0.41
11:1K:36:MET:HE2	11:1K:36:MET:HB2	1.95	0.41
12:1L:60:GLU:O	41:1p:114:GLN:NE2	2.54	0.41
12:1L:145:GLU:HG2	12:1L:176:ARG:NH1	2.36	0.41
12:1L:586:LEU:HD12	24:1Y:41:ALA:O	2.21	0.41
13:1M:279:GLN:NE2	13:1M:284:SER:OG	2.32	0.41
13:1M:411:LEU:HD12	13:1M:411:LEU:HA	1.90	0.41
14:1N:95:MET:HE1	14:1N:145:ILE:HD12	2.03	0.41
14:1N:259:GLY:O	14:1N:262:PRO:HD2	2.21	0.41
15:1O:160:ALA:HA	15:1O:163:TYR:HD1	1.85	0.41
17:1Q:76:ALA:O	17:1Q:78:PRO:HD3	2.21	0.41
21:1V:65:LYS:HE3	21:1V:65:LYS:HB3	1.65	0.41
29:1d:17:GLU:OE1	29:1d:81:TYR:OH	2.20	0.41
30:1e:16:TRP:CH2	30:1e:17:MET:HE3	2.55	0.41
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.56	0.41
35:1j:6:HIS:O	35:1j:7:ILE:HD13	2.21	0.41
43:1r:28:GLN:HE21	43:1r:28:GLN:HB3	1.64	0.41
2:1B:94:ASN:HB3	3:1C:174:LEU:HD11	2.03	0.40
6:1F:91:LYS:CD	6:1F:219:PRO:HB2	2.51	0.40
6:1F:121:GLY:HA2	6:1F:232:PRO:HD3	2.03	0.40
6:1F:231:SER:N	6:1F:232:PRO:HD2	2.36	0.40
6:1F:399:ILE:H	6:1F:399:ILE:HG13	1.72	0.40
9:1I:164:GLU:OE2	42:1q:87:HIS:ND1	2.52	0.40
10:1J:100:GLU:HA	10:1J:103:MET:HG3	2.03	0.40
12:1L:298:ILE:HD11	12:1L:359:MET:CE	2.51	0.40
12:1L:435:PRO:HG2	36:1k:56:PHE:CG	2.56	0.40
12:1L:482:MET:HB3	12:1L:486:MET:SD	2.61	0.40
16:1P:177:ARG:H	16:1P:180:ASN:HD21	1.69	0.40
17:1Q:72:TRP:HA	17:1Q:72:TRP:CE3	2.56	0.40
18:1R:95:HIS:O	18:1R:95:HIS:ND1	2.53	0.40
23:1X:22:SER:HB3	23:1X:88:ILE:HG22	2.01	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:1X:101:LYS:HB2	23:1X:101:LYS:HE2	1.87	0.40
23:1X:120:ASP:N	23:1X:123:GLU:OE1	2.49	0.40
24:1Y:43:LYS:HD3	45:1Y:201:3PE:HN2	1.86	0.40
33:1h:36:VAL:O	33:1h:40:ILE:HG13	2.20	0.40
37:1l:65:ASP:OD2	37:1l:73:TRP:N	2.54	0.40
38:1m:45:GLU:HA	38:1m:48:LEU:HD12	2.03	0.40
40:1o:7:ARG:HH21	40:1o:17:ASP:HA	1.85	0.40
41:1p:34:LYS:O	41:1p:38:LEU:HD12	2.21	0.40
1:1A:53:MET:O	1:1A:57:LEU:N	2.44	0.40
2:1B:176:TRP:HB2	2:1B:179:ARG:HH21	1.86	0.40
4:1D:166:PRO:HA	4:1D:169:TRP:HB2	2.03	0.40
4:1D:205:LEU:O	43:1r:35:GLN:HG3	2.20	0.40
6:1F:97:ALA:HB1	6:1F:111:ILE:HD11	2.03	0.40
6:1F:101:GLU:OE1	6:1F:104:THR:HG23	2.21	0.40
7:1G:59:ILE:HD12	7:1G:59:ILE:HA	1.98	0.40
7:1G:70:ALA:O	7:1G:72:PRO:HD3	2.21	0.40
8:1H:74:ALA:HB3	8:1H:75:PRO:HD3	2.02	0.40
10:1J:99:MET:H	10:1J:99:MET:HE3	1.86	0.40
13:1M:121:LEU:H	13:1M:121:LEU:HD12	1.86	0.40
14:1N:341:PRO:HB2	29:1d:79:GLN:HE22	1.84	0.40
15:1O:29:GLY:O	15:1O:126:ARG:NH1	2.50	0.40
16:1P:216:ASN:HA	16:1P:219:LYS:HG2	2.02	0.40
17:1Q:28:GLU:OE1	17:1Q:28:GLU:N	2.44	0.40
18:1R:55:ARG:HE	18:1R:55:ARG:HB3	1.76	0.40
20:1T:12:LYS:HD2	20:1T:77:VAL:HG21	2.02	0.40
20:1T:83:LYS:HG3	20:1T:84:LYS:N	2.36	0.40
22:1W:54:ILE:HG12	22:1W:107:PHE:HE2	1.85	0.40
23:1X:46:ARG:HD2	23:1X:46:ARG:HA	1.79	0.40
33:1h:44:ASN:O	41:1p:51:ILE:HD11	2.22	0.40
34:1i:84:TYR:O	34:1i:89:VAL:HG23	2.21	0.40
38:1m:18:ASP:OD2	38:1m:18:ASP:C	2.64	0.40
39:1n:34:ASP:OD1	39:1n:34:ASP:N	2.55	0.40
39:1n:163:PRO:HA	39:1n:164:PRO:HD3	1.94	0.40
42:1q:32:ASP:OD1	42:1q:33:VAL:N	2.54	0.40
2:1B:39:TRP:CD1	2:1B:39:TRP:C	2.98	0.40
5:1E:108:CYS:HA	5:1E:111:ARG:CZ	2.51	0.40
6:1F:92:TYR:CE1	6:1F:133:ALA:HB3	2.57	0.40
6:1F:179:ARG:HD2	44:1s:51:PHE:CD2	2.56	0.40
7:1G:91:GLU:OE2	7:1G:125:SER:N	2.54	0.40
7:1G:415:LEU:O	7:1G:416:THR:OG1	2.33	0.40
12:1L:15:LEU:O	12:1L:18:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:152:PHE:CD1	12:1L:168:ALA:HB1	2.56	0.40
13:1M:27:ALA:O	13:1M:31:SER:OG	2.25	0.40
13:1M:75:LEU:HD13	13:1M:440:HIS:NE2	2.36	0.40
13:1M:387:SER:O	38:1m:111:LYS:NZ	2.38	0.40
14:1N:106:LEU:HD23	14:1N:106:LEU:HA	1.90	0.40
14:1N:124:LEU:HD12	14:1N:124:LEU:HA	1.84	0.40
15:1O:234:VAL:O	15:1O:238:ILE:HG12	2.21	0.40
15:1O:265:ASN:HD22	15:1O:268:GLU:N	2.14	0.40
16:1P:250:TYR:CD2	16:1P:326:TRP:HB3	2.57	0.40
19:1S:85:GLN:O	19:1S:88:ARG:HB3	2.21	0.40
26:1a:1:MET:HE2	52:1r:201:CDL:HB21	2.03	0.40
26:1a:7:PRO:HD3	52:1r:201:CDL:H172	2.03	0.40
29:1d:61:GLN:HA	29:1d:64:TYR:HD2	1.86	0.40
31:1f:28:ARG:HH12	50:1f:101:PC1:H112	1.86	0.40
33:1h:91:MET:HG2	41:1p:85:PHE:CD2	2.56	0.40
33:1h:132:LEU:HD23	33:1h:132:LEU:HA	1.85	0.40
35:1j:33:TRP:CZ2	36:1k:67:LEU:HA	2.57	0.40
37:1l:37:TYR:CG	37:1l:44:TYR:HD2	2.39	0.40
38:1m:45:GLU:O	38:1m:49:GLN:HG3	2.21	0.40
38:1m:65:ILE:H	38:1m:65:ILE:HG13	1.73	0.40
39:1n:122:GLU:OE1	39:1n:123:GLN:NE2	2.54	0.40
4:1D:366:ALA:HB1	4:1D:373:GLU:OE1	2.21	0.40
6:1F:317:MET:O	6:1F:317:MET:HG3	2.20	0.40
7:1G:122:MET:N	7:1G:122:MET:SD	2.94	0.40
7:1G:239:VAL:HG13	7:1G:251:LEU:HB2	2.04	0.40
8:1H:11:ILE:N	8:1H:12:PRO:HD2	2.36	0.40
8:1H:127:TYR:HE1	8:1H:207:LEU:HA	1.86	0.40
11:1K:61:ILE:O	11:1K:65:VAL:HG22	2.21	0.40
13:1M:47:GLU:HB3	41:1p:92:ARG:NE	2.33	0.40
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.22	0.40
13:1M:222:GLU:OE2	13:1M:222:GLU:HA	2.21	0.40
13:1M:329:LEU:HD12	13:1M:359:TRP:CE3	2.57	0.40
13:1M:367:LEU:CD2	13:1M:404:ALA:HA	2.51	0.40
15:1O:250:ASP:OD1	15:1O:250:ASP:N	2.53	0.40
23:1X:3:ILE:HD13	25:1Z:105:LYS:NZ	2.36	0.40
23:1X:44:LEU:HD22	23:1X:130:VAL:HG13	2.03	0.40
23:1X:81:PHE:CG	23:1X:106:PHE:HE2	2.39	0.40
24:1Y:43:LYS:HZ3	45:1Y:201:3PE:P	2.43	0.40
32:1g:71:VAL:O	32:1g:74:SER:OG	2.39	0.40
34:1i:49:PHE:CZ	34:1i:57:LYS:HG3	2.56	0.40
39:1n:51:LYS:HD2	57:1n:201:EHZ:O5	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:106:ARG:HA	40:1o:109:GLN:NE2	2.26	0.40
40:1o:112:LYS:O	40:1o:116:GLN:HG2	2.21	0.40
41:1p:50:PHE:O	41:1p:53:GLN:HG3	2.21	0.40
43:1r:57:ASP:O	43:1r:60:ARG:N	2.55	0.40
4:1D:220:PHE:O	4:1D:224:GLU:HG2	2.22	0.40
4:1D:242:ILE:HD12	4:1D:409:HIS:CD2	2.57	0.40
4:1D:387:TYR:CE1	21:1V:113:TRP:HH2	2.39	0.40
5:1E:103:CYS:CB	5:1E:153:MET:HB2	2.51	0.40
6:1F:98:ASP:HB3	6:1F:187:GLY:HA2	2.03	0.40
6:1F:112:ARG:HB2	6:1F:145:GLU:HG2	2.03	0.40
6:1F:246:GLY:HA3	6:1F:250:ASN:O	2.22	0.40
7:1G:58:GLU:OE2	7:1G:85:LYS:HB3	2.21	0.40
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.62	0.40
8:1H:136:VAL:O	8:1H:140:ILE:HG23	2.21	0.40
8:1H:241:LEU:HD23	8:1H:241:LEU:HA	1.98	0.40
10:1J:164:GLY:HA2	14:1N:38:LEU:HD11	2.02	0.40
12:1L:395:ILE:O	12:1L:399:VAL:HG13	2.22	0.40
12:1L:452:ASN:HB3	12:1L:456:ARG:HH12	1.86	0.40
13:1M:10:MET:O	13:1M:13:PRO:HD2	2.21	0.40
17:1Q:56:LYS:HA	17:1Q:84:LEU:O	2.21	0.40
19:1S:55:ARG:HD2	19:1S:55:ARG:N	2.37	0.40
22:1W:127:ASP:HA	22:1W:128:PRO:HD2	1.90	0.40
25:1Z:75:PHE:CZ	26:1a:50:ARG:HD2	2.57	0.40
29:1d:14:LEU:HD11	29:1d:77:LYS:HE2	2.04	0.40
30:1e:28:ILE:HG22	33:1h:139:THR:HB	2.03	0.40
32:1g:72:LEU:HD11	33:1h:32:THR:HG21	2.03	0.40
33:1h:7:ARG:HE	34:1i:27:LEU:HD12	1.86	0.40
33:1h:30:LEU:O	33:1h:34:ILE:HG12	2.21	0.40
38:1m:25:SER:C	38:1m:27:GLU:H	2.29	0.40
38:1m:32:GLN:HE22	39:1n:8:TYR:HA	1.87	0.40
39:1n:50:HIS:O	39:1n:50:HIS:ND1	2.51	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%)	106 (94%)	6 (5%)	1 (1%)	14	46
2	1B	153/258 (59%)	144 (94%)	9 (6%)	0	100	100
3	1C	207/264 (78%)	190 (92%)	17 (8%)	0	100	100
4	1D	427/476 (90%)	397 (93%)	29 (7%)	1 (0%)	43	72
5	1E	212/249 (85%)	193 (91%)	18 (8%)	1 (0%)	24	57
6	1F	430/464 (93%)	399 (93%)	31 (7%)	0	100	100
7	1G	697/727 (96%)	656 (94%)	37 (5%)	4 (1%)	21	54
8	1H	316/318 (99%)	295 (93%)	18 (6%)	3 (1%)	14	46
9	1I	174/239 (73%)	162 (93%)	12 (7%)	0	100	100
10	1J	173/175 (99%)	160 (92%)	12 (7%)	1 (1%)	21	54
11	1K	96/98 (98%)	92 (96%)	4 (4%)	0	100	100
12	1L	604/606 (100%)	555 (92%)	48 (8%)	1 (0%)	43	72
13	1M	457/459 (100%)	440 (96%)	17 (4%)	0	100	100
14	1N	345/347 (99%)	323 (94%)	22 (6%)	0	100	100
15	1O	318/357 (89%)	297 (93%)	21 (7%)	0	100	100
16	1P	340/377 (90%)	323 (95%)	17 (5%)	0	100	100
17	1Q	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
18	1R	94/123 (76%)	77 (82%)	17 (18%)	0	100	100
19	1S	85/99 (86%)	81 (95%)	4 (5%)	0	100	100
20	1T	83/156 (53%)	79 (95%)	4 (5%)	0	100	100
20	1U	84/156 (54%)	77 (92%)	7 (8%)	0	100	100
21	1V	113/116 (97%)	101 (89%)	12 (11%)	0	100	100
22	1W	113/128 (88%)	103 (91%)	10 (9%)	0	100	100
23	1X	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
24	1Y	137/141 (97%)	133 (97%)	4 (3%)	0	100	100
25	1Z	139/144 (96%)	130 (94%)	9 (6%)	0	100	100
26	1a	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
27	1b	81/84 (96%)	75 (93%)	6 (7%)	0	100	100
28	1c	47/76 (62%)	44 (94%)	3 (6%)	0	100	100
29	1d	117/123 (95%)	111 (95%)	5 (4%)	1 (1%)	14	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
30	1e	97/106 (92%)	92 (95%)	5 (5%)	0	100	100
31	1f	55/135 (41%)	52 (94%)	2 (4%)	1 (2%)	6	34
32	1g	98/154 (64%)	85 (87%)	12 (12%)	1 (1%)	12	45
33	1h	136/189 (72%)	131 (96%)	5 (4%)	0	100	100
34	1i	124/128 (97%)	117 (94%)	7 (6%)	0	100	100
35	1j	69/105 (66%)	67 (97%)	2 (3%)	0	100	100
36	1k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	1l	154/186 (83%)	143 (93%)	11 (7%)	0	100	100
38	1m	126/129 (98%)	120 (95%)	6 (5%)	0	100	100
39	1n	170/179 (95%)	165 (97%)	5 (3%)	0	100	100
40	1o	120/137 (88%)	119 (99%)	1 (1%)	0	100	100
41	1p	171/176 (97%)	169 (99%)	2 (1%)	0	100	100
42	1q	143/145 (99%)	134 (94%)	8 (6%)	1 (1%)	18	51
43	1r	90/114 (79%)	81 (90%)	9 (10%)	0	100	100
44	1s	43/471 (9%)	41 (95%)	2 (5%)	0	100	100
All	All	8194/9744 (84%)	7679 (94%)	499 (6%)	16 (0%)	44	72

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1E	97	LYS
8	1H	68	ILE
8	1H	92	PRO
29	1d	53	VAL
42	1q	142	THR
1	1A	52	SER
4	1D	87	THR
7	1G	47	SER
7	1G	186	TYR
8	1H	208	VAL
32	1g	25	ARG
7	1G	696	GLN
12	1L	464	ALA
31	1f	36	ALA
7	1G	367	THR
10	1J	116	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%)	99 (100%)	0	100	100
2	1B	131/212 (62%)	130 (99%)	1 (1%)	73	77
3	1C	190/227 (84%)	189 (100%)	1 (0%)	81	80
4	1D	371/405 (92%)	370 (100%)	1 (0%)	86	83
5	1E	183/207 (88%)	183 (100%)	0	100	100
6	1F	346/368 (94%)	344 (99%)	2 (1%)	78	79
7	1G	588/610 (96%)	584 (99%)	4 (1%)	76	78
8	1H	274/274 (100%)	272 (99%)	2 (1%)	76	78
9	1I	151/201 (75%)	151 (100%)	0	100	100
10	1J	140/140 (100%)	140 (100%)	0	100	100
11	1K	84/84 (100%)	84 (100%)	0	100	100
12	1L	539/539 (100%)	535 (99%)	4 (1%)	76	78
13	1M	408/408 (100%)	405 (99%)	3 (1%)	76	78
14	1N	310/310 (100%)	310 (100%)	0	100	100
15	1O	283/307 (92%)	281 (99%)	2 (1%)	76	78
16	1P	296/323 (92%)	293 (99%)	3 (1%)	68	75
17	1Q	117/152 (77%)	117 (100%)	0	100	100
18	1R	79/97 (81%)	79 (100%)	0	100	100
19	1S	77/82 (94%)	77 (100%)	0	100	100
20	1T	79/133 (59%)	78 (99%)	1 (1%)	61	72
20	1U	79/133 (59%)	79 (100%)	0	100	100
21	1V	100/101 (99%)	99 (99%)	1 (1%)	68	75
22	1W	107/112 (96%)	107 (100%)	0	100	100
23	1X	153/154 (99%)	153 (100%)	0	100	100
24	1Y	101/102 (99%)	100 (99%)	1 (1%)	68	75
25	1Z	123/124 (99%)	121 (98%)	2 (2%)	55	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	57
27	1b	69/70 (99%)	69 (100%)	0	100	100
28	1c	45/66 (68%)	45 (100%)	0	100	100
29	1d	107/109 (98%)	106 (99%)	1 (1%)	70	76
30	1e	87/94 (93%)	87 (100%)	0	100	100
31	1f	54/113 (48%)	54 (100%)	0	100	100
32	1g	92/129 (71%)	92 (100%)	0	100	100
33	1h	121/158 (77%)	120 (99%)	1 (1%)	73	77
34	1i	119/120 (99%)	119 (100%)	0	100	100
35	1j	62/84 (74%)	62 (100%)	0	100	100
36	1k	63/76 (83%)	63 (100%)	0	100	100
37	1l	141/161 (88%)	140 (99%)	1 (1%)	76	78
38	1m	113/114 (99%)	111 (98%)	2 (2%)	51	68
39	1n	156/160 (98%)	156 (100%)	0	100	100
40	1o	110/120 (92%)	110 (100%)	0	100	100
41	1p	154/156 (99%)	153 (99%)	1 (1%)	78	79
42	1q	131/131 (100%)	131 (100%)	0	100	100
43	1r	85/98 (87%)	85 (100%)	0	100	100
44	1s	44/351 (12%)	44 (100%)	0	100	100
All	All	7219/8272 (87%)	7183 (100%)	36 (0%)	78	80

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	1B	129	SER
3	1C	74	SER
4	1D	224	GLU
6	1F	192	LEU
6	1F	279	LEU
7	1G	77	TRP
7	1G	332	LYS
7	1G	525	LEU
7	1G	684	MET
8	1H	20	LEU
8	1H	32	GLN

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Mol	Chain	Res	Type
12	1L	26	ILE
12	1L	66	TRP
12	1L	88	MET
12	1L	409	LEU
13	1M	188	ASN
13	1M	218	LYS
13	1M	263	MET
15	1O	164	LEU
15	1O	251	GLN
16	1P	44	GLN
16	1P	83	LYS
16	1P	145	TYR
20	1T	70	LEU
21	1V	99	TRP
24	1Y	54	ARG
25	1Z	24	ASN
25	1Z	127	LEU
26	1a	1	MET
26	1a	9	ILE
29	1d	25	LYS
33	1h	25	MET
37	1l	83	MET
38	1m	116	GLN
38	1m	126	ILE
41	1p	46	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	106	GLN
3	1C	104	GLN
4	1D	84	HIS
4	1D	98	GLN
4	1D	149	ASN
4	1D	273	GLN
4	1D	421	GLN
5	1E	74	GLN
5	1E	99	HIS
5	1E	121	GLN
6	1F	148	ASN
6	1F	224	ASN
7	1G	255	HIS

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Mol	Chain	Res	Type
7	1G	392	ASN
8	1H	235	ASN
10	1J	175	ASN
11	1K	50	ASN
11	1K	92	ASN
12	1L	2	ASN
12	1L	25	ASN
12	1L	59	GLN
12	1L	135	ASN
12	1L	165	ASN
12	1L	323	HIS
12	1L	332	HIS
12	1L	444	ASN
12	1L	579	ASN
13	1M	30	HIS
13	1M	81	GLN
13	1M	103	GLN
13	1M	144	ASN
13	1M	415	GLN
13	1M	422	HIS
14	1N	36	ASN
14	1N	83	GLN
14	1N	120	GLN
14	1N	134	GLN
14	1N	144	GLN
14	1N	289	ASN
14	1N	309	ASN
14	1N	322	GLN
15	1O	120	GLN
15	1O	251	GLN
16	1P	36	ASN
16	1P	119	GLN
16	1P	131	HIS
16	1P	203	GLN
16	1P	288	HIS
16	1P	306	GLN
17	1Q	9	GLN
17	1Q	50	ASN
19	1S	24	GLN
20	1T	33	ASN
20	1U	47	GLN
21	1V	70	GLN

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Mol	Chain	Res	Type
22	1W	48	HIS
23	1X	63	ASN
23	1X	98	HIS
24	1Y	88	ASN
25	1Z	8	GLN
26	1a	31	ASN
26	1a	46	ASN
28	1c	35	HIS
29	1d	46	ASN
29	1d	61	GLN
29	1d	79	GLN
30	1e	69	GLN
31	1f	5	GLN
31	1f	13	HIS
32	1g	103	ASN
35	1j	13	GLN
36	1k	90	GLN
37	1l	55	GLN
37	1l	66	HIS
37	1l	126	GLN
38	1m	54	ASN
39	1n	61	GLN
41	1p	55	HIS
41	1p	160	GLN
42	1q	13	GLN
43	1r	8	GLN
44	1s	35	ASN
44	1s	40	ASN

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	$\# Z > 2$
13	FME	1M	1	13	8,9,10	0.55	0	8,9,11	0.95	1 (12%)
11	FME	1K	1	11	8,9,10	0.56	0	8,9,11	1.02	1 (12%)
12	FME	1L	1	12	8,9,10	0.54	0	8,9,11	0.96	1 (12%)
1	FME	1A	1	1	8,9,10	0.54	0	8,9,11	0.99	1 (12%)
14	FME	1N	1	14	8,9,10	0.55	0	8,9,11	0.97	1 (12%)
34	SAC	1i	1	-	7,8,9	0.57	0	7,9,11	1.15	1 (14%)
8	FME	1H	1	8	8,9,10	0.54	0	8,9,11	1.03	1 (12%)
10	FME	1J	1	10	8,9,10	0.56	0	8,9,11	0.94	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
13	FME	1M	1	13	-	3/7/9/11	-
11	FME	1K	1	11	-	1/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
1	FME	1A	1	1	-	0/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
8	FME	1H	1	8	-	0/7/9/11	-
10	FME	1J	1	10	-	0/7/9/11	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	1i	1	SAC	O-C-CA	-2.99	117.08	124.77
11	1K	1	FME	O-C-CA	-2.80	117.57	124.77
8	1H	1	FME	O-C-CA	-2.68	117.87	124.77
14	1N	1	FME	O-C-CA	-2.56	118.19	124.77
1	1A	1	FME	O-C-CA	-2.53	118.27	124.77
13	1M	1	FME	O-C-CA	-2.52	118.28	124.77
12	1L	1	FME	O-C-CA	-2.50	118.34	124.77
10	1J	1	FME	O-C-CA	-2.40	118.60	124.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	1M	1	FME	O-C-CA-CB
13	1M	1	FME	N-CA-CB-CG
11	1K	1	FME	CA-CB-CG-SD
13	1M	1	FME	CB-CA-N-CN

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1M	1	FME	2	0
11	1K	1	FME	2	0
1	1A	1	FME	6	0
14	1N	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
45	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.39	0
50	PC1	1L	702	-	43,43,53	0.30	0	49,51,61	0.38	0
47	FES	1G	804	7	0,4,4	-	-	-		
53	GTP	1O	401	15,54	33,34,34	0.61	0	50,54,54	0.57	0
47	FES	1E	301	5	0,4,4	-	-	-		
45	3PE	1L	701	-	45,45,50	0.30	0	48,50,55	0.32	0
45	3PE	1A	201	-	46,46,50	0.28	0	49,51,55	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
51	PGT	1M	501	-	50,50,50	0.49	0	53,56,56	0.47	0
57	EHZ	1W	201	-	31,36,37	0.18	0	36,44,47	1.47	1 (2%)
57	EHZ	1n	201	-	31,36,37	0.21	0	36,44,47	1.11	1 (2%)
46	SF4	1G	802	7	0,12,12	-	-	-		
50	PC1	1I	203	-	53,53,53	0.28	0	59,61,61	0.32	0
52	CDL	1N	402	14	76,76,99	0.30	0	82,88,111	0.39	0
52	CDL	1r	201	42,26,43	60,60,99	0.32	0	66,72,111	0.49	0
46	SF4	1F	502	6	0,12,12	-	-	-		
48	FMN	1F	501	-	33,33,33	0.59	0	48,50,50	0.63	1 (2%)
50	PC1	1f	101	31	45,45,53	0.28	0	51,53,61	0.34	0
46	SF4	1B	201	2	0,12,12	-	-	-		
46	SF4	1I	202	9	0,12,12	-	-	-		
45	3PE	1Y	202	-	50,50,50	0.27	0	53,55,55	0.42	0
45	3PE	1Y	201	-	30,30,50	0.35	0	33,35,55	0.60	1 (3%)
55	NDP	1P	501	-	51,52,52	0.53	0	71,80,80	0.76	2 (2%)
46	SF4	1I	201	9	0,12,12	-	-	-		
58	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.30	0
50	PC1	1I	204	9	43,43,53	0.28	0	49,51,61	0.40	0
46	SF4	1G	801	7	0,12,12	-	-	-		
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.34	0
45	3PE	1L	703	-	41,41,50	0.30	0	44,46,55	1.27	5 (11%)

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
45	3PE	1N	401	-	-	10/54/54/54	-
50	PC1	1L	702	-	-	4/47/47/57	-
47	FES	1G	804	7	-	-	0/1/1/1
53	GTP	1O	401	15,54	-	3/22/38/38	0/3/3/3
47	FES	1E	301	5	-	-	0/1/1/1
45	3PE	1L	701	-	-	4/49/49/54	-
45	3PE	1A	201	-	-	2/50/50/54	-
51	PGT	1M	501	-	-	23/55/55/55	-
57	EHZ	1W	201	-	-	3/42/44/45	-
57	EHZ	1n	201	-	-	10/42/44/45	-
46	SF4	1G	802	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	PC1	1I	203	-	-	4/57/57/57	-
52	CDL	1N	402	14	-	6/87/87/110	-
52	CDL	1r	201	42,26,43	-	10/71/71/110	-
46	SF4	1F	502	6	-	-	0/6/5/5
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
50	PC1	1f	101	31	-	4/49/49/57	-
46	SF4	1B	201	2	-	-	0/6/5/5
46	SF4	1I	202	9	-	-	0/6/5/5
45	3PE	1Y	202	-	-	8/54/54/54	-
45	3PE	1Y	201	-	-	6/34/34/54	-
55	NDP	1P	501	-	-	6/34/77/77	0/5/5/5
58	MYR	1l	201	-	-	2/12/12/13	-
46	SF4	1I	201	9	-	-	0/6/5/5
50	PC1	1I	204	9	-	5/47/47/57	-
46	SF4	1G	801	7	-	-	0/6/5/5
50	PC1	1J	201	-	-	3/38/38/57	-
45	3PE	1L	703	-	-	7/45/45/54	-

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	1W	201	EHZ	C10-S1-C9	7.92	125.26	101.84
57	1n	201	EHZ	C10-S1-C9	6.14	120.00	101.84
45	1L	703	3PE	O21-C21-C22	6.14	124.76	111.48
55	1P	501	NDP	P2B-O2B-C2B	-3.81	113.25	123.43
45	1L	703	3PE	O21-C21-O22	-2.75	117.28	123.70
45	1L	703	3PE	C2-O21-C21	2.60	124.01	117.80
55	1P	501	NDP	O4D-C1D-C2D	-2.52	101.22	106.62
45	1L	703	3PE	O21-C2-C1	2.30	116.61	108.34
45	1L	703	3PE	O21-C2-C3	2.10	115.87	108.34
48	1F	501	FMN	C4-N3-C2	-2.09	121.93	125.64
45	1Y	201	3PE	O21-C21-C22	2.09	116.00	111.48

There are no chirality outliers.

All (121) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	C22-C21-O21-C2
45	1Y	201	3PE	C1-O11-P-O14
45	1Y	201	3PE	O32-C31-O31-C3
45	1Y	201	3PE	C32-C31-O31-C3
45	1Y	201	3PE	O22-C21-O21-C2
45	1Y	201	3PE	C22-C21-O21-C2
45	1Y	202	3PE	C1-O11-P-O14
50	1I	204	PC1	C1-O11-P-O14
50	1I	204	PC1	C1-O11-P-O13
50	1J	201	PC1	C1-O11-P-O14
50	1J	201	PC1	C1-O11-P-O13
50	1L	702	PC1	C1-O11-P-O14
50	1f	101	PC1	O32-C31-O31-C3
50	1f	101	PC1	C32-C31-O31-C3
51	1M	501	PGT	C32-C31-O2-C2
51	1M	501	PGT	O31-C31-O2-C2
51	1M	501	PGT	C1-O3P-P-O4P
51	1M	501	PGT	C4-O4P-P-O3P
51	1M	501	PGT	C5-C4-O4P-P
51	1M	501	PGT	C4-C5-C6-O6
51	1M	501	PGT	C12-C11-O3-C3
52	1N	402	CDL	OA6-CA4-CA6-OA8
52	1r	201	CDL	OB6-CB4-CB6-OB8
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
58	1l	201	MYR	O1-C1-C2-C3
51	1M	501	PGT	O11-C11-O3-C3
45	1Y	202	3PE	C2-C1-O11-P
55	1P	501	NDP	C2D-C1D-N1N-C2N
55	1P	501	NDP	C2D-C1D-N1N-C6N
53	1O	401	GTP	O4'-C4'-C5'-O5'
51	1M	501	PGT	C15-C16-C17-C18
51	1M	501	PGT	C40-C41-C42-C43
51	1M	501	PGT	O5-C5-C6-O6
51	1M	501	PGT	C14-C15-C16-C17
51	1M	501	PGT	C21-C22-C23-C24
45	1L	701	3PE	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
45	1Y	202	3PE	C35-C36-C37-C38
57	1n	201	EHZ	C21-C1-C2-C3
50	1I	203	PC1	C24-C25-C26-C27
52	1r	201	CDL	CB3-CB4-CB6-OB8
45	1Y	202	3PE	C3C-C3D-C3E-C3F
50	1f	101	PC1	C32-C33-C34-C35
51	1M	501	PGT	C34-C35-C36-C37
55	1P	501	NDP	C1B-C2B-O2B-P2B
45	1L	703	3PE	O11-C1-C2-O21
52	1r	201	CDL	C53-C54-C55-C56
45	1N	401	3PE	O31-C31-C32-C33
50	1I	203	PC1	O31-C31-C32-C33
53	1O	401	GTP	C3'-C4'-C5'-O5'
52	1r	201	CDL	C52-C51-CB5-OB6
52	1N	402	CDL	CA3-CA4-CA6-OA8
45	1N	401	3PE	O11-C1-C2-O21
57	1n	201	EHZ	O3-C12-C13-C14
51	1M	501	PGT	C44-C45-C46-C47
57	1W	201	EHZ	C6-C7-C8-C9
55	1P	501	NDP	C3B-C2B-O2B-P2B
45	1L	701	3PE	C22-C23-C24-C25
45	1Y	202	3PE	O11-C1-C2-O21
45	1A	201	3PE	C12-C11-O13-P
45	1Y	202	3PE	C12-C11-O13-P
50	1J	201	PC1	O13-C11-C12-N
52	1N	402	CDL	C55-C56-C57-C58
45	1N	401	3PE	C2-C3-O31-C31
55	1P	501	NDP	O4D-C1D-N1N-C2N
55	1P	501	NDP	O4D-C1D-N1N-C6N
45	1N	401	3PE	C34-C35-C36-C37
52	1r	201	CDL	C19-C20-C21-C22
50	1L	702	PC1	C1-C2-C3-O31
52	1r	201	CDL	C51-C52-C53-C54
51	1M	501	PGT	C32-C33-C34-C35
45	1N	401	3PE	C1-O11-P-O14
50	1L	702	PC1	C1-O11-P-O13
50	1f	101	PC1	C11-O13-P-O14
51	1M	501	PGT	C1-O3P-P-O1P
51	1M	501	PGT	C4-O4P-P-O1P
52	1r	201	CDL	CA3-OA5-PA1-OA3
45	1L	701	3PE	C31-C32-C33-C34
45	1L	703	3PE	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	C1-C2-C3-O31
57	1n	201	EHZ	N1-C12-C13-C14
45	1N	401	3PE	C3A-C3B-C3C-C3D
57	1n	201	EHZ	C13-C14-N2-C15
51	1M	501	PGT	C22-C23-C24-C25
45	1N	401	3PE	C2-C1-O11-P
53	1O	401	GTP	C4'-C5'-O5'-PA
45	1L	703	3PE	C1-C2-O21-C21
52	1r	201	CDL	C17-C18-C19-C20
51	1M	501	PGT	C16-C17-C18-C19
45	1A	201	3PE	O21-C2-C3-O31
45	1N	401	3PE	O21-C2-C3-O31
57	1n	201	EHZ	C12-C13-C14-N2
45	1L	701	3PE	C37-C38-C39-C3A
45	1Y	202	3PE	O11-C1-C2-C3
45	1Y	201	3PE	O21-C2-C3-O31
51	1M	501	PGT	C2-C1-O3P-P
52	1r	201	CDL	C52-C51-CB5-OB7
52	1N	402	CDL	C75-C76-C77-C78
52	1N	402	CDL	C32-C33-C34-C35
50	1I	203	PC1	C3D-C3E-C3F-C3G
50	1I	204	PC1	C34-C35-C36-C37
52	1N	402	CDL	C53-C54-C55-C56
50	1I	203	PC1	O32-C31-C32-C33
45	1L	703	3PE	C32-C33-C34-C35
45	1N	401	3PE	C39-C3A-C3B-C3C
58	1l	201	MYR	C3-C4-C5-C6
51	1M	501	PGT	C20-C21-C22-C23
50	1L	702	PC1	O31-C31-C32-C33
48	1F	501	FMN	N10-C1'-C2'-O2'
45	1N	401	3PE	O32-C31-C32-C33
45	1Y	202	3PE	C24-C25-C26-C27
50	1I	204	PC1	C25-C26-C27-C28
52	1r	201	CDL	C13-C14-C15-C16
50	1I	204	PC1	C11-C12-N-C13
51	1M	501	PGT	C18-C19-C20-C21

There are no ring outliers.

24 monomers are involved in 77 short contacts:

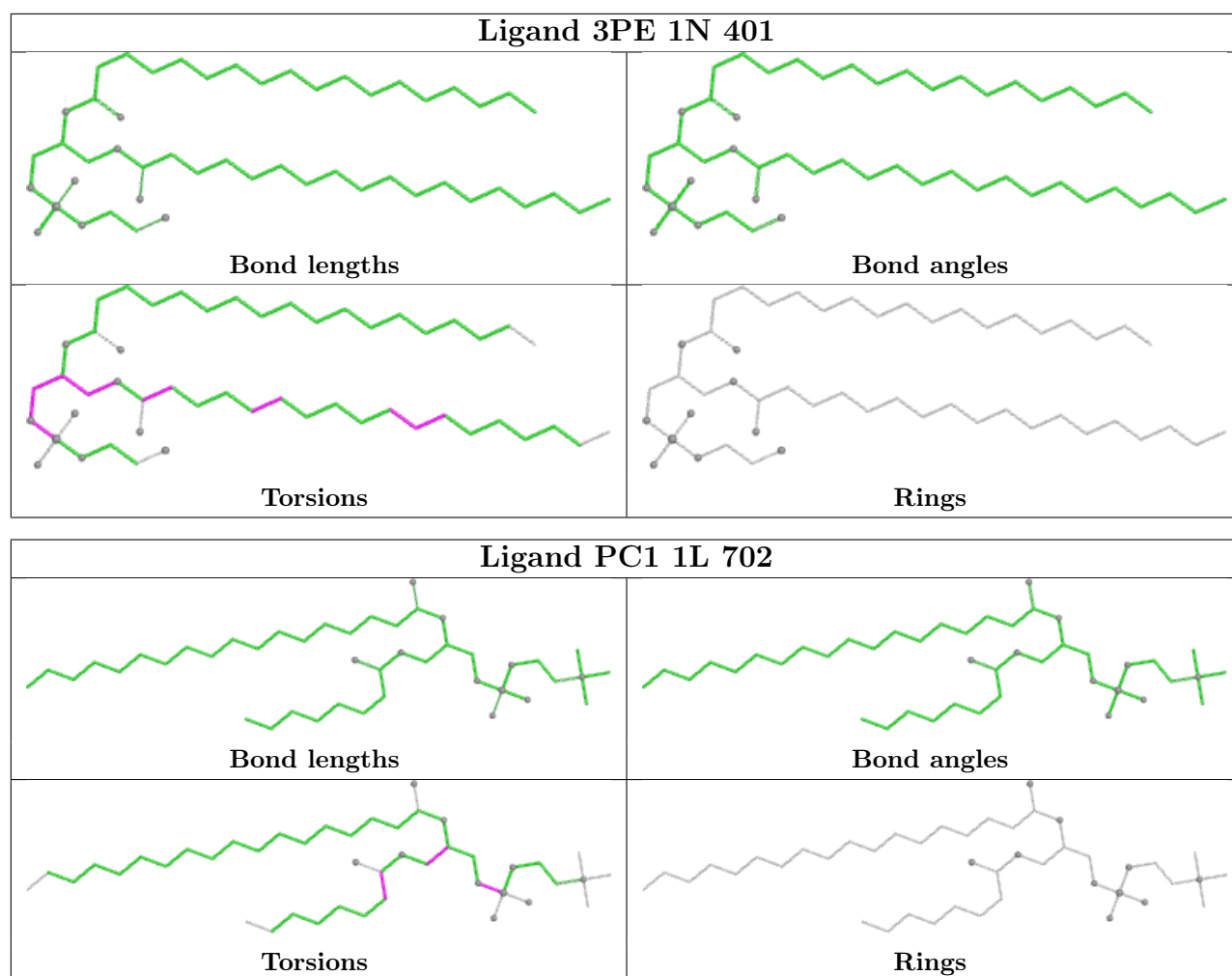
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	1N	401	3PE	3	0

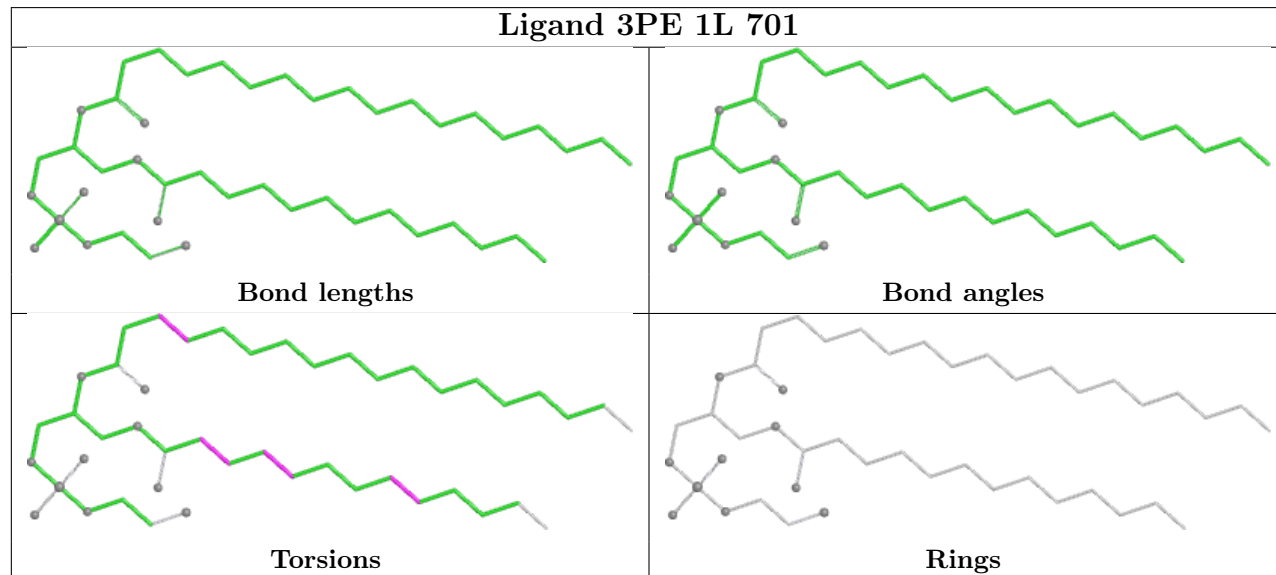
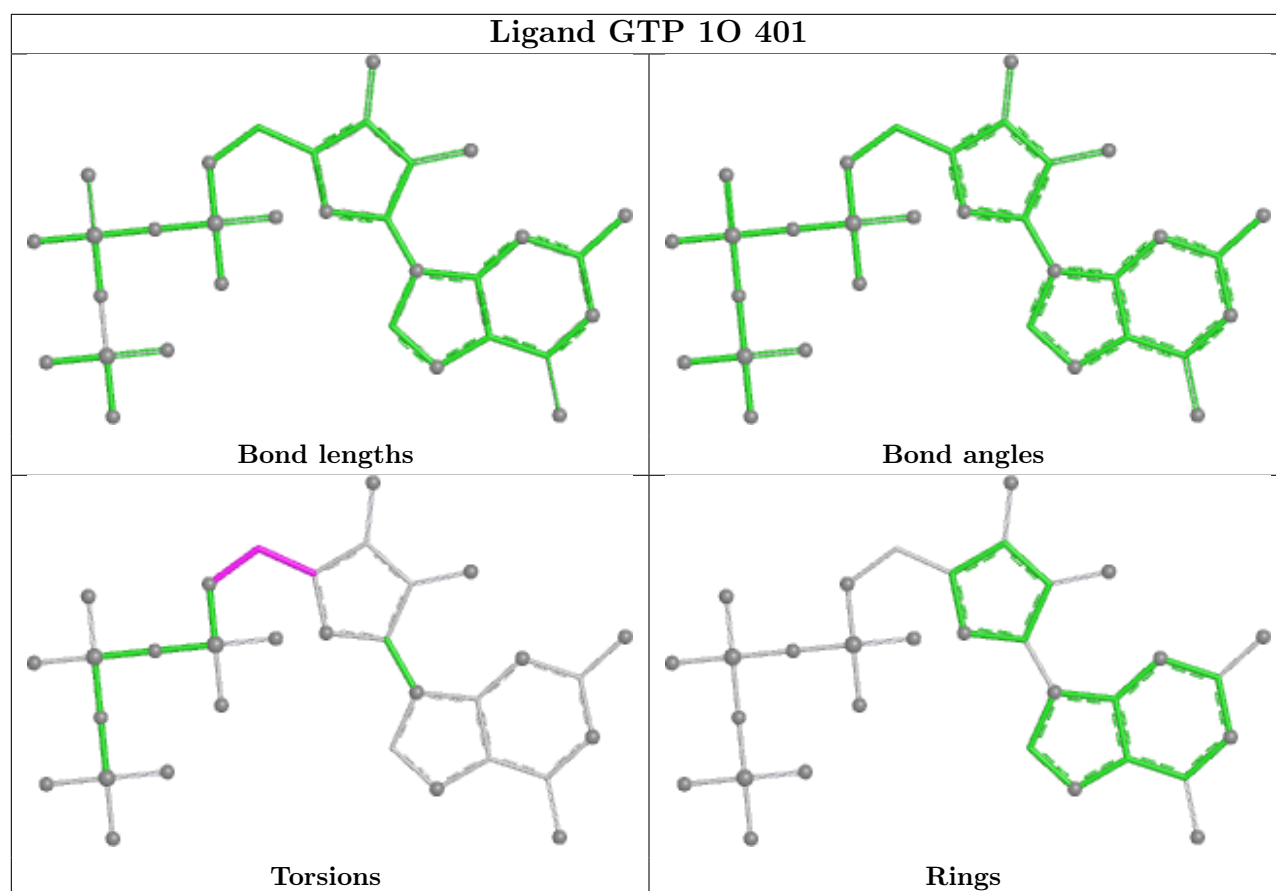
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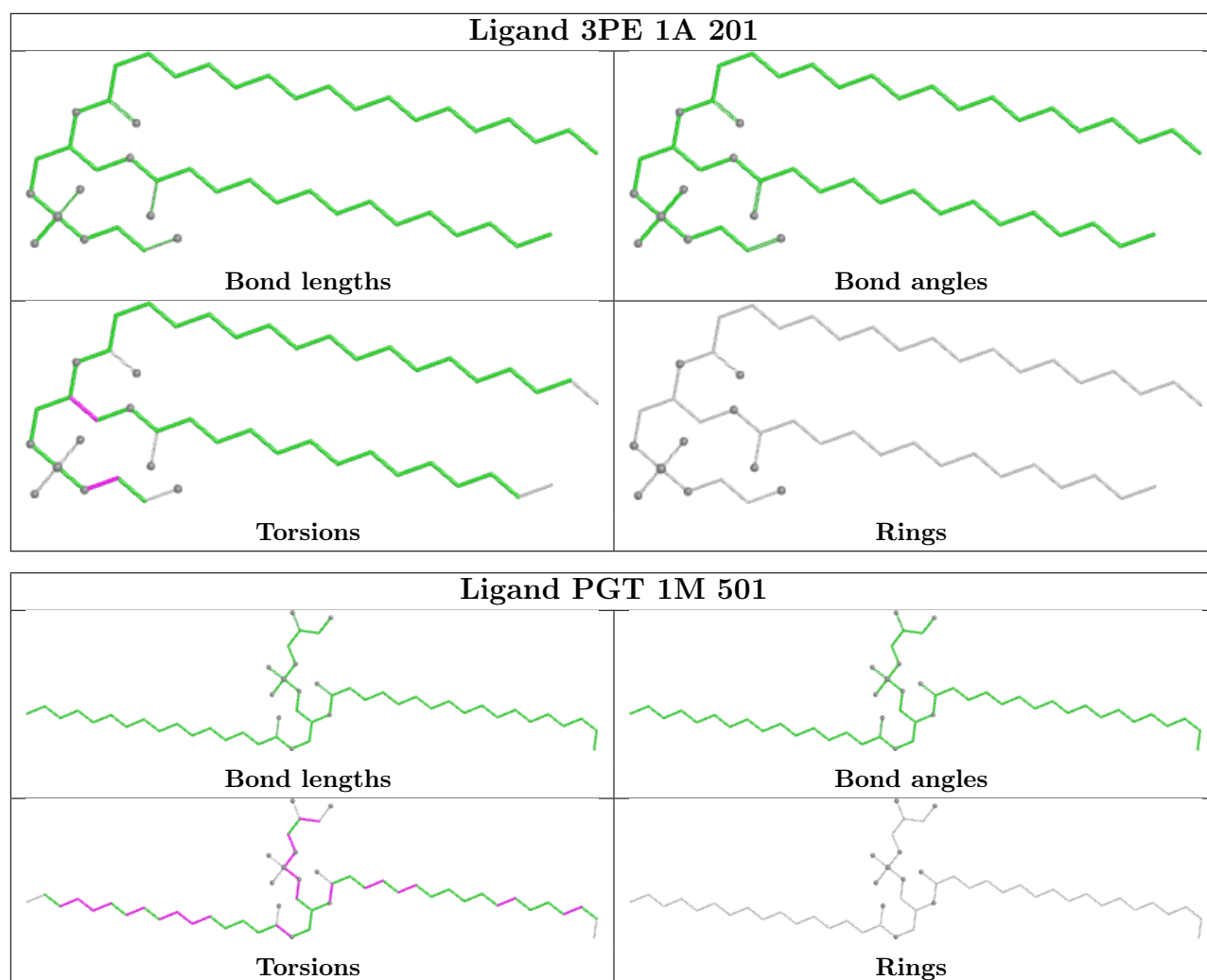
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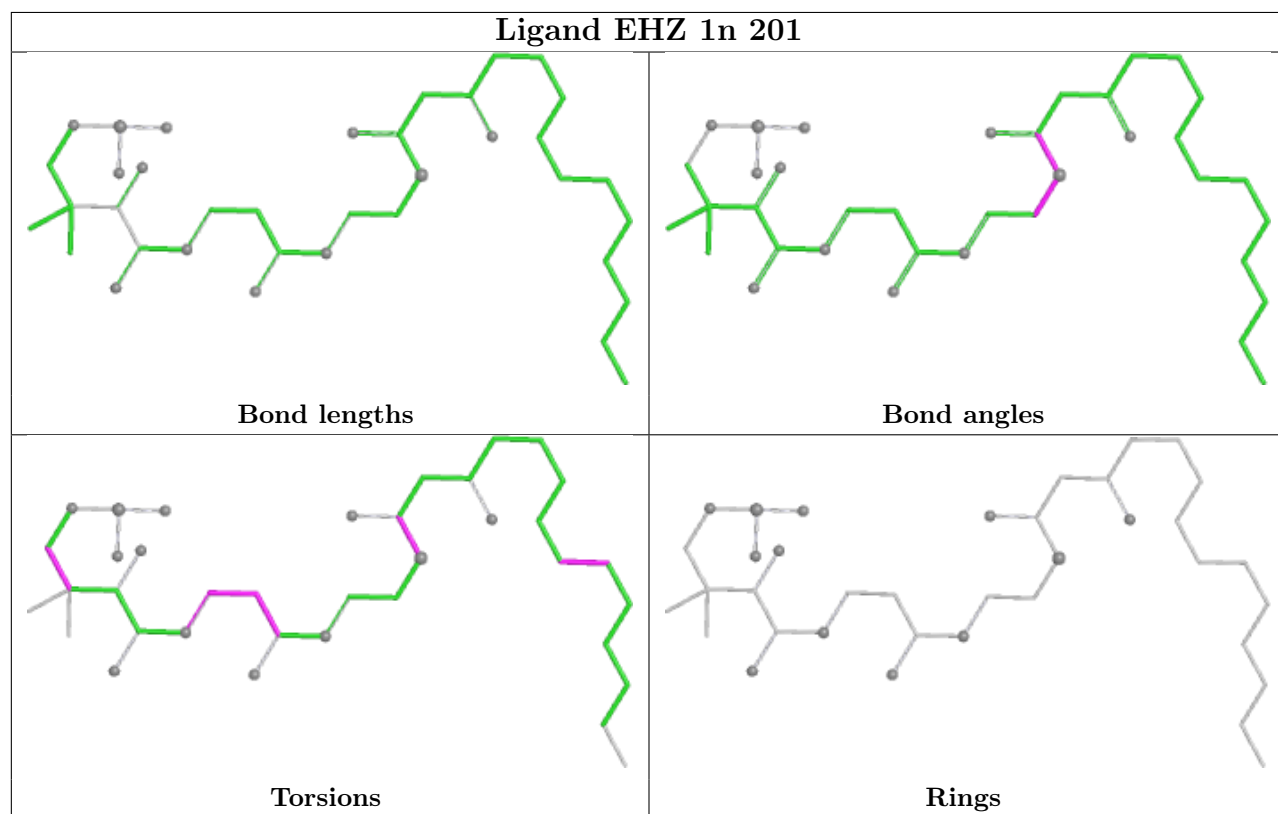
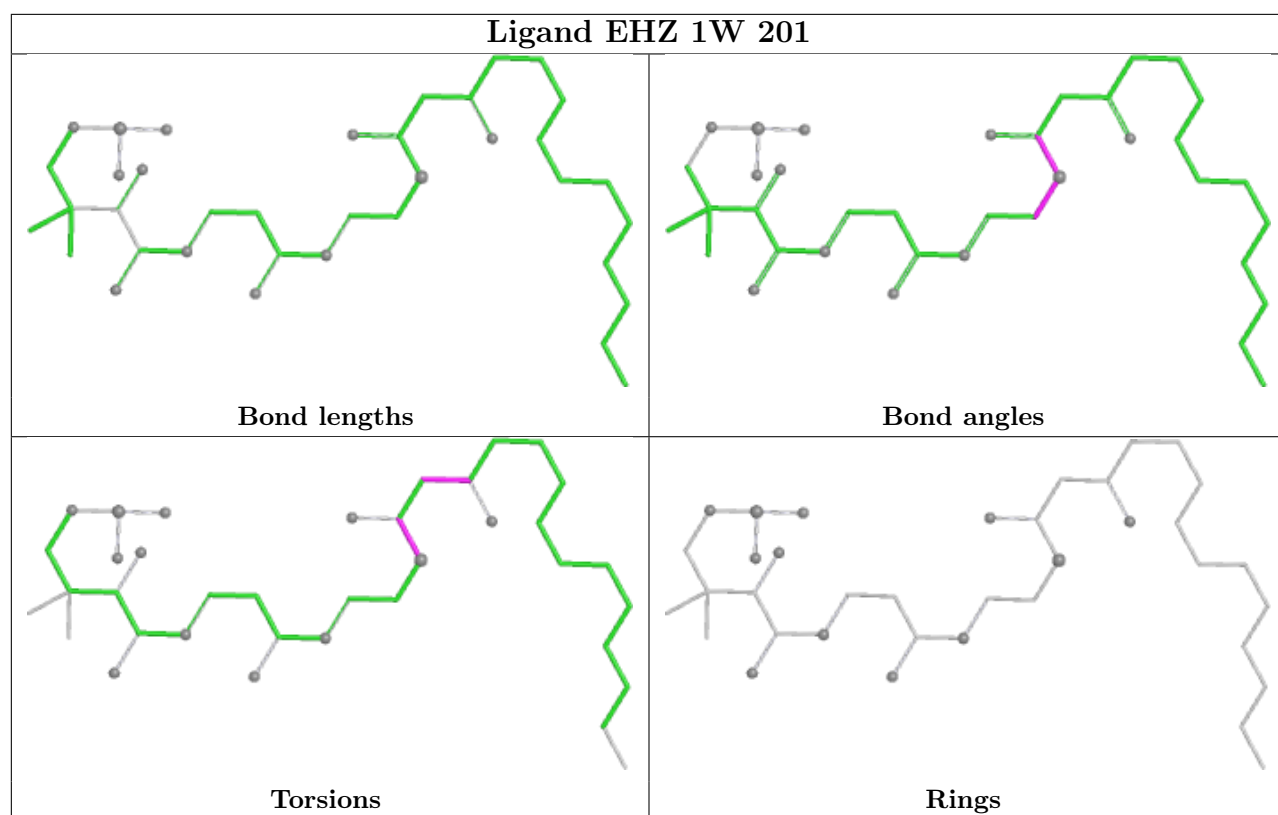
Mol	Chain	Res	Type	Clashes	Symm-Clashes
50	1L	702	PC1	1	0
47	1G	804	FES	3	0
53	1O	401	GTP	3	0
47	1E	301	FES	1	0
45	1L	701	3PE	6	0
45	1A	201	3PE	1	0
51	1M	501	PGT	8	0
57	1n	201	EHZ	2	0
46	1G	802	SF4	1	0
50	1I	203	PC1	4	0
52	1N	402	CDL	2	0
52	1r	201	CDL	7	0
46	1F	502	SF4	1	0
48	1F	501	FMN	4	0
50	1f	101	PC1	2	0
46	1B	201	SF4	2	0
46	1I	202	SF4	2	0
45	1Y	202	3PE	1	0
45	1Y	201	3PE	8	0
55	1P	501	NDP	7	0
46	1I	201	SF4	2	0
58	1l	201	MYR	1	0
50	1I	204	PC1	5	0

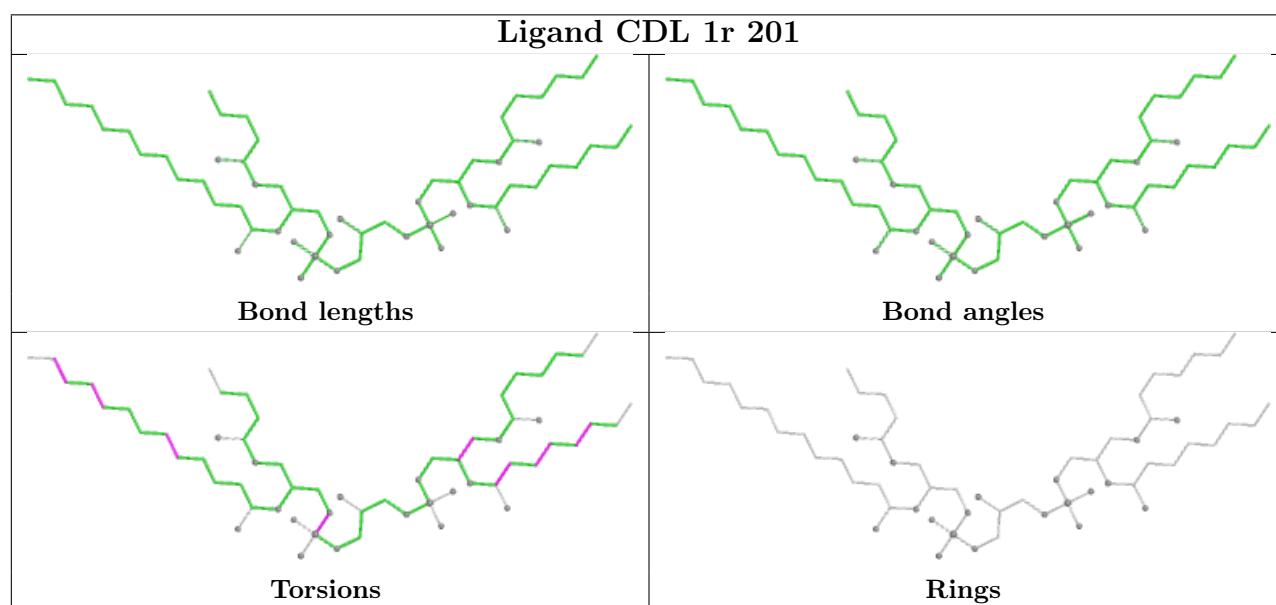
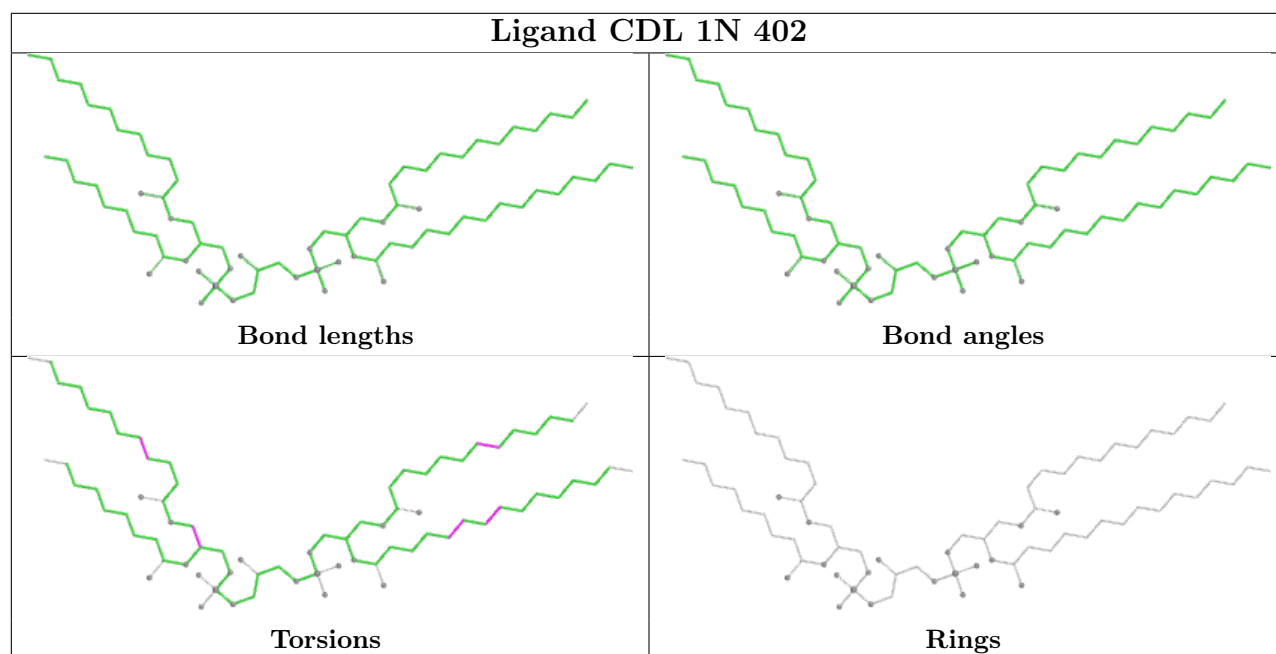
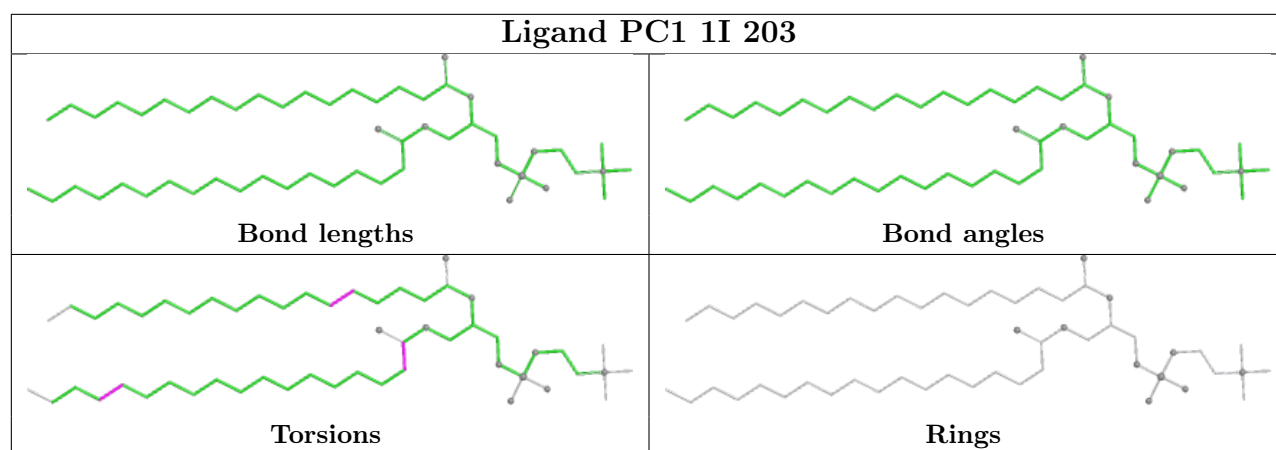
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

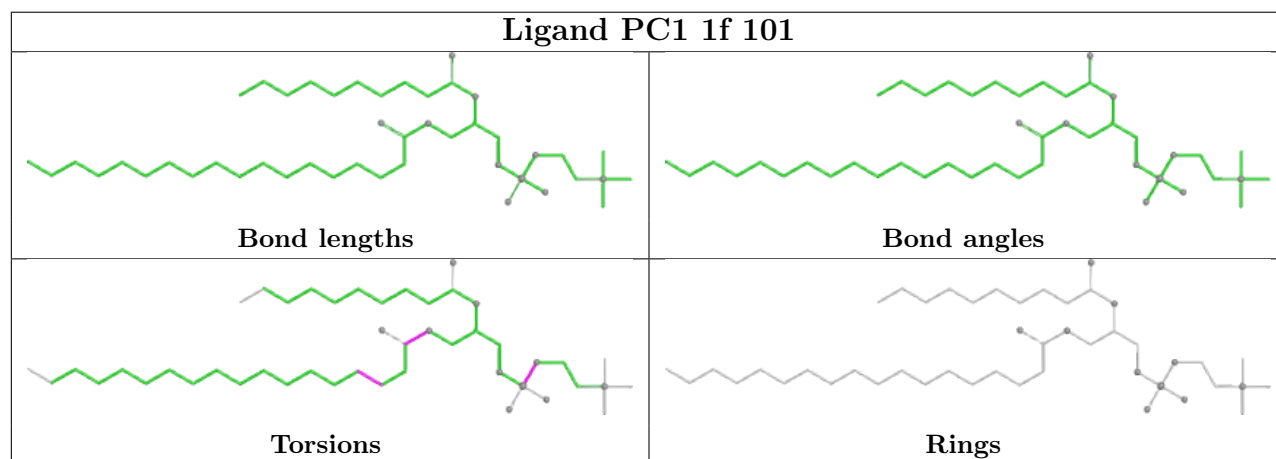
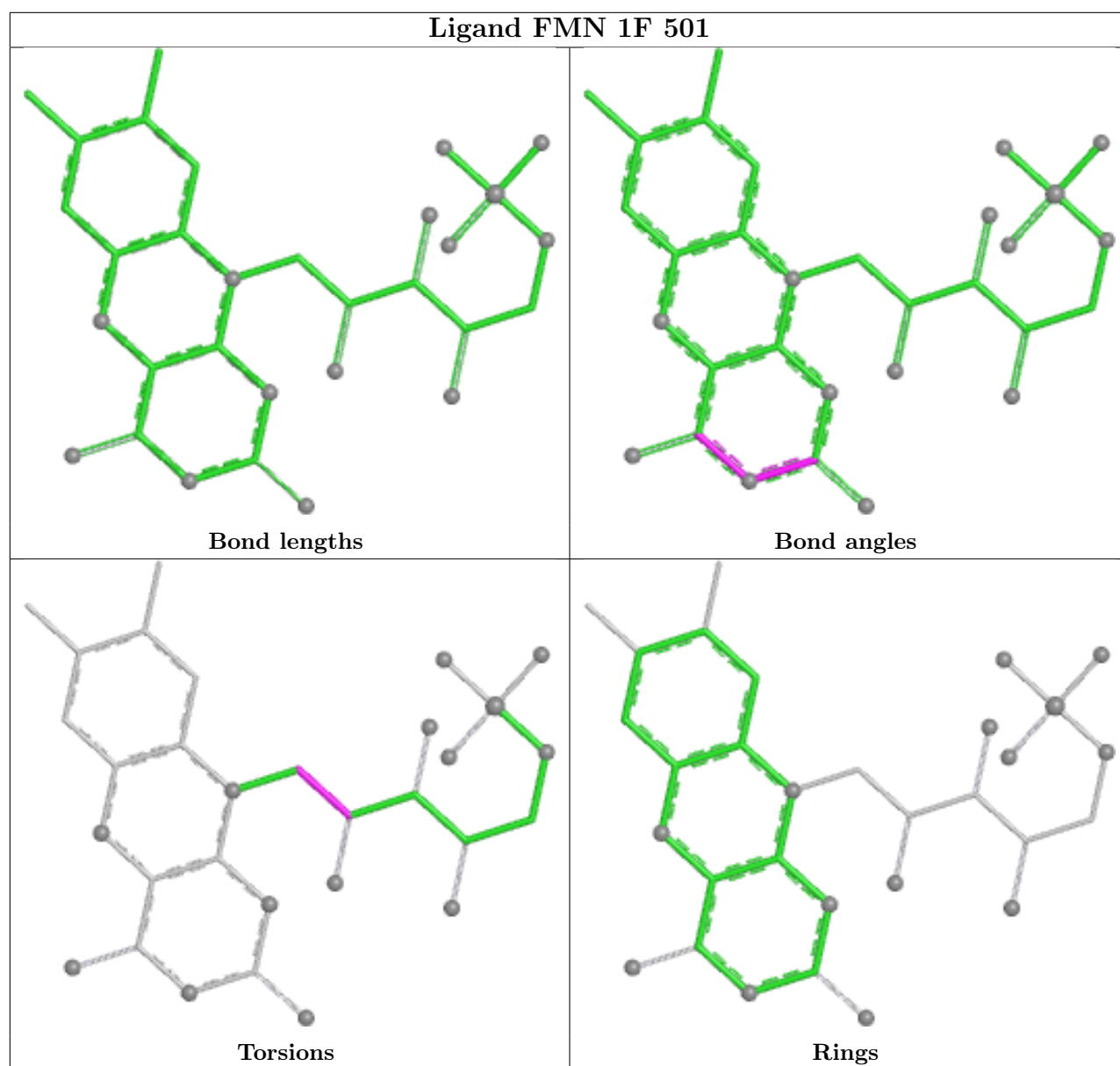


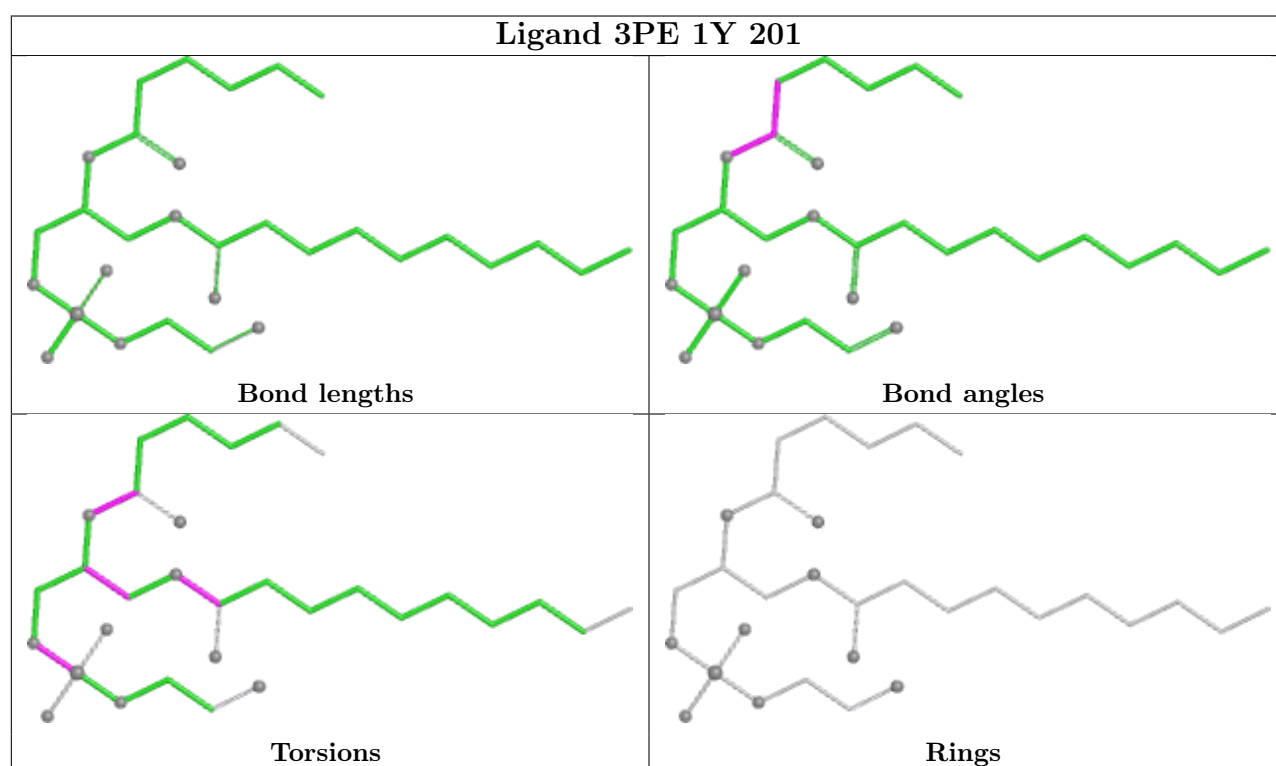
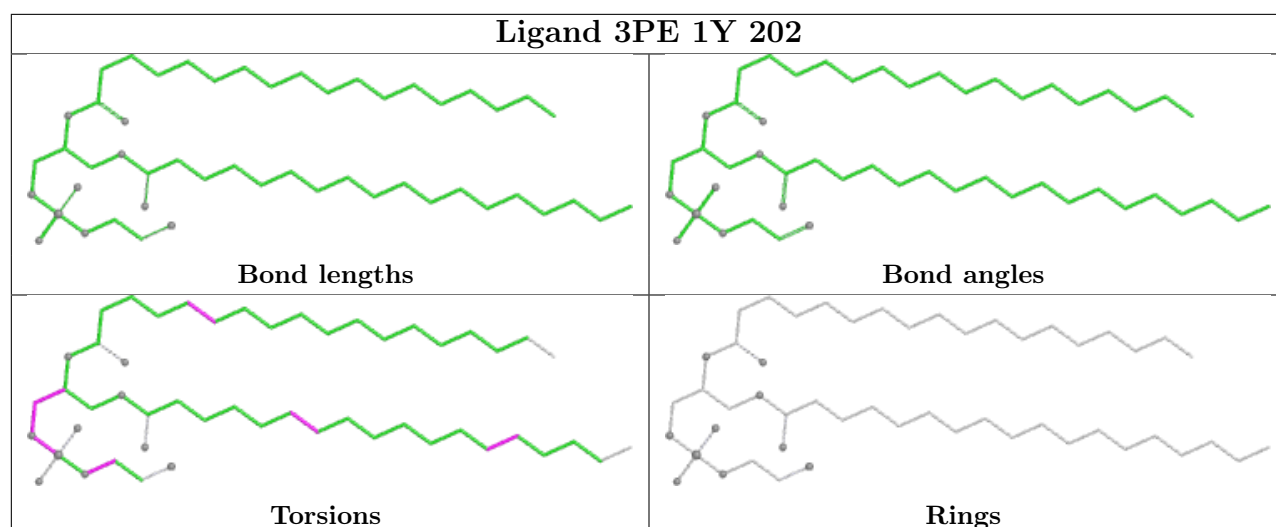


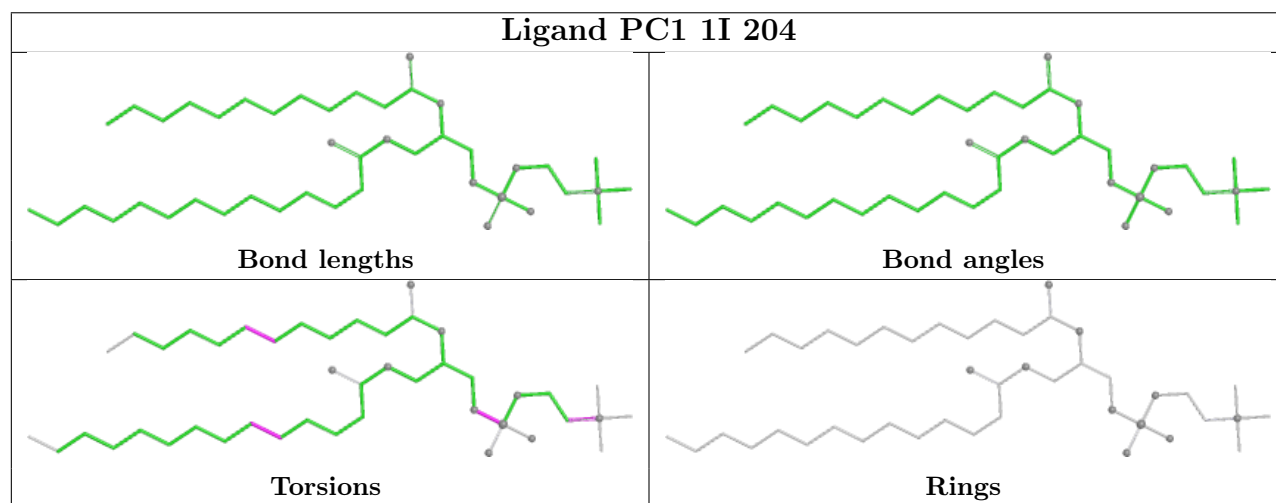
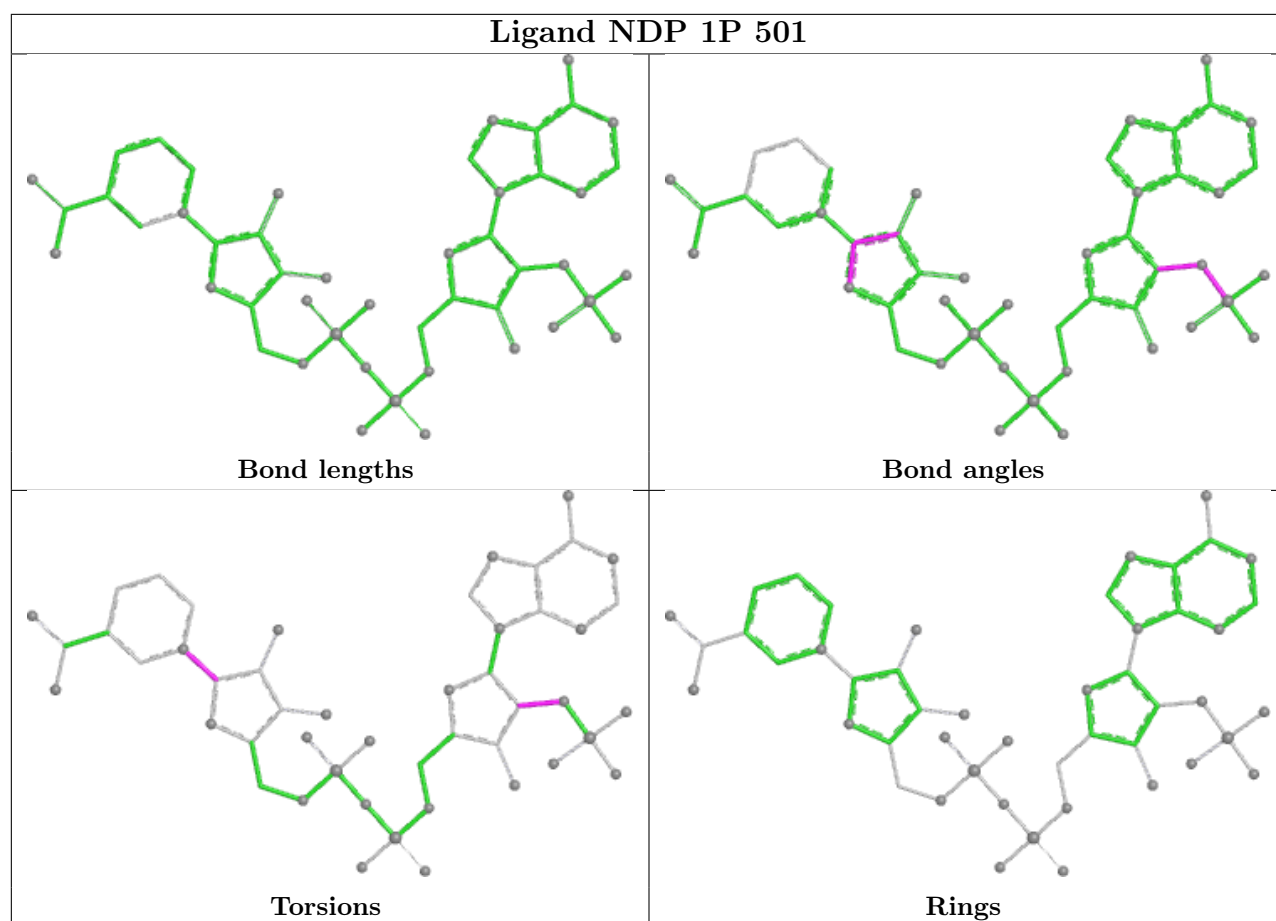


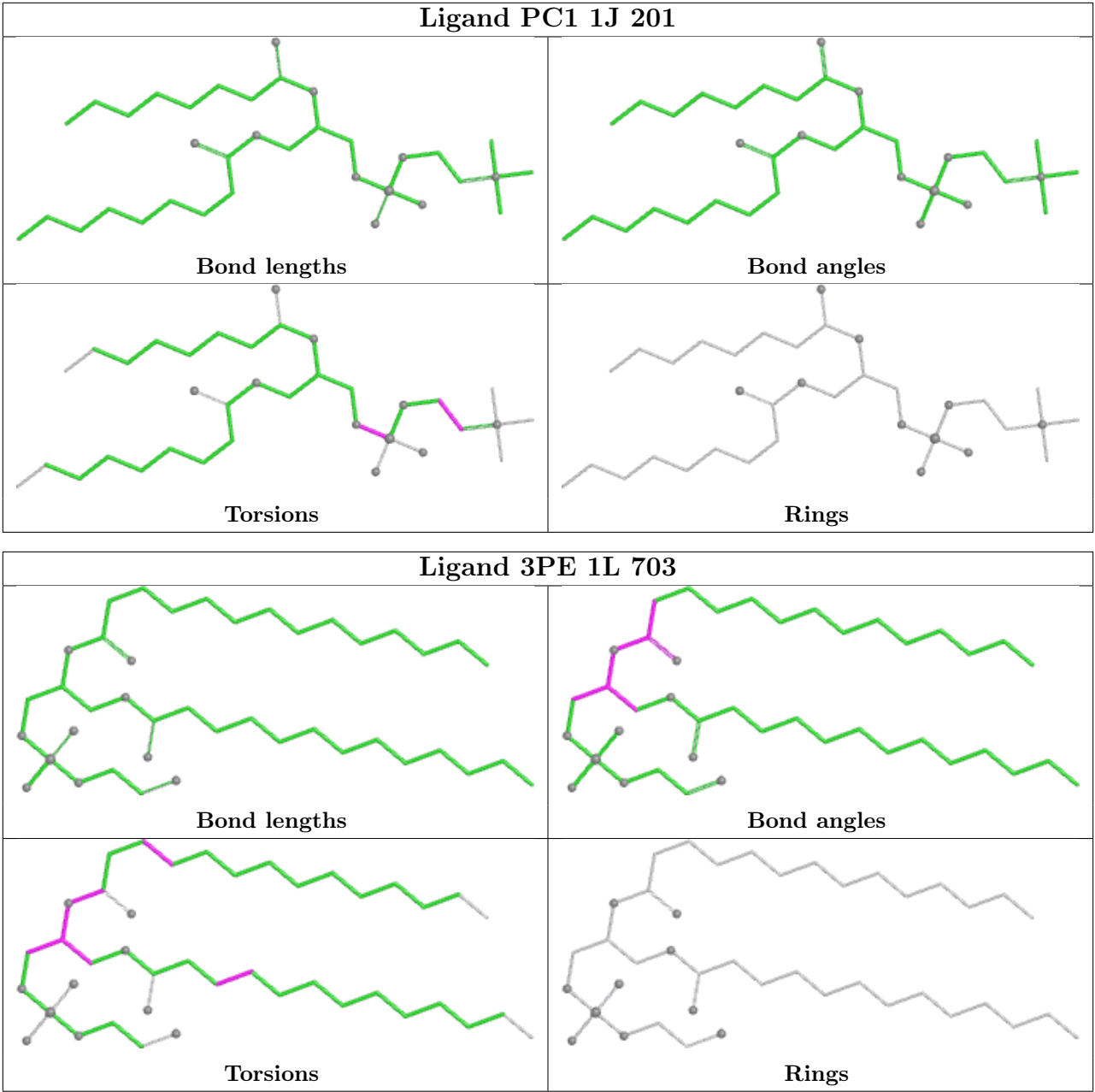












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
34	1i	1

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Mol	Chain	Number of breaks
43	1r	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	4.86
1	1r	1:ALA	C	2:SER	N	3.06

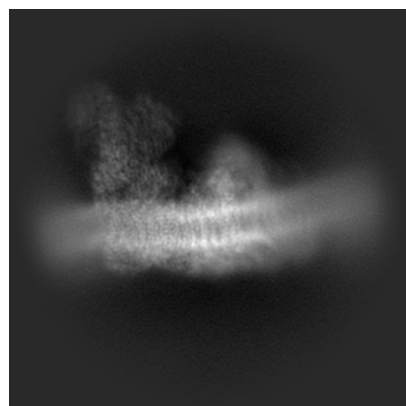
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42173. These allow visual inspection of the internal detail of the map and identification of artifacts.

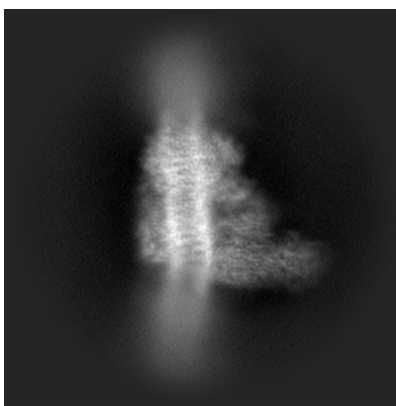
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

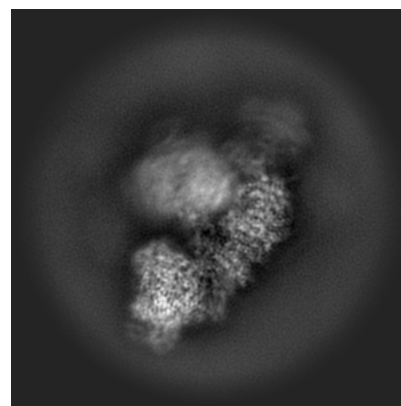
6.1.1 Primary map



X

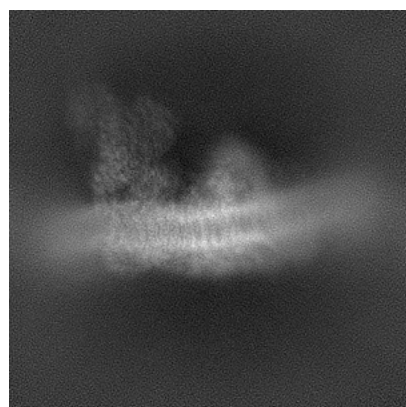


Y

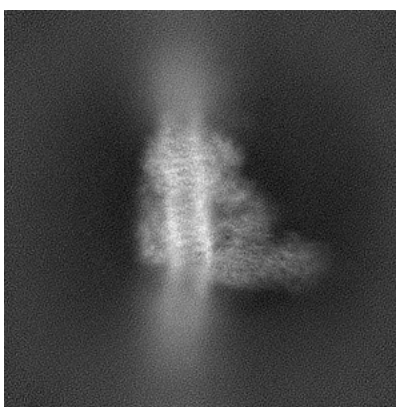


Z

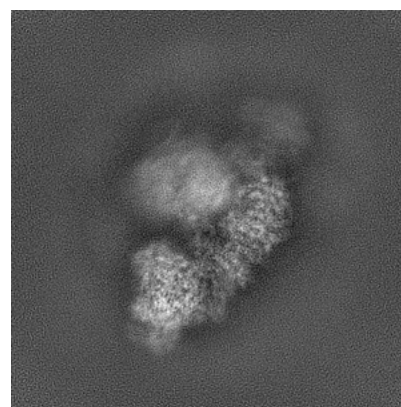
6.1.2 Raw map



X



Y

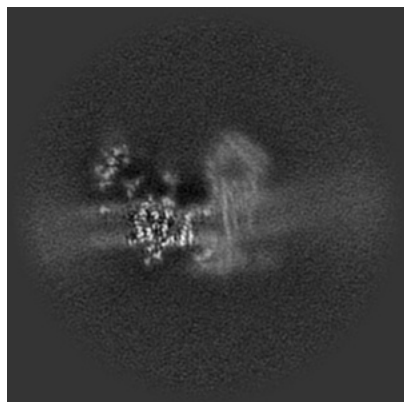


Z

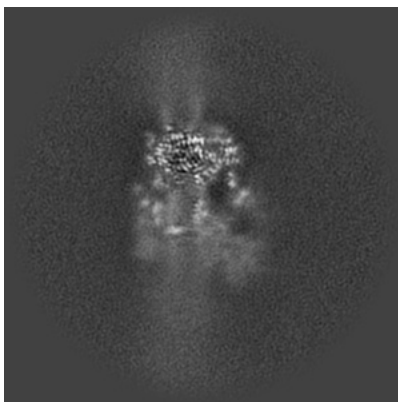
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

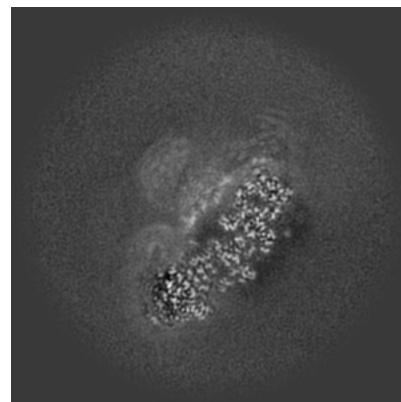
6.2.1 Primary map



X Index: 160



Y Index: 160

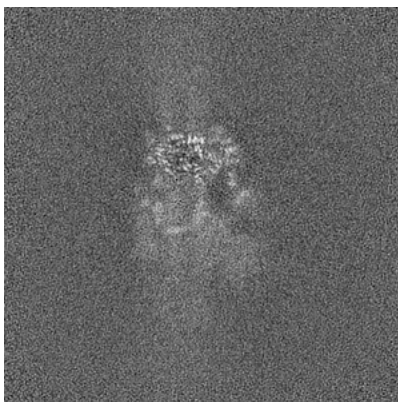


Z Index: 160

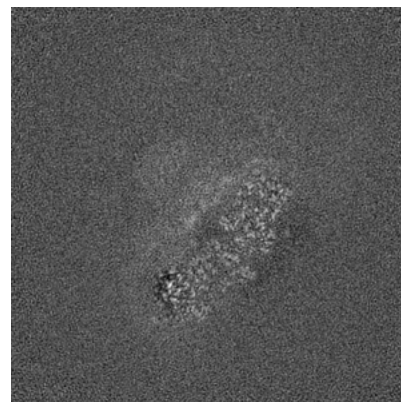
6.2.2 Raw map



X Index: 160



Y Index: 160

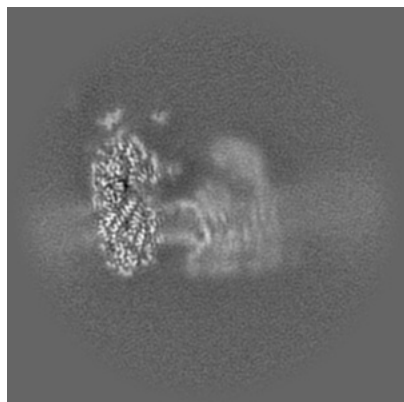


Z Index: 160

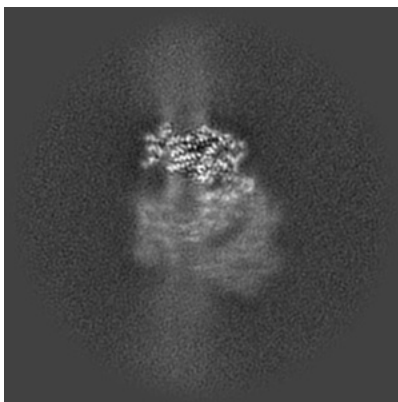
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

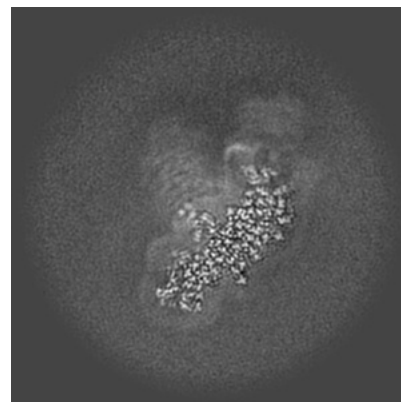
6.3.1 Primary map



X Index: 140

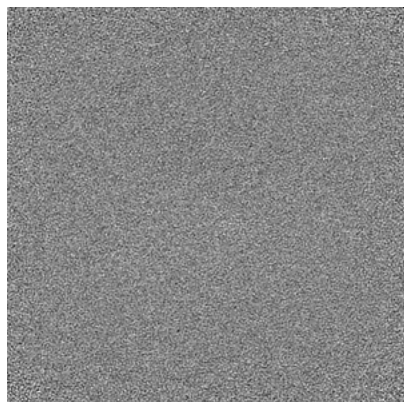


Y Index: 171

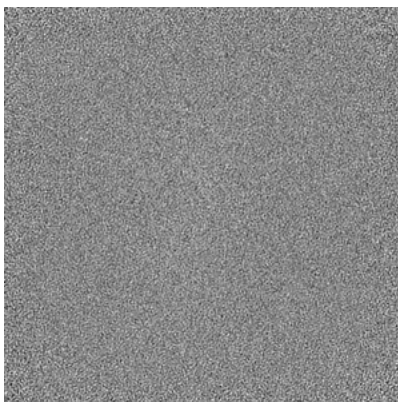


Z Index: 134

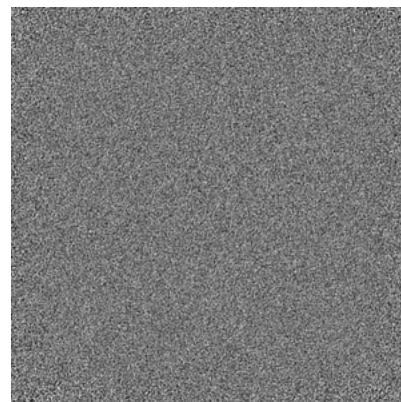
6.3.2 Raw map



X Index: 0



Y Index: 0

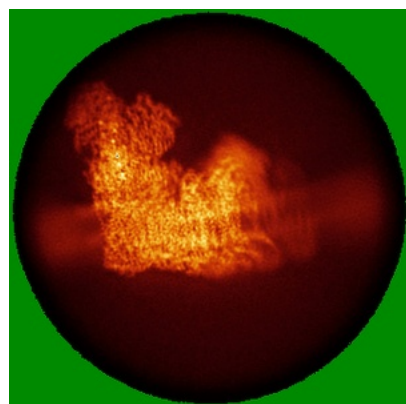


Z Index: 0

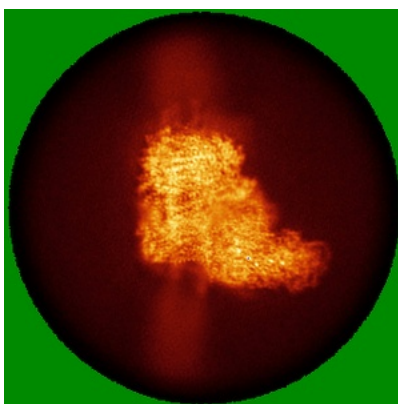
The images above show the largest variance slices of the map in three orthogonal directions.

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

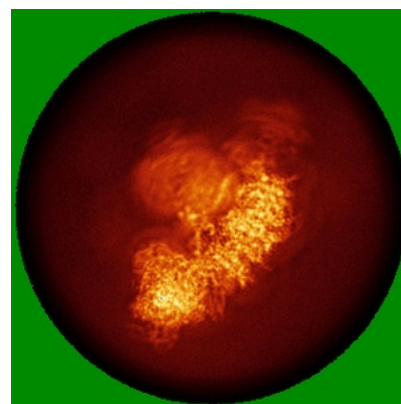
6.4.1 Primary map



X

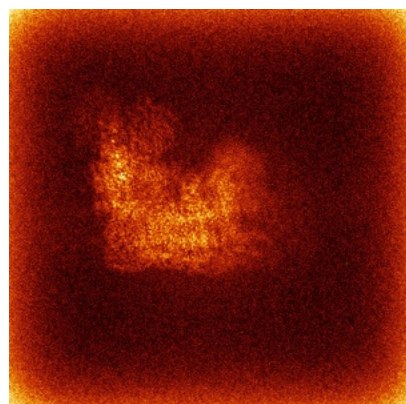


Y

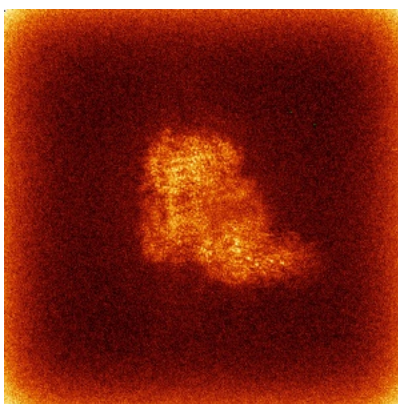


Z

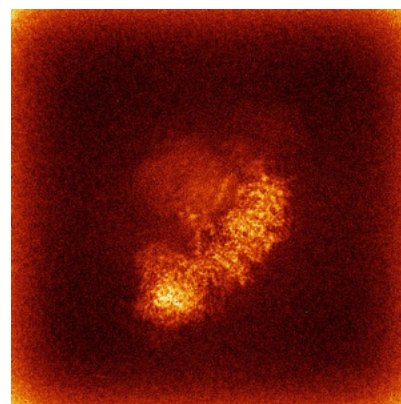
6.4.2 Raw map



X



Y



Z

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

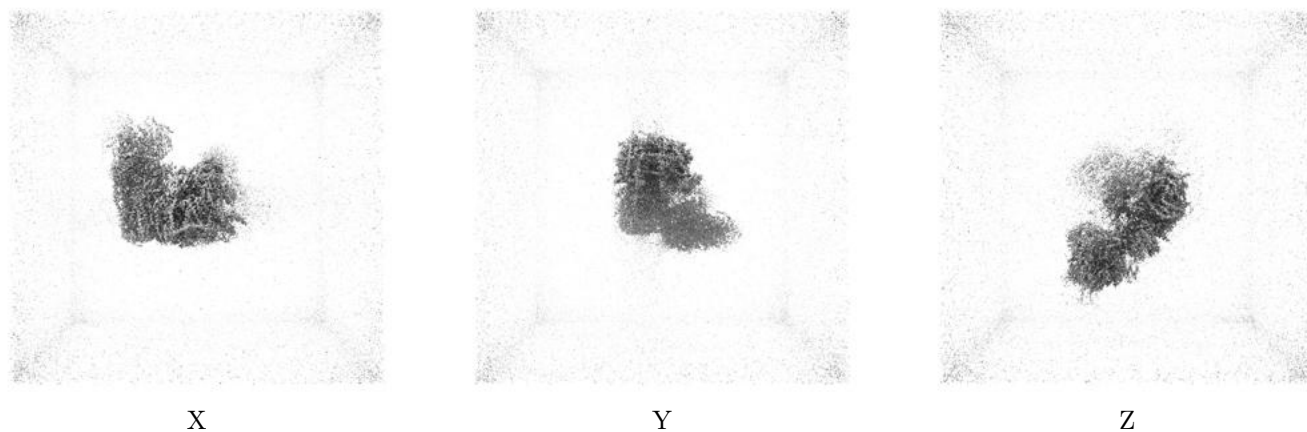
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.09. 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.

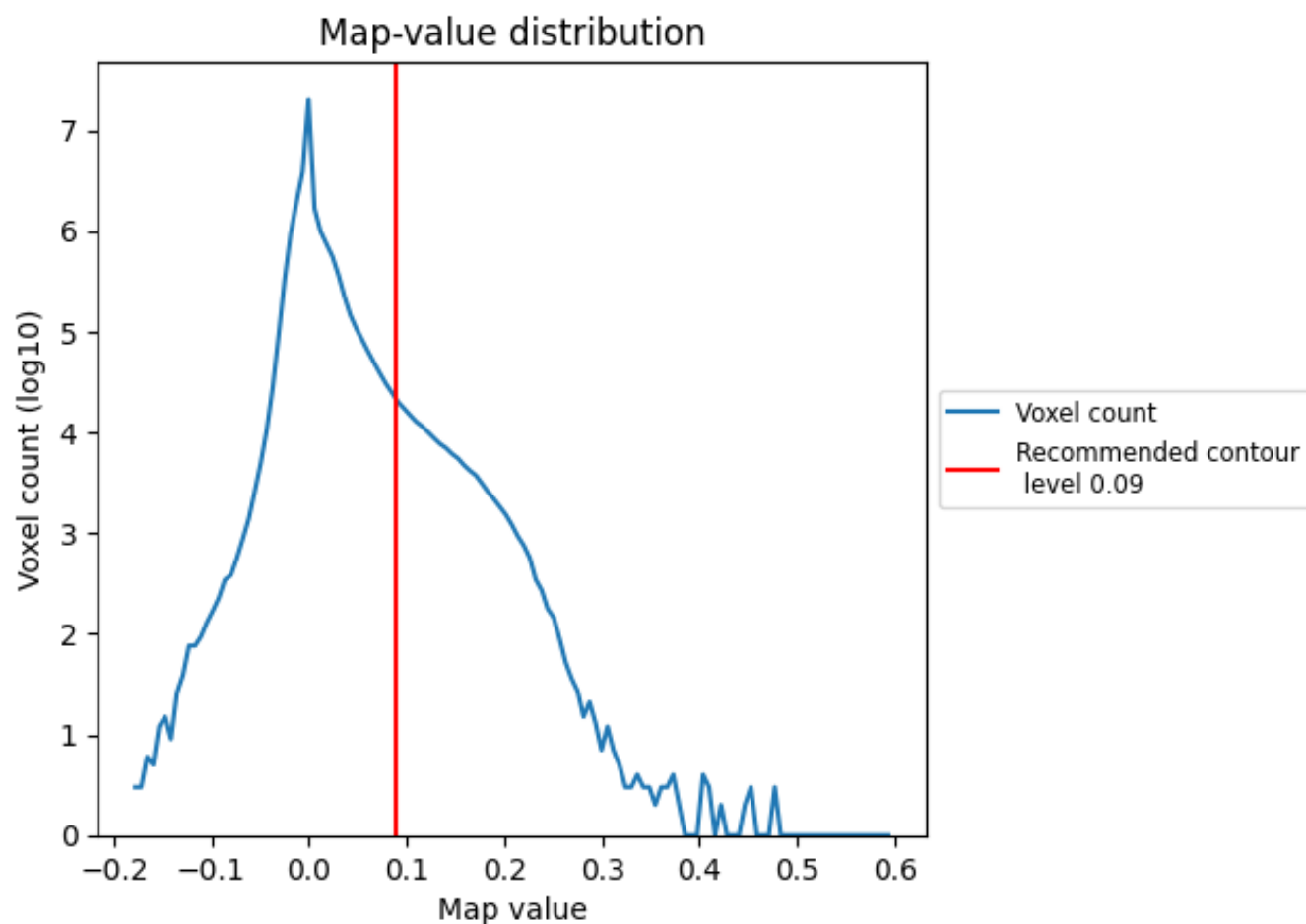
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

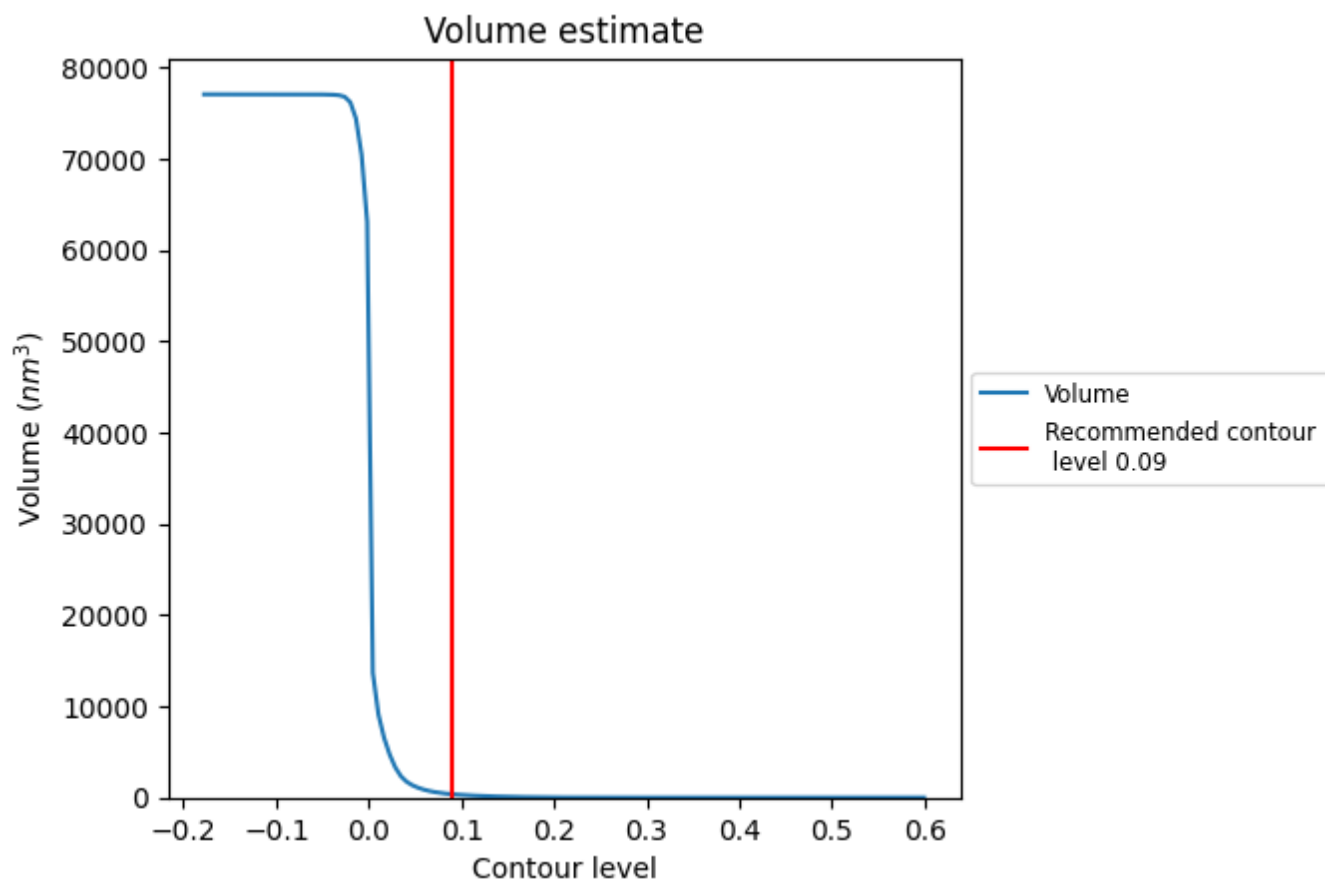
This section contains the results of statistical analysis of the map.

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.

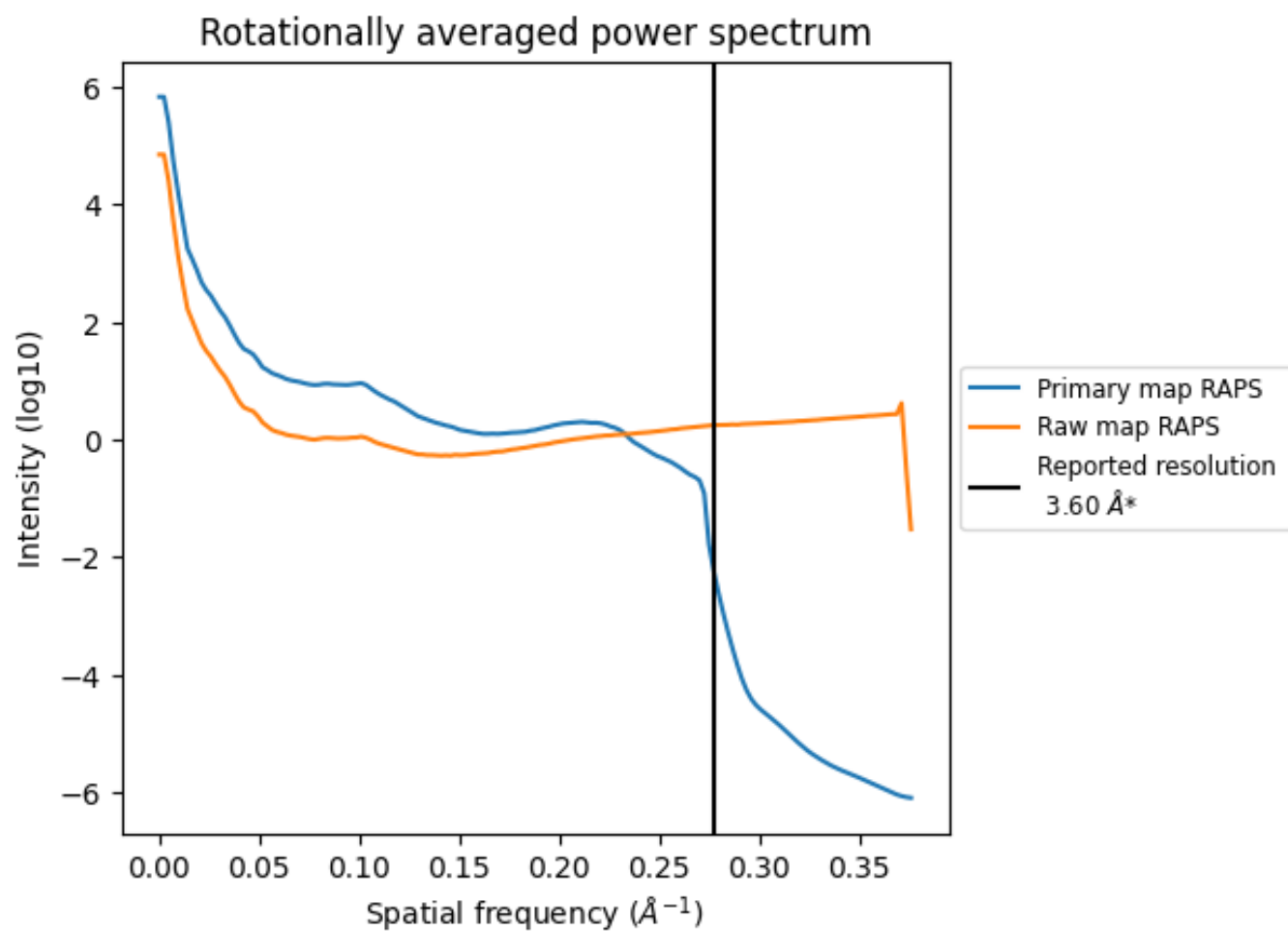
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 366 nm^3 ; this corresponds to an approximate mass of 330 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](#)

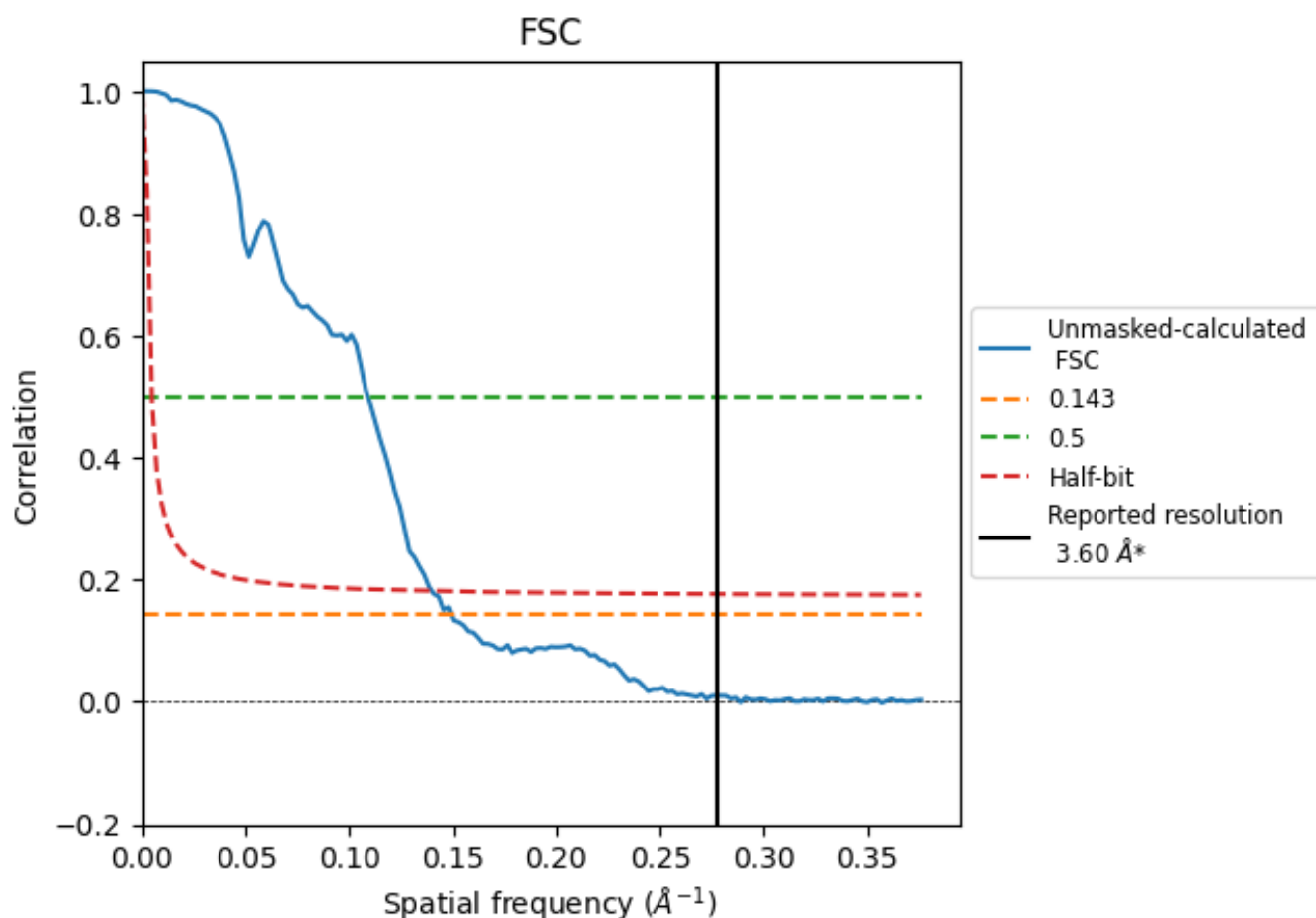


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

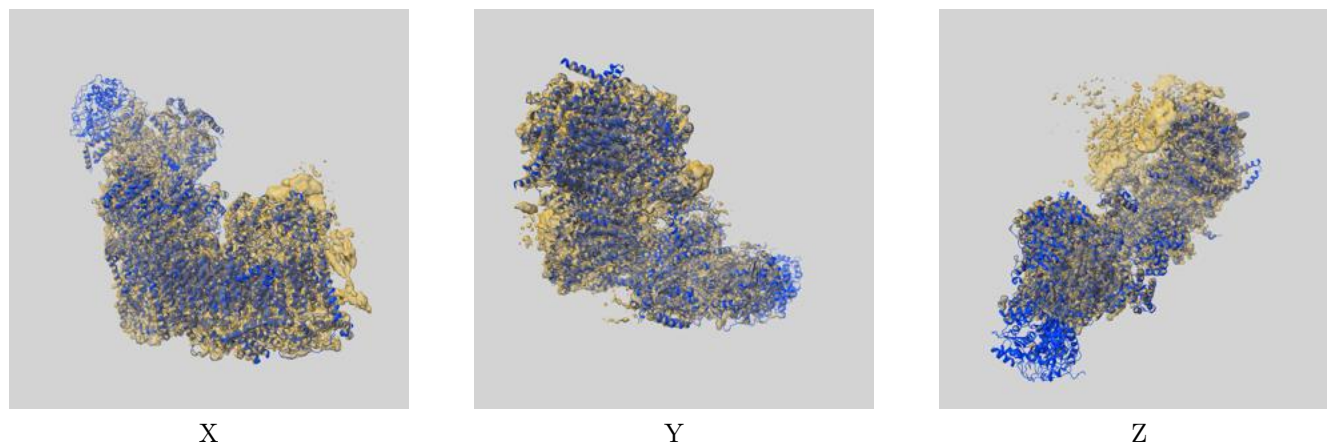
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.70	9.17	7.14

*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 6.70 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

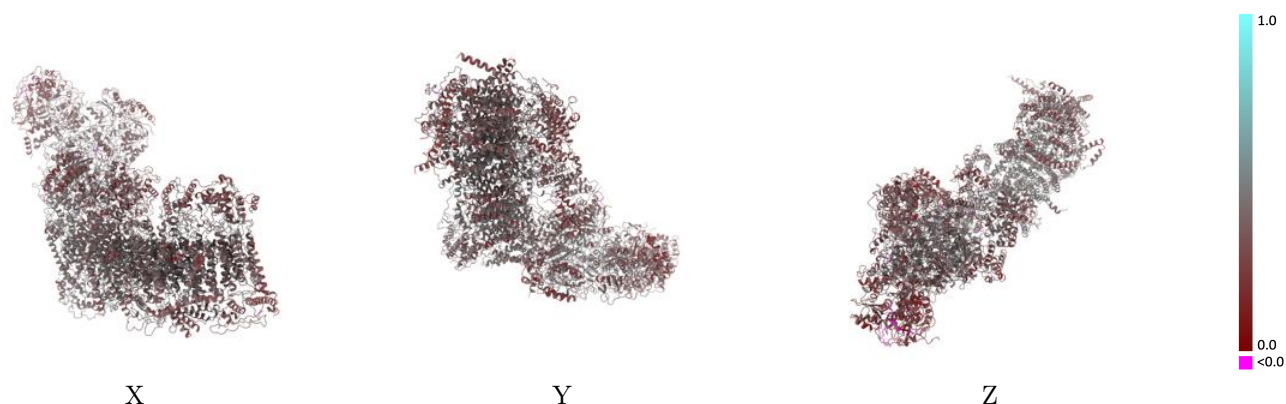
This section contains information regarding the fit between EMDB map EMD-42173 and PDB model 8UEW. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



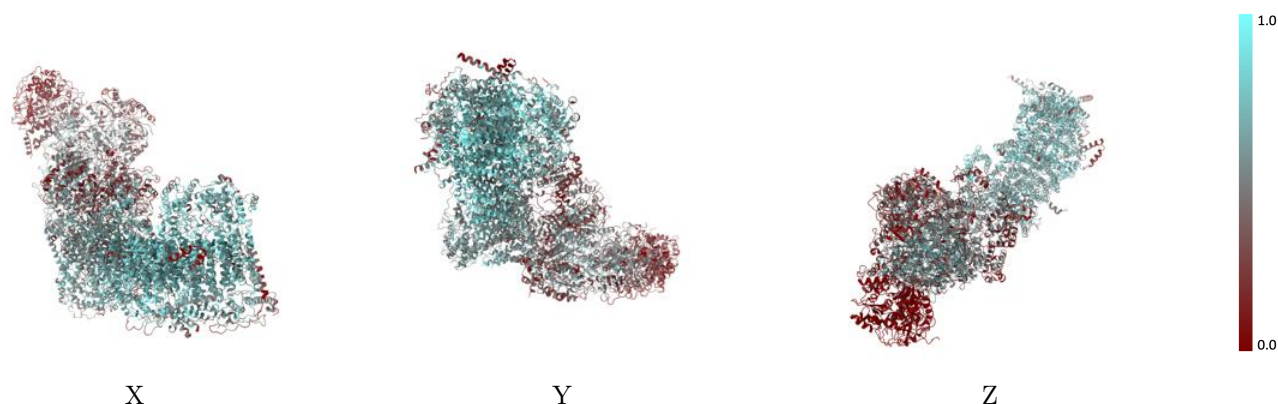
The images above show the 3D surface view of the map at the recommended contour level 0.09 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



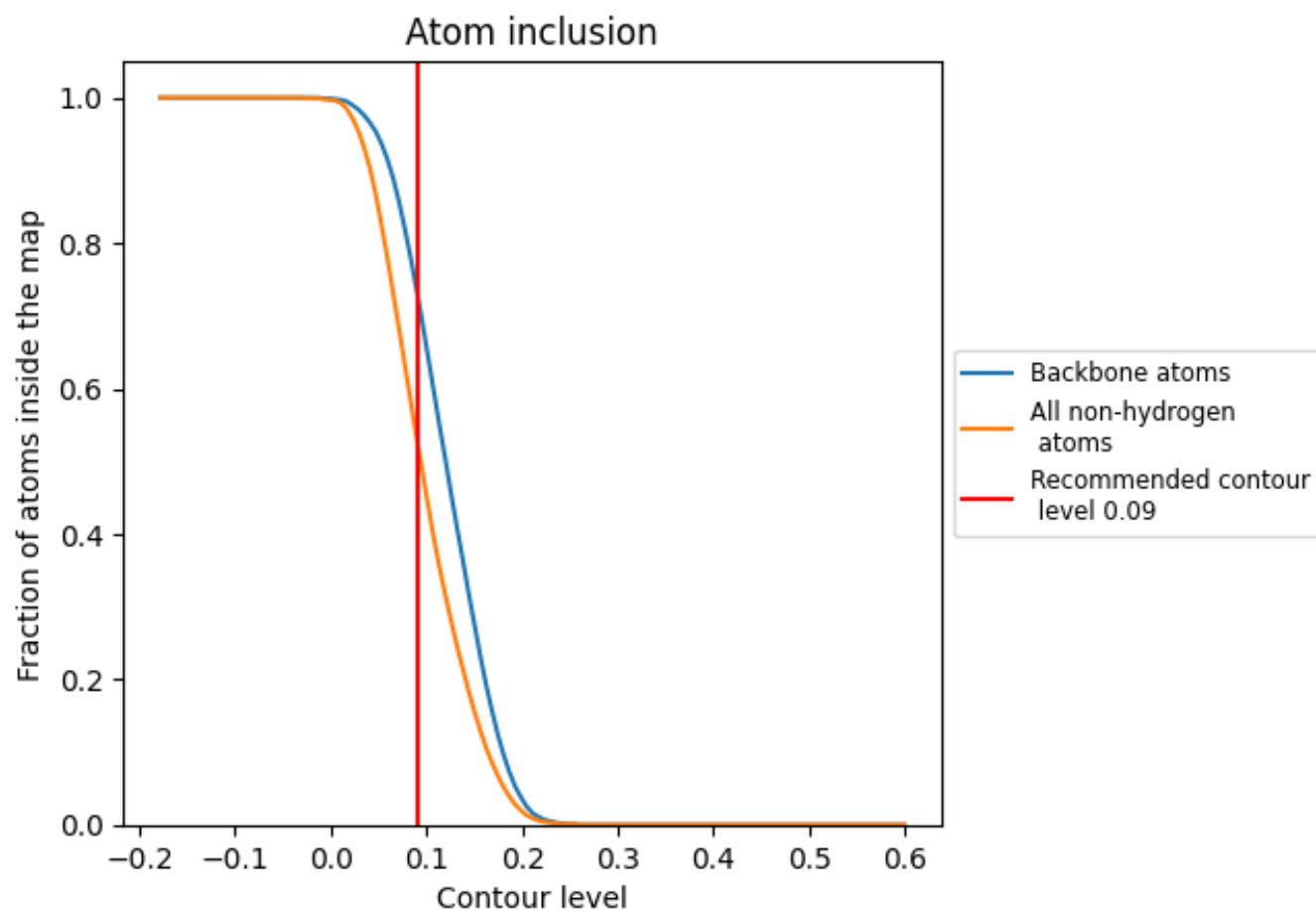
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.09).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 53% 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 (0.09) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5300	 0.3790
1A	 0.4350	 0.3830
1B	 0.5760	 0.4270
1C	 0.4720	 0.4080
1D	 0.5640	 0.4080
1E	 0.0810	 0.2870
1F	 0.0840	 0.2730
1G	 0.3820	 0.3650
1H	 0.6470	 0.4150
1I	 0.6200	 0.4220
1J	 0.5380	 0.3750
1K	 0.6490	 0.4090
1L	 0.7380	 0.4020
1M	 0.7860	 0.4370
1N	 0.7010	 0.4260
1O	 0.4410	 0.3600
1P	 0.3610	 0.3440
1Q	 0.3840	 0.3750
1R	 0.4030	 0.4090
1S	 0.2310	 0.2900
1T	 0.2750	 0.2800
1U	 0.6600	 0.3430
1V	 0.2980	 0.3340
1W	 0.3550	 0.3430
1X	 0.6010	 0.4040
1Y	 0.7050	 0.3720
1Z	 0.6260	 0.4100
1a	 0.7020	 0.4140
1b	 0.6030	 0.4170
1c	 0.5150	 0.3690
1d	 0.7100	 0.4140
1e	 0.6240	 0.4330
1f	 0.5420	 0.3700
1g	 0.6460	 0.3810
1h	 0.7080	 0.4120



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Chain	Atom inclusion	Q-score
1i	 0.4450	 0.3430
1j	 0.5770	 0.3610
1k	 0.5500	 0.3450
1l	 0.6910	 0.3950
1m	 0.7380	 0.3780
1n	 0.7000	 0.3580
1o	 0.5760	 0.3140
1p	 0.6650	 0.3840
1q	 0.5260	 0.4110
1r	 0.4600	 0.4020
1s	 0.0110	 0.2470