



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:37 PM UTC

PDB ID : 8UES / pdb_00008ues
EMDB ID : EMD-42169
Title : In-situ complex I, Deactive class01
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:

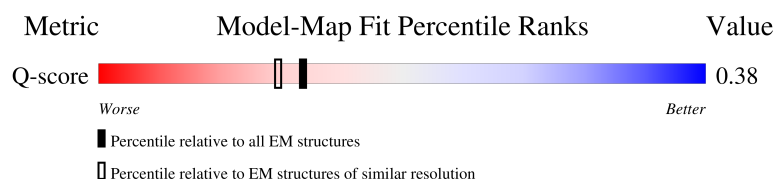
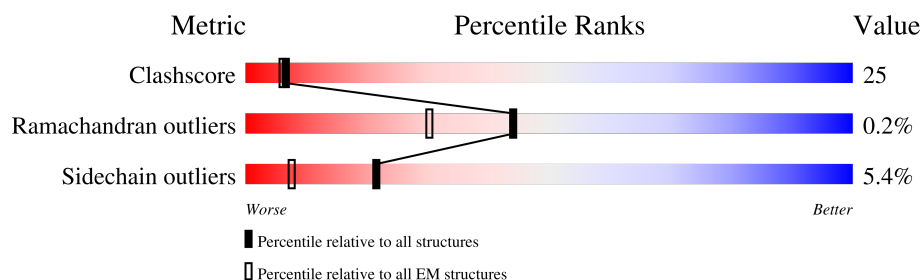
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	1G	801	-	-	X	-
47	FES	1E	301	-	-	X	-
47	FES	1G	803	-	-	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		
			1062	691	182	189	0	0

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

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

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

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

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

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

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

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

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

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

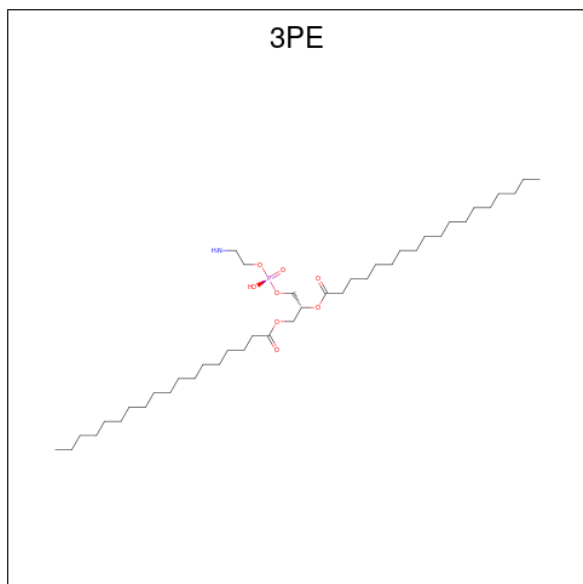
There is a discrepancy between the modelled and reference sequences:

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

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

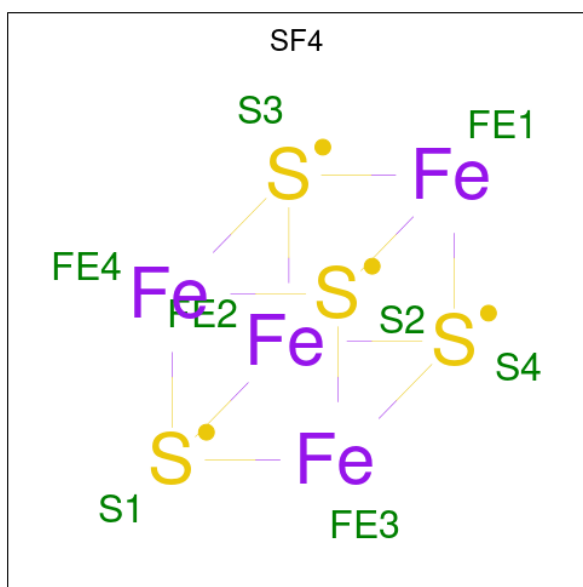
Mol	Chain	Residues	Atoms					AltConf	Trace
44	1s	45	Total	C	N	O	S	0	0
			382	238	70	73	1		

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



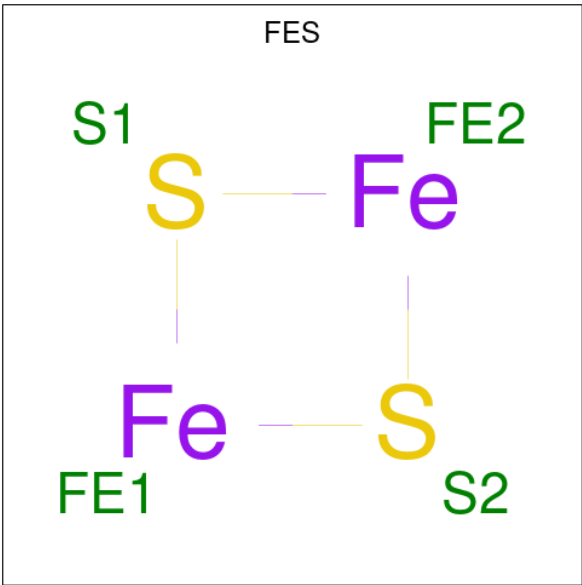
Mol	Chain	Residues	Atoms					AltConf
45	1A	1	Total	C	N	O	P	0
			47	37	1	8	1	
45	1L	1	Total	C	N	O	P	0
			46	36	1	8	1	
45	1L	1	Total	C	N	O	P	0
			42	32	1	8	1	
45	1N	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			31	21	1	8	1	
45	1Y	1	Total	C	N	O	P	0
			51	41	1	8	1	

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



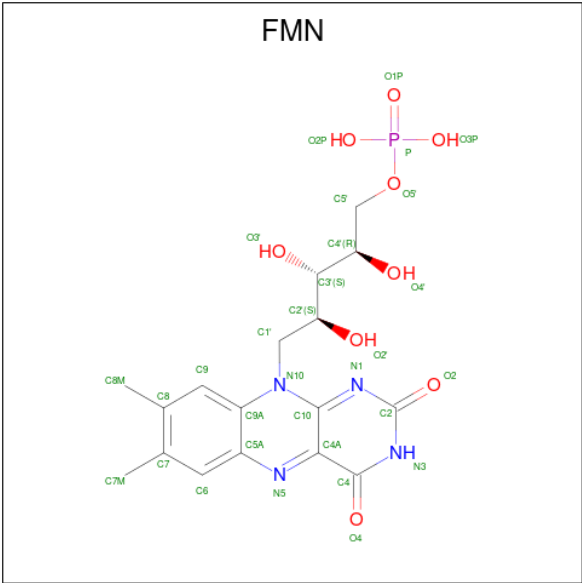
Mol	Chain	Residues	Atoms			AltConf
46	1B	1	Total	Fe	S	0
			8	4	4	
46	1F	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1G	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	
46	1I	1	Total	Fe	S	0
			8	4	4	

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

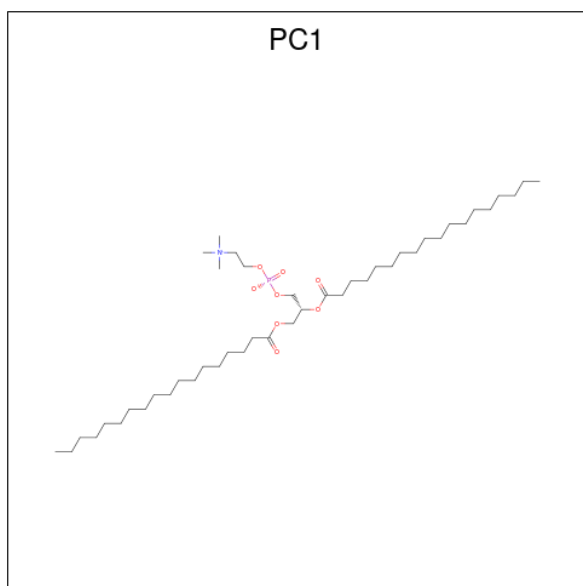


Mol	Chain	Residues	Atoms					AltConf
48	1F	1	Total	C	N	O	P	0
			31	17	4	9	1	

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

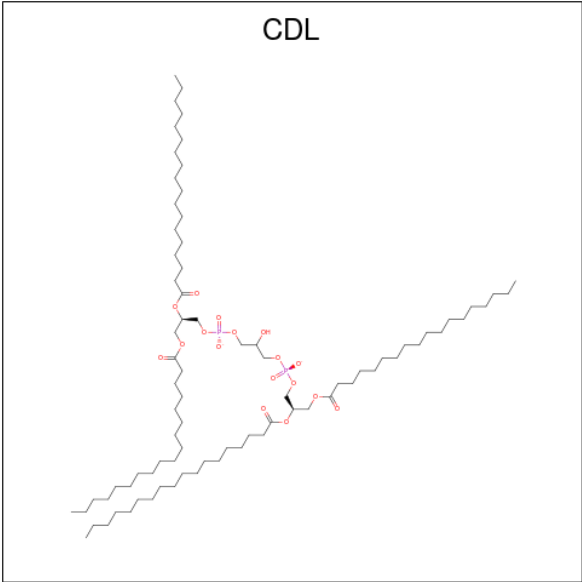
Mol	Chain	Residues	Atoms		AltConf
49	1G	1	Total	K	0
			1	1	

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



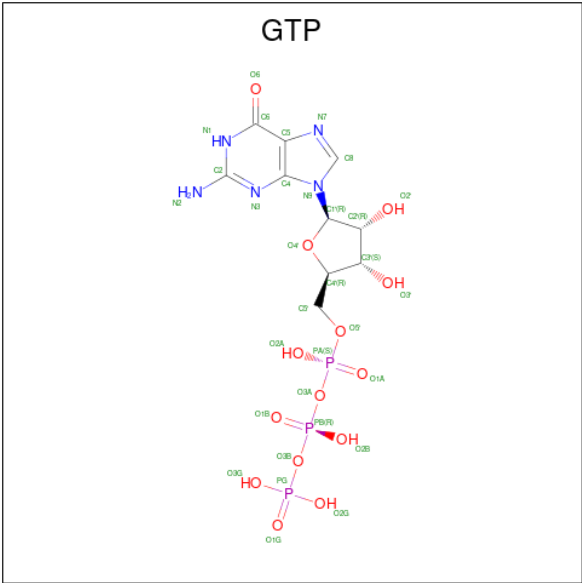
Mol	Chain	Residues	Atoms					AltConf
50	1I	1	Total	C	N	O	P	0
			54	44	1	8	1	
50	1I	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1J	1	Total	C	N	O	P	0
			35	25	1	8	1	
50	1L	1	Total	C	N	O	P	0
			44	34	1	8	1	
50	1f	1	Total	C	N	O	P	0
			46	36	1	8	1	

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



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

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

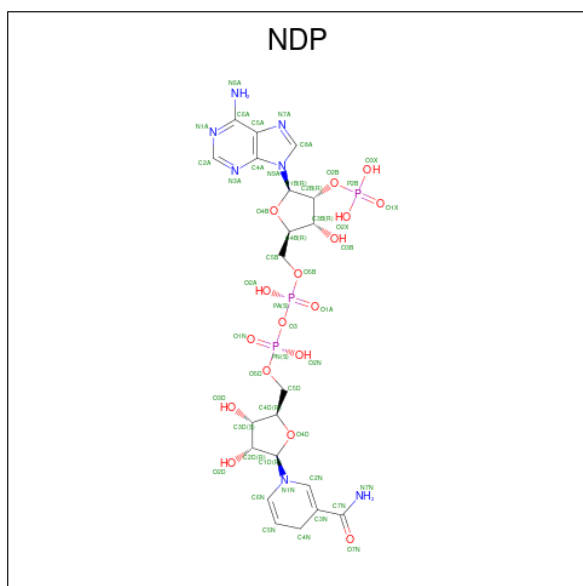


Mol	Chain	Residues	Atoms					AltConf
52	1O	1	Total	C	N	O	P	0
			32	10	5	14	3	

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

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

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

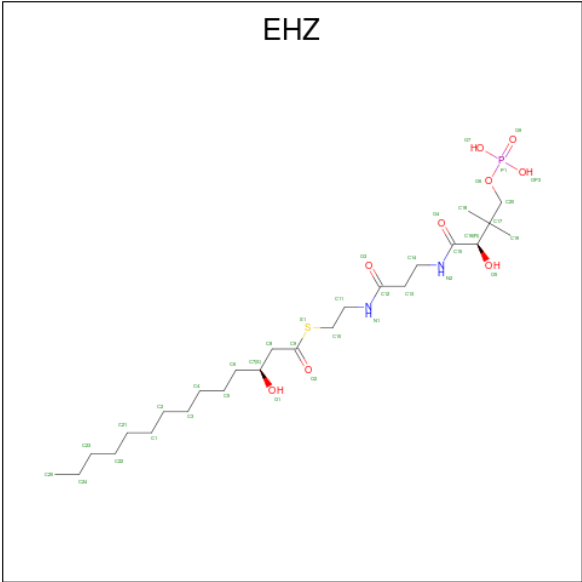


Mol	Chain	Residues	Atoms					AltConf
54	1P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

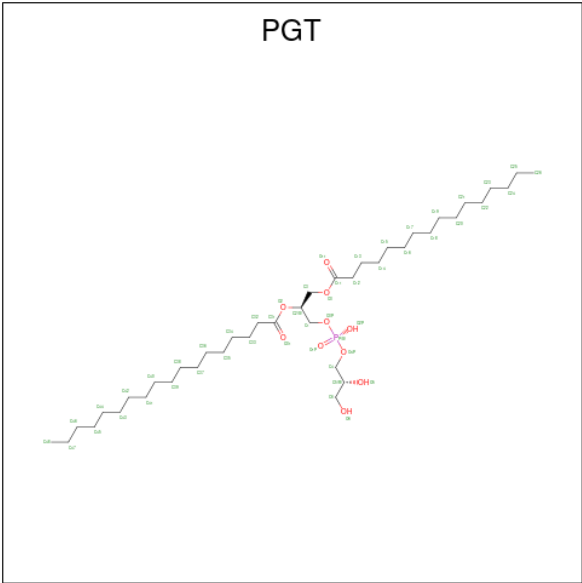
Mol	Chain	Residues	Atoms		AltConf
55	1R	1	Total	Zn	0
			1	1	

- Molecule 56 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$).



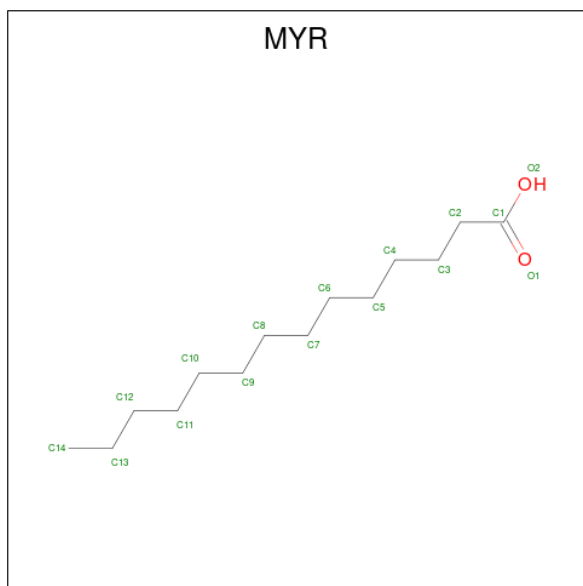
Mol	Chain	Residues	Atoms						AltConf
56	1W	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	
56	1n	1	Total	C	N	O	P	S	0
			37	25	2	8	1	1	

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



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

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

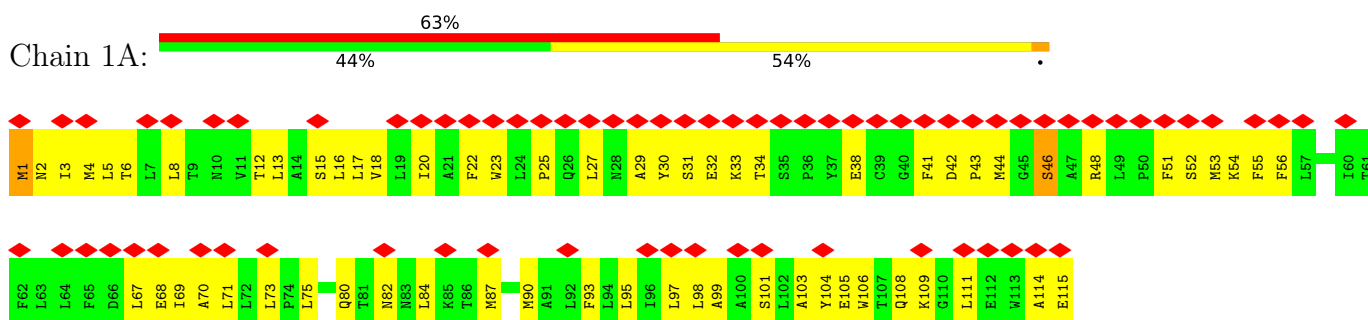


Mol	Chain	Residues	Atoms			AltConf
58	1l	1	Total	C	O	0
			15	14	1	

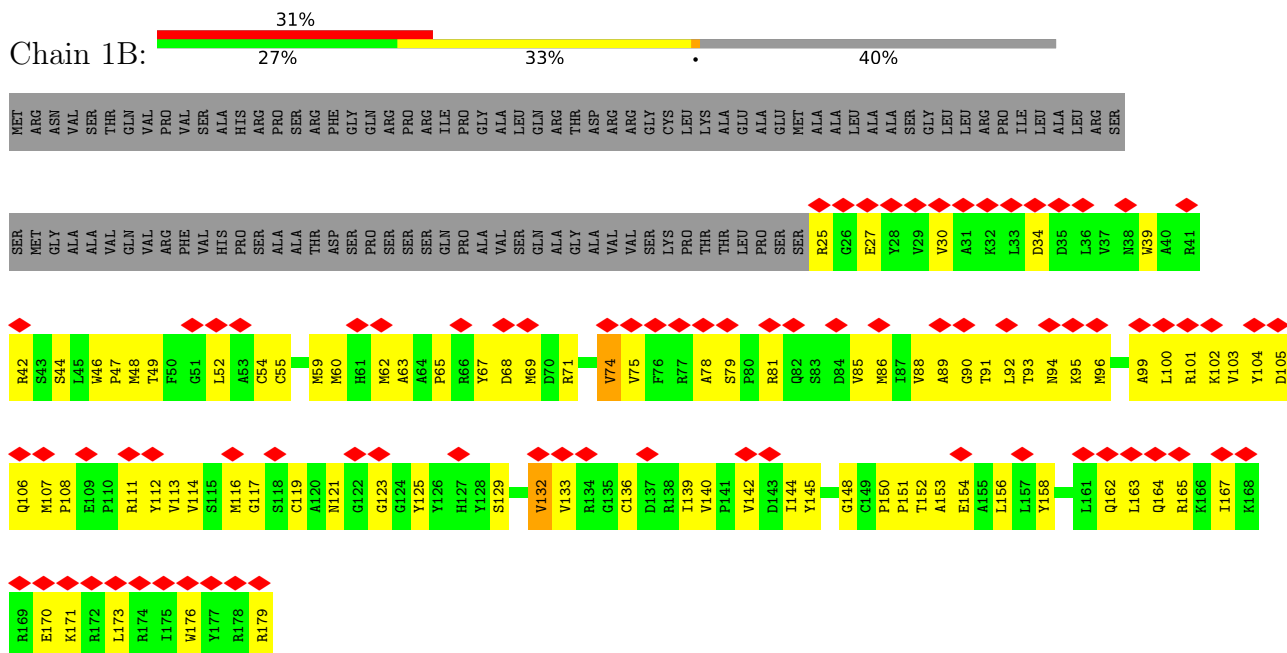
3 Residue-property plots

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

- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



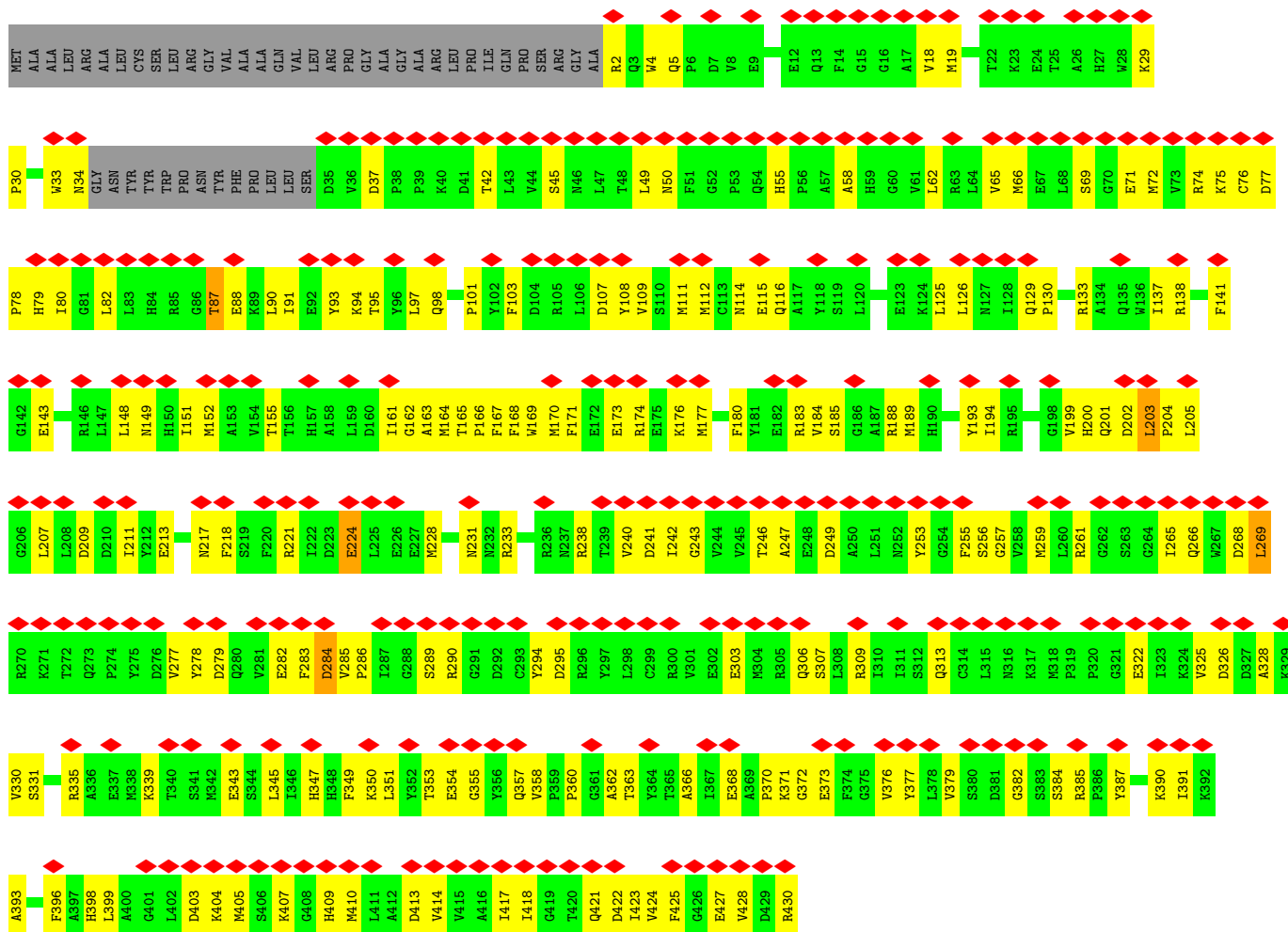
- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



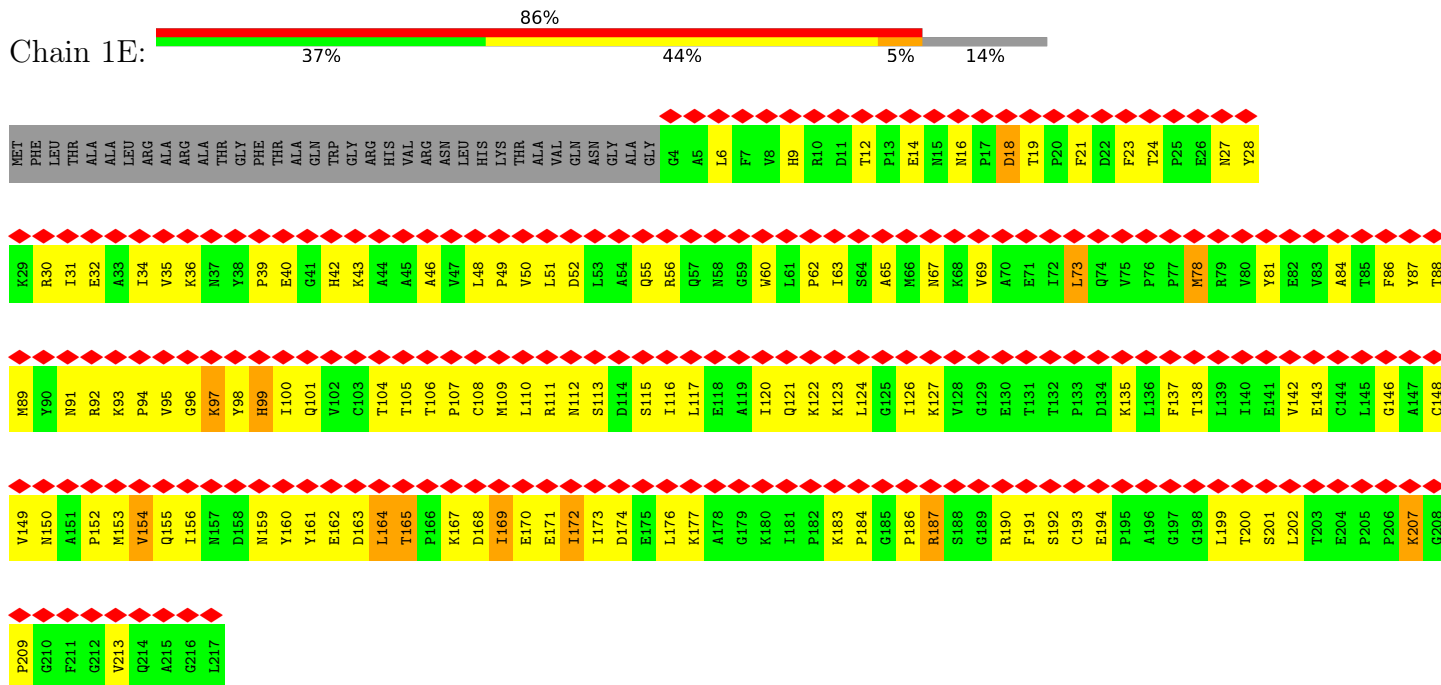
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial



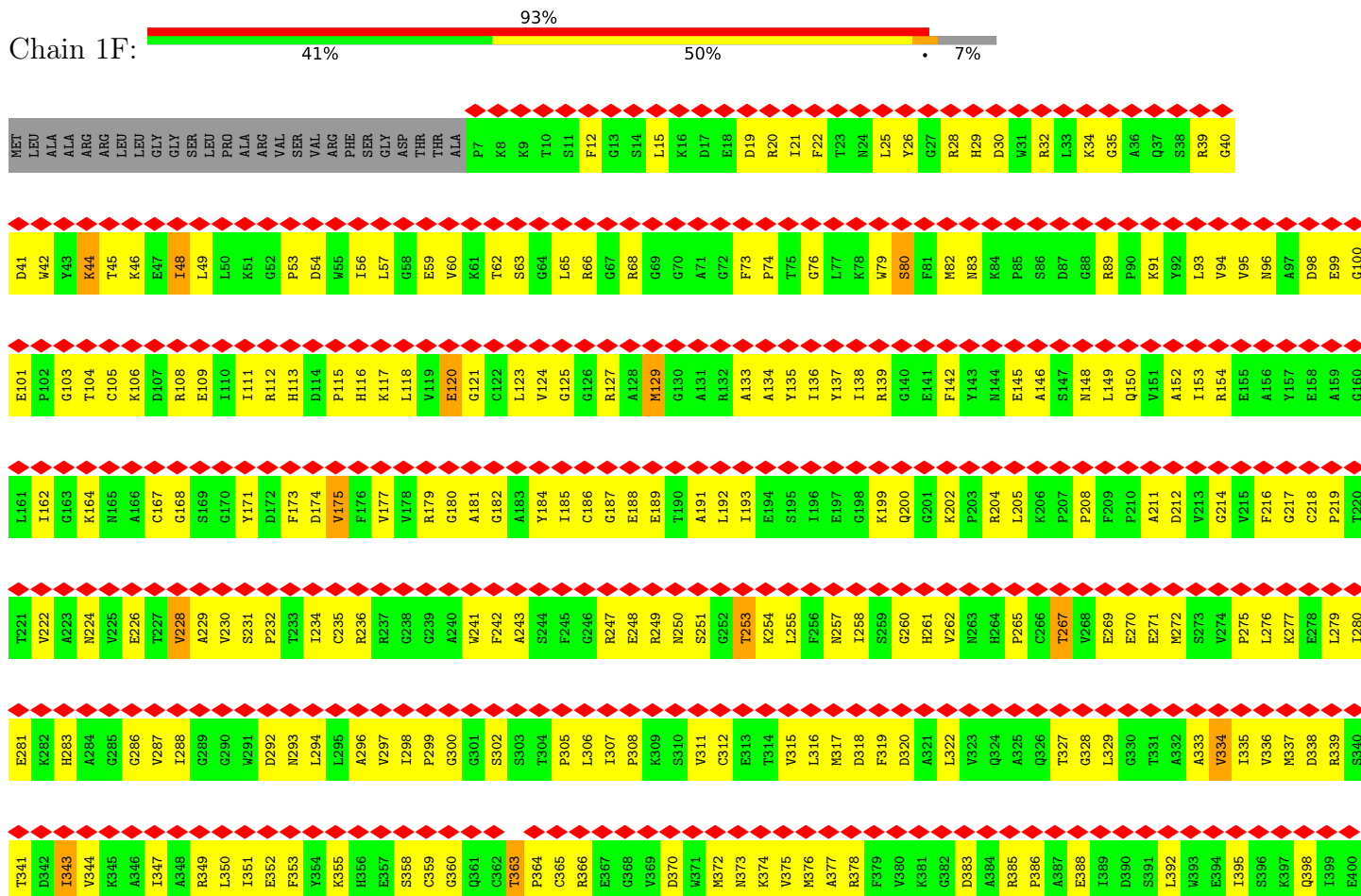
- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

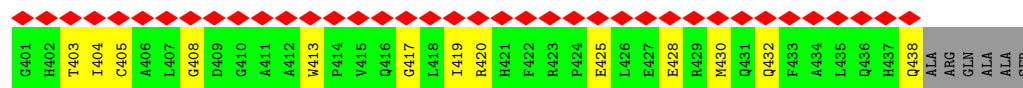


Chain 1E:

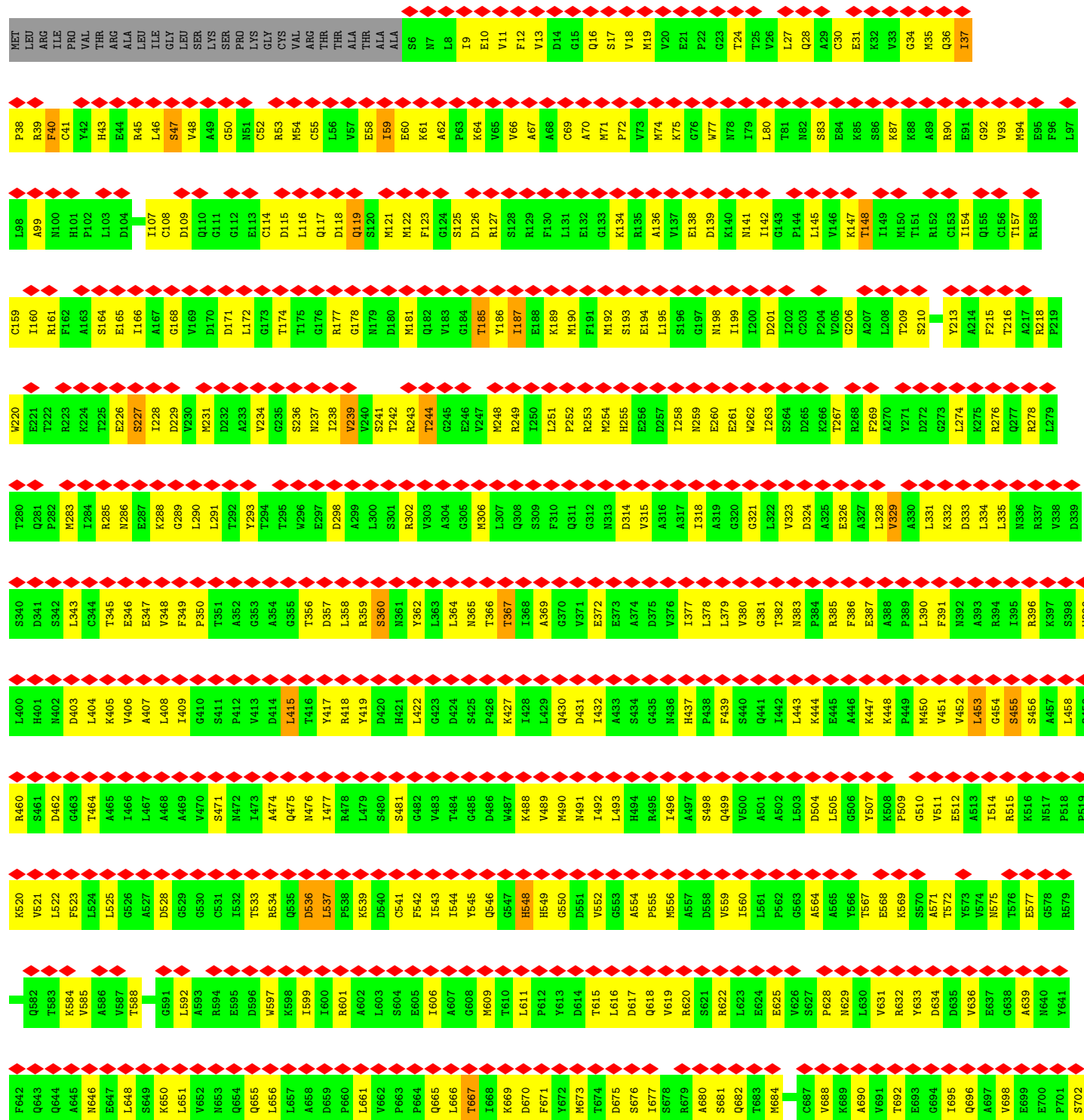


Chain 1F:



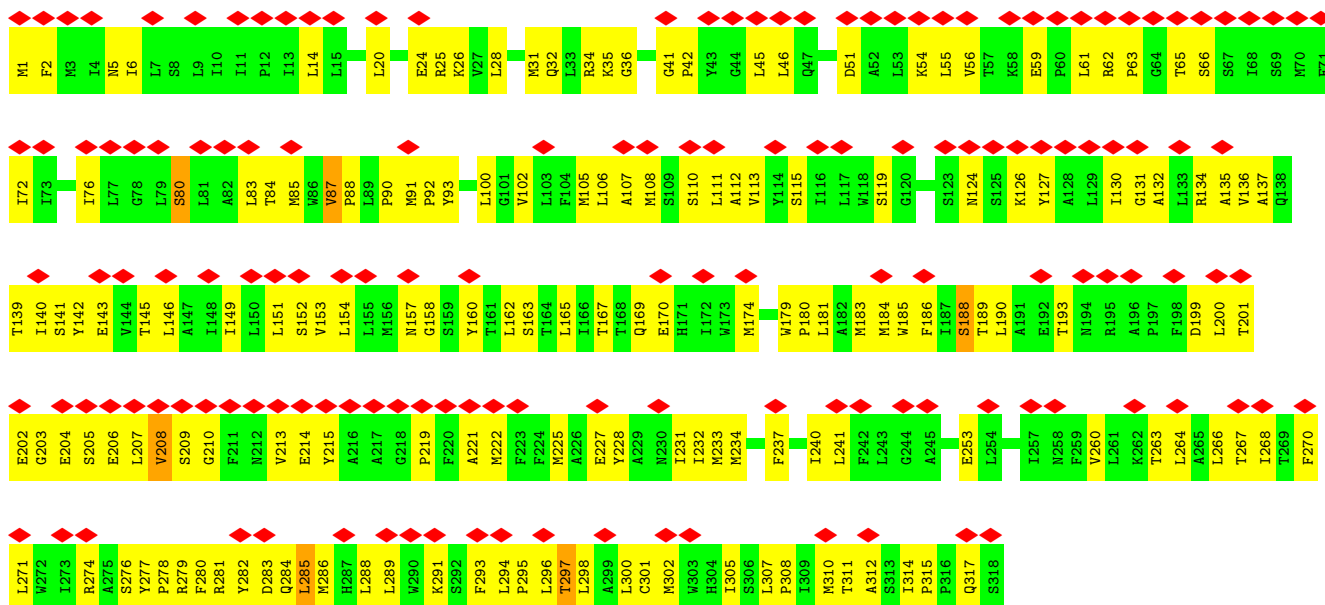


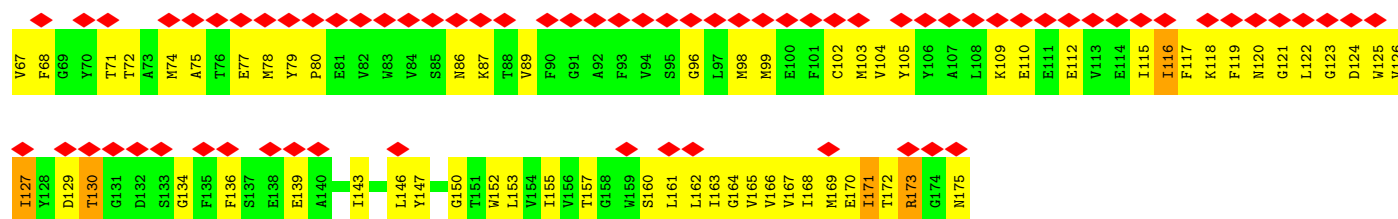
• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



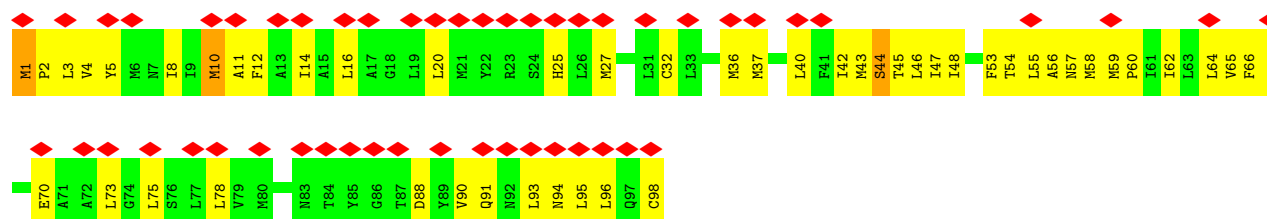


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

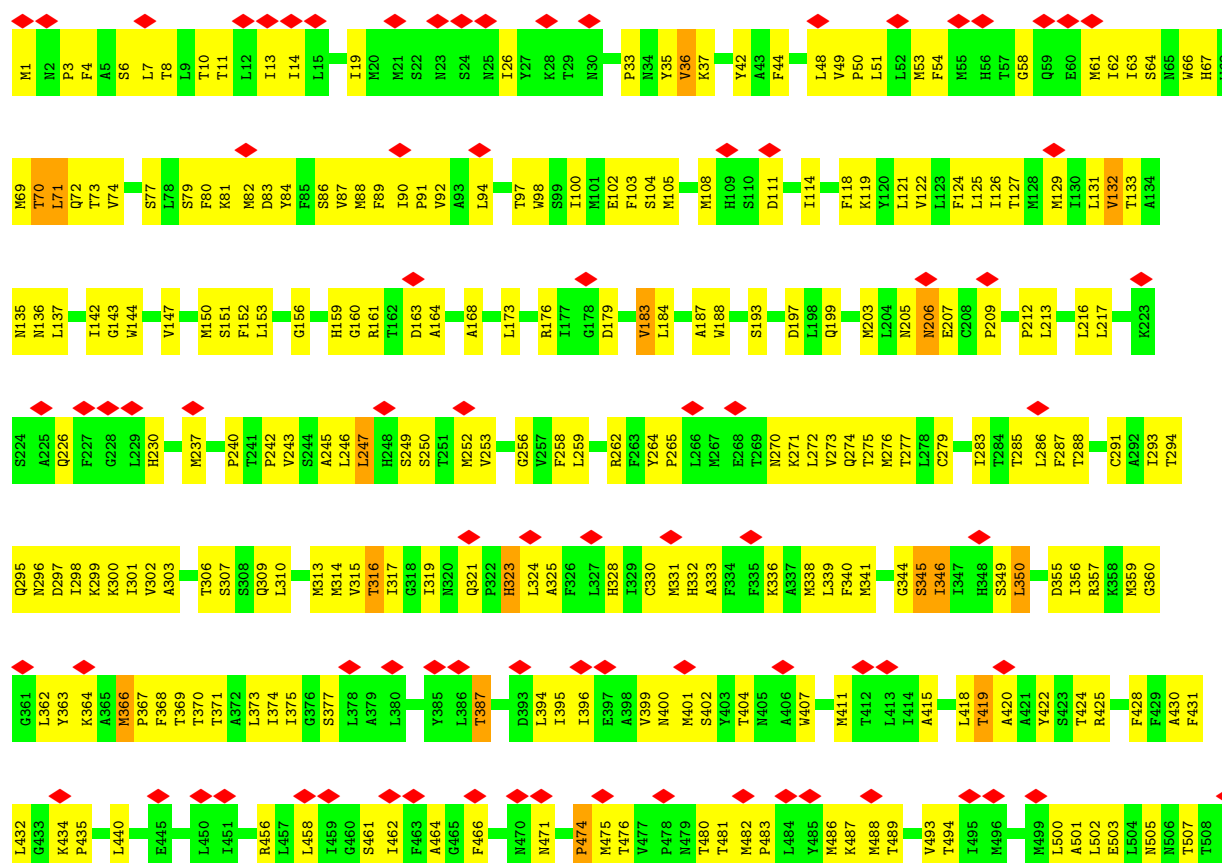


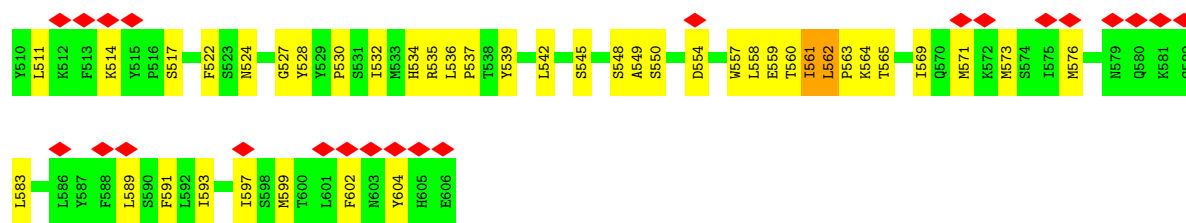


• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

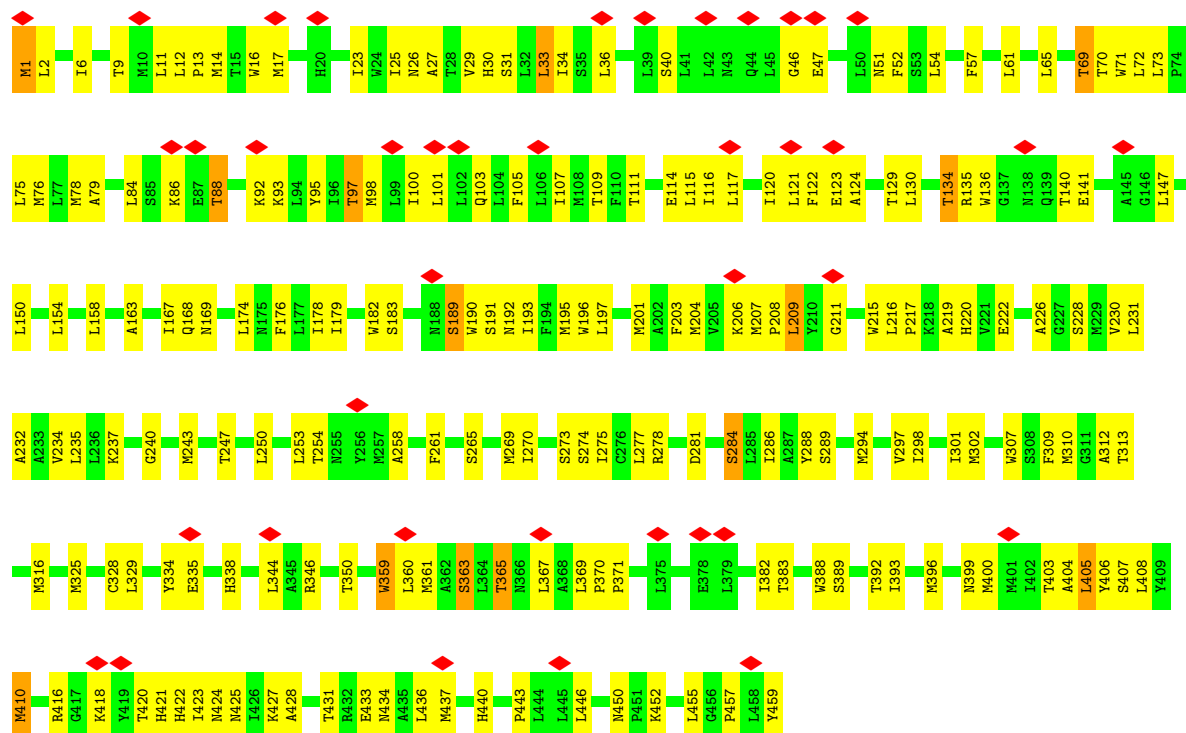


• Molecule 12: NADH-ubiquinone oxidoreductase chain 5

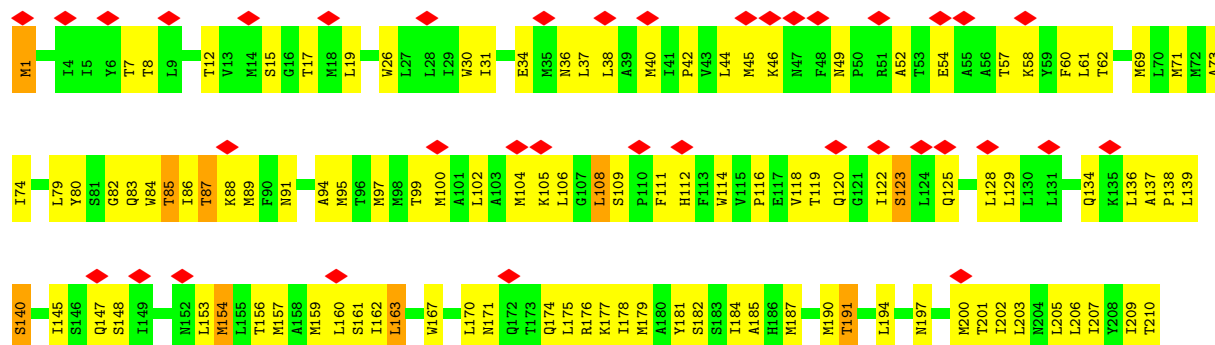


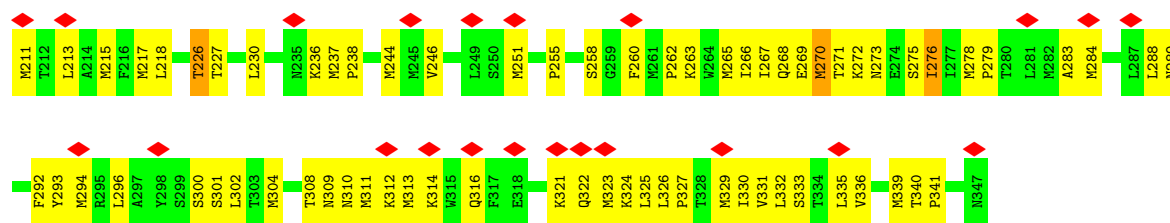


• Molecule 13: NADH-ubiquinone oxidoreductase chain 4

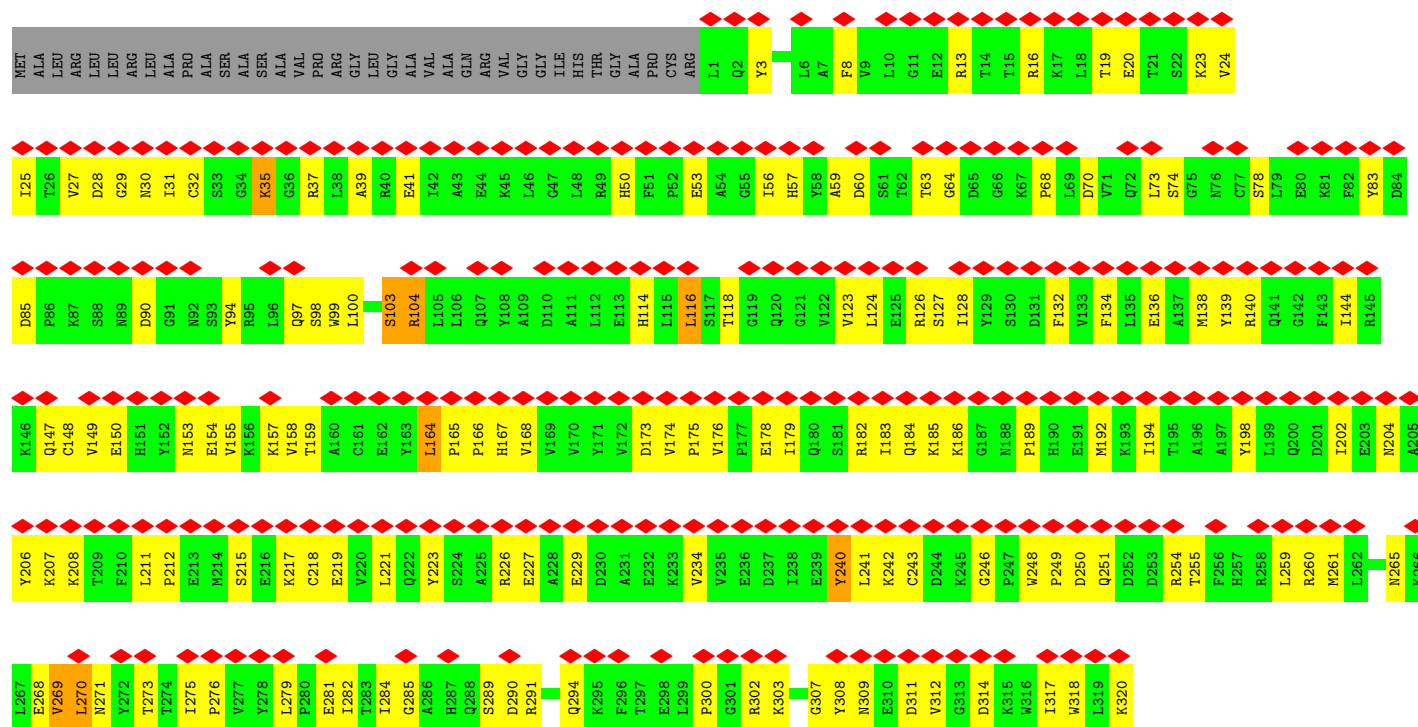
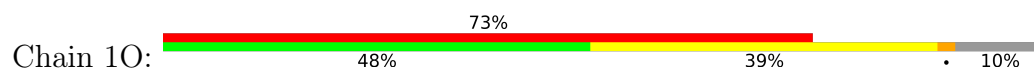


• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

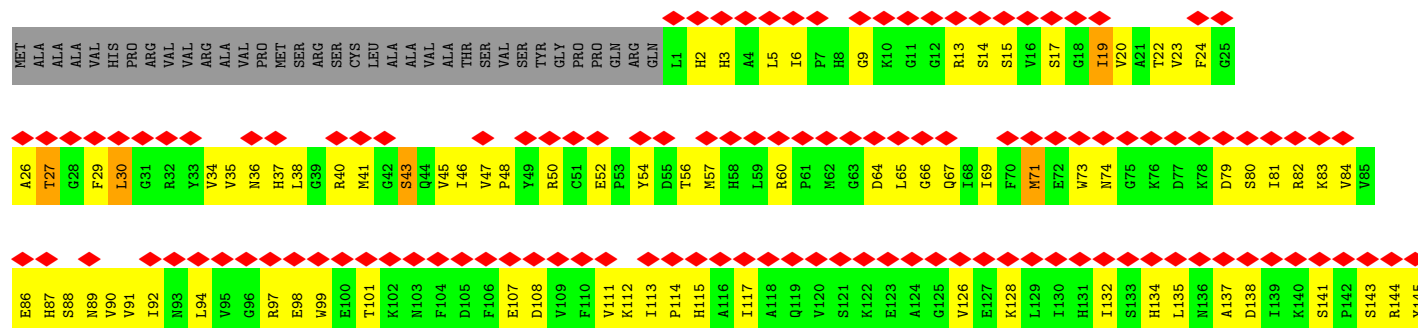
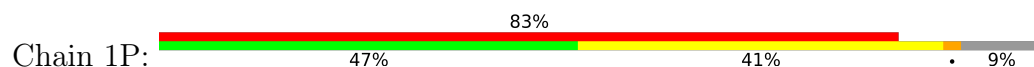


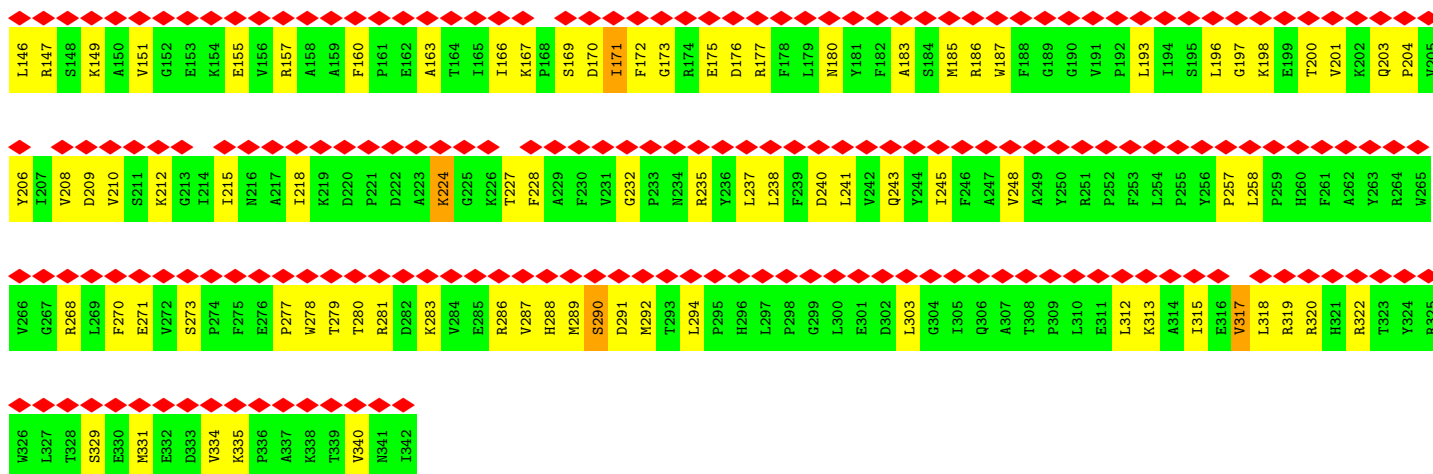


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

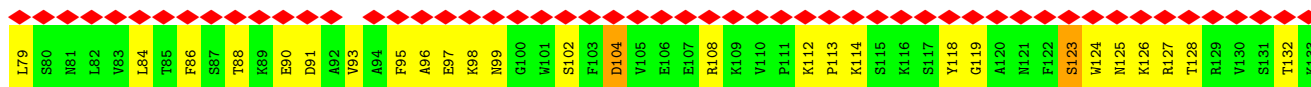
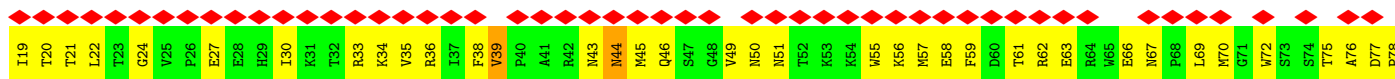
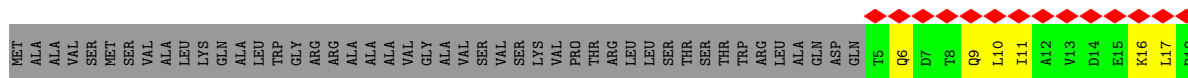


- Molecule 16: NADH:ubiquinone oxidoreductase subunit A9

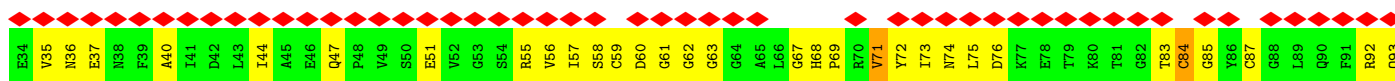
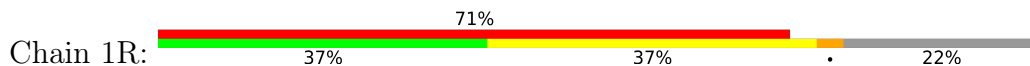




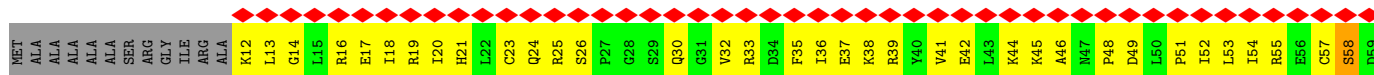
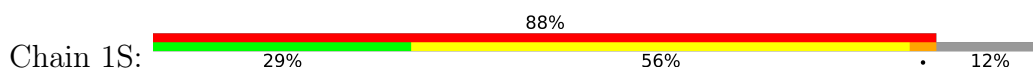
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

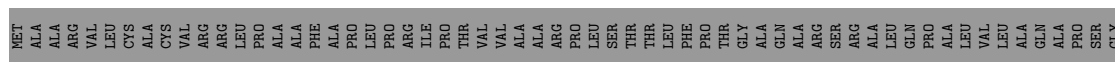


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

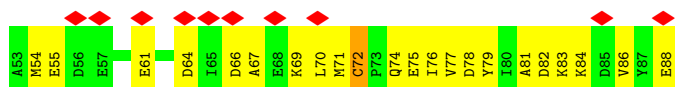
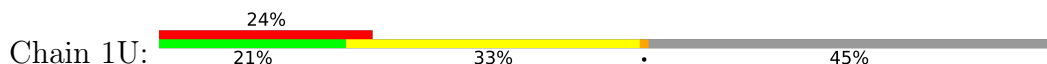




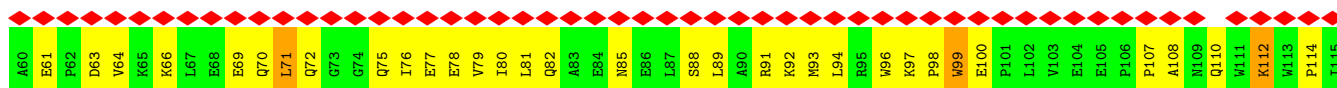
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1



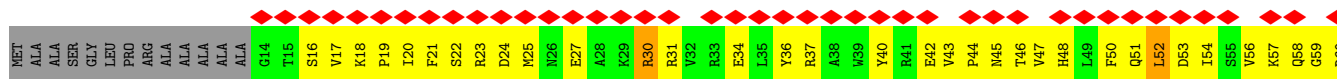
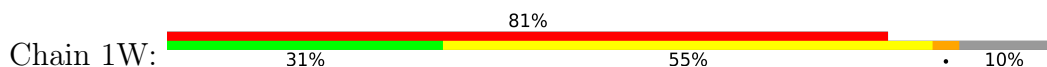
• Molecule 20: NADH:ubiquinone oxidoreductase subunit AB1

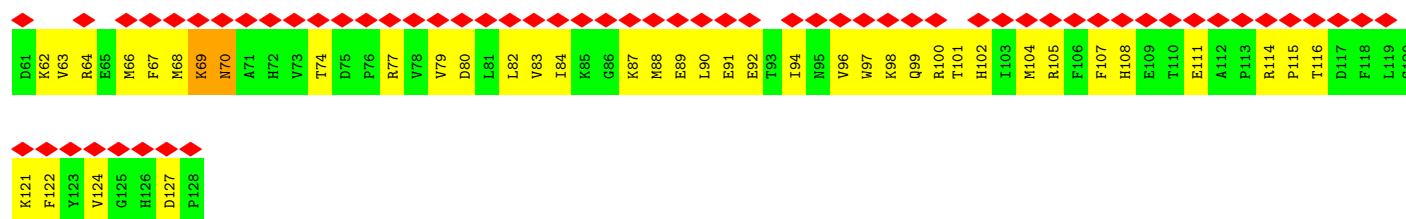


• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5 isoform X1

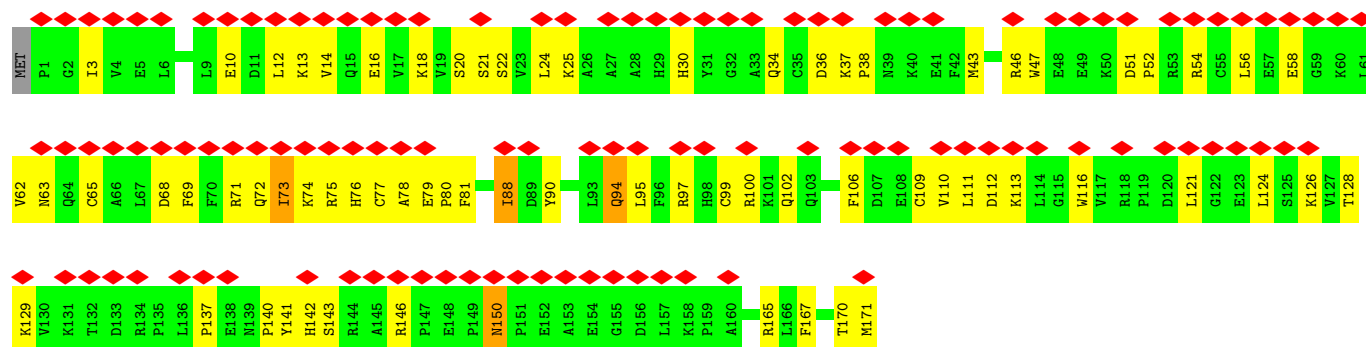


• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

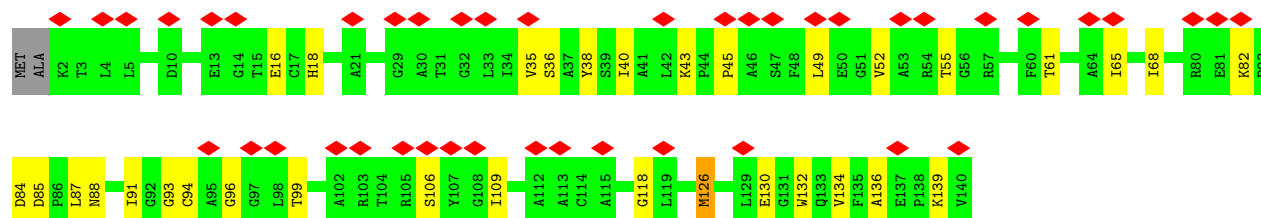
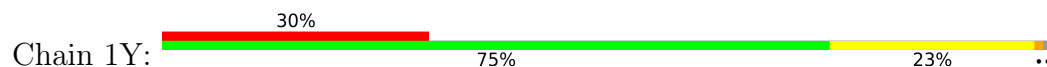




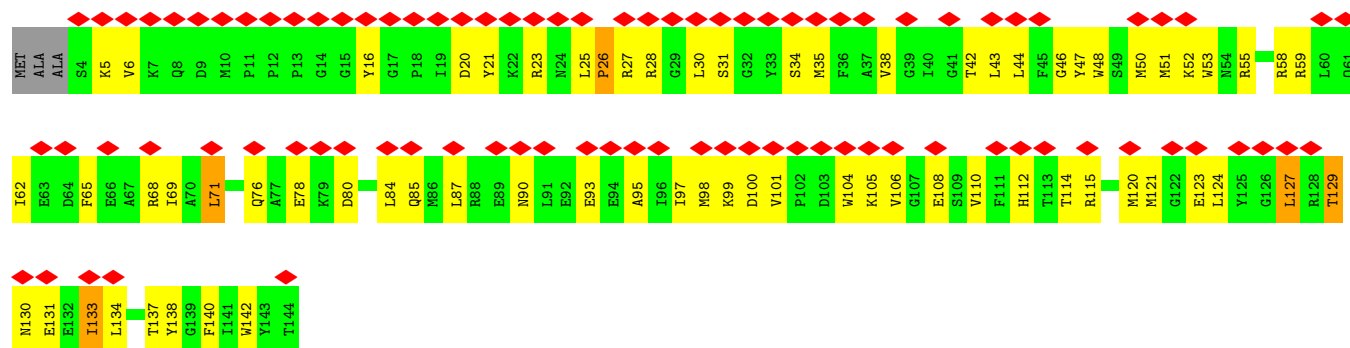
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



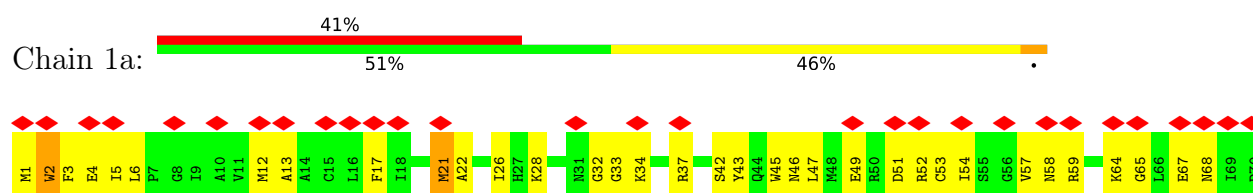
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



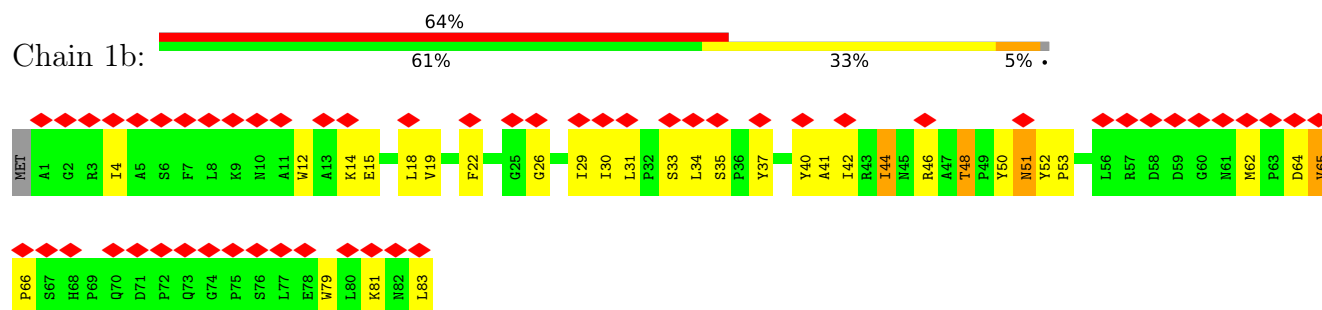
- Molecule 25: NADH:ubiquinone oxidoreductase subunit A13



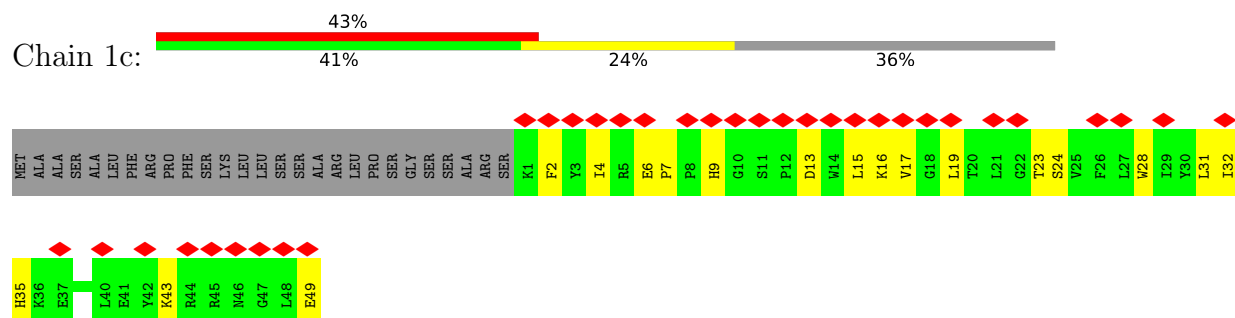
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



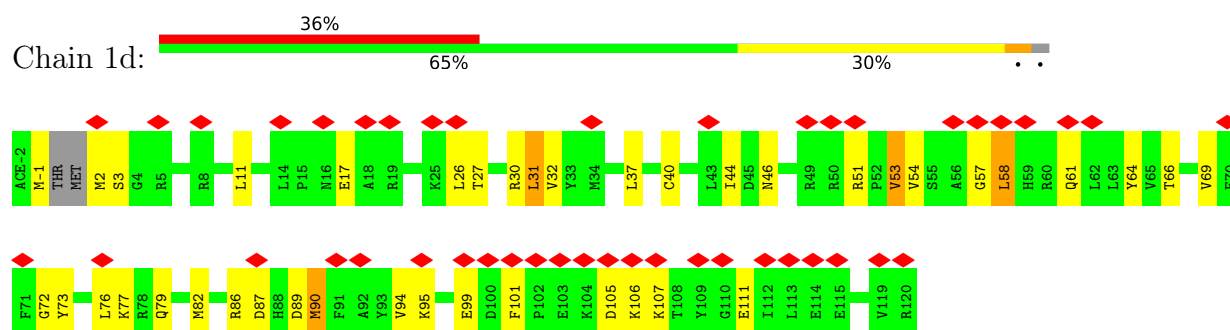
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



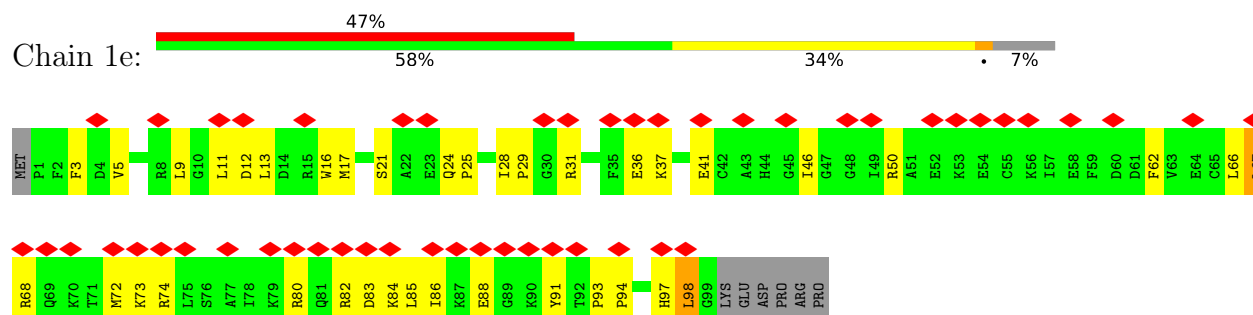
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial



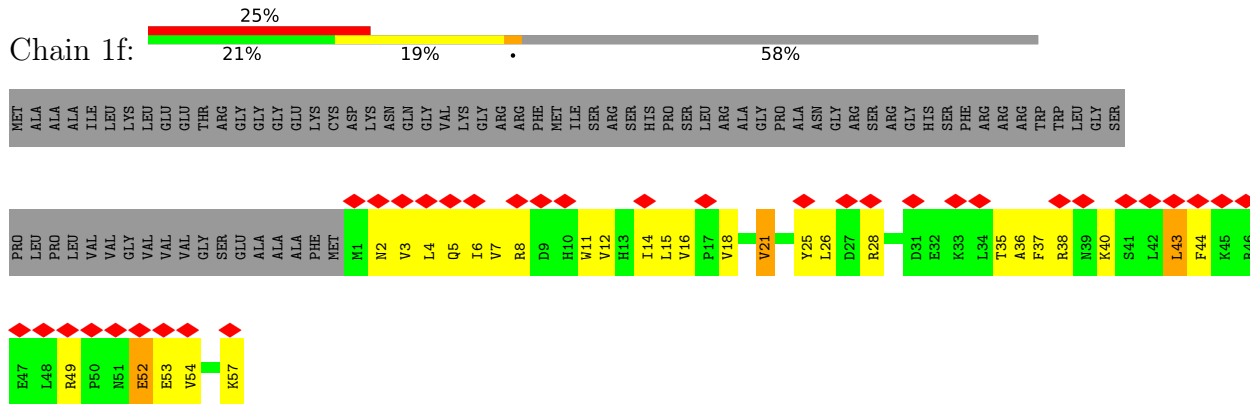
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C2



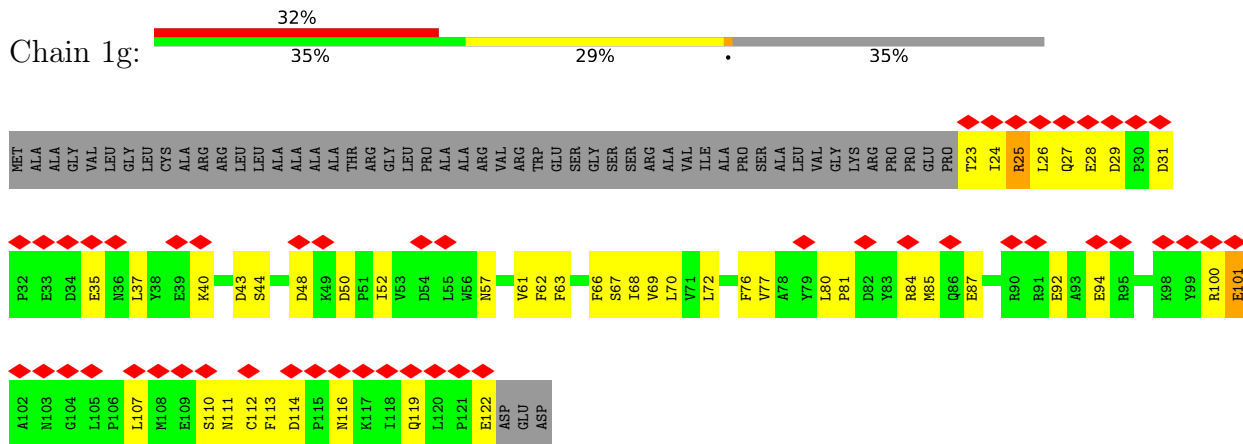
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



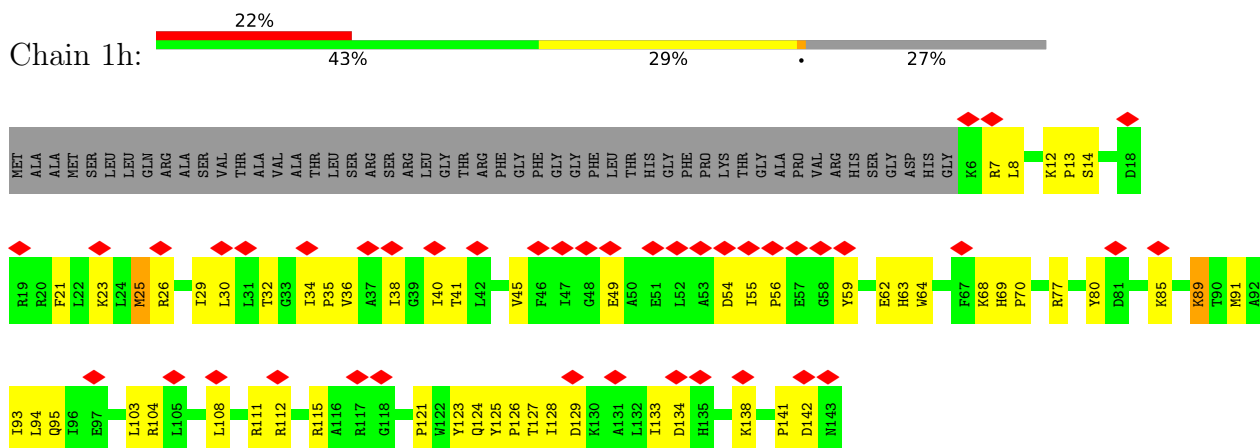
● Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1 [Sus scrofa]



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



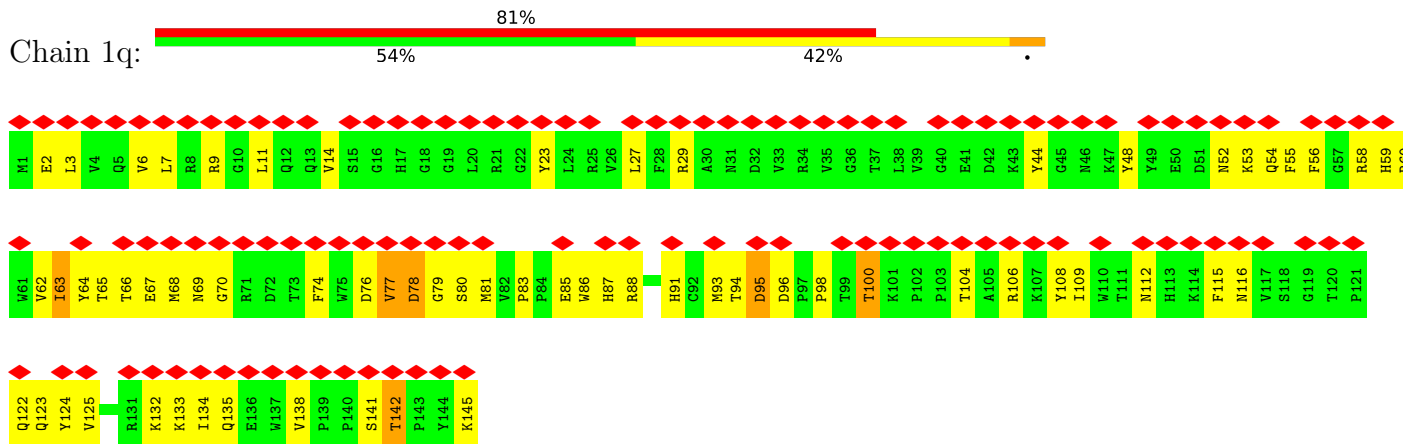
- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



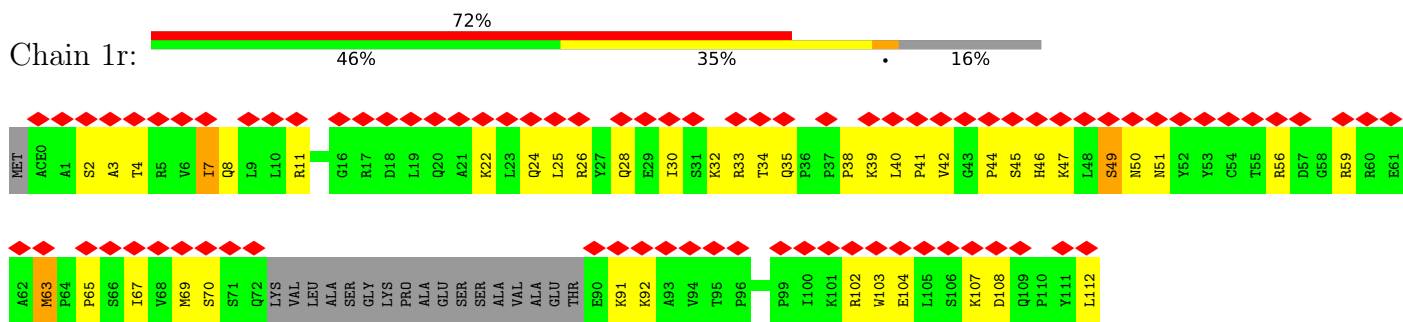
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



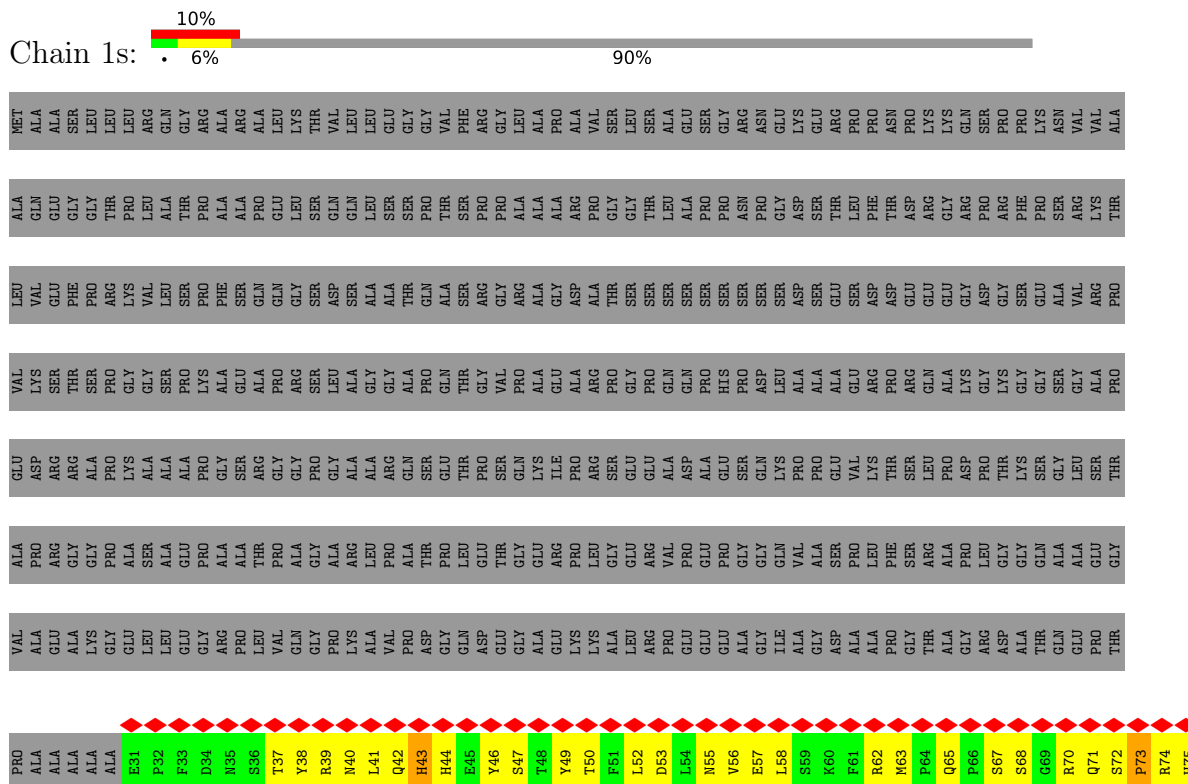
• Molecule 42: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



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



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	35000	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	0.594	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.015	Depositor
Recommended contour level	0.12	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: SAC, MYR, PC1, GTP, CDL, NDP, SF4, FMN, 3PE, EH3, FES, ZN, PGT, FME, MG, ACE, K

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	0.20	0/930	0.54	0/1271
2	1B	0.21	0/1273	0.52	0/1722
3	1C	0.18	0/1791	0.44	0/2439
4	1D	0.17	0/3545	0.43	0/4806
5	1E	0.16	0/1698	0.45	0/2311
6	1F	0.14	0/3401	0.40	0/4595
7	1G	0.15	0/5451	0.43	0/7387
8	1H	0.17	0/2566	0.42	0/3509
9	1I	0.20	0/1443	0.44	0/1952
10	1J	0.16	0/1364	0.42	0/1850
11	1K	0.20	0/751	0.50	0/1018
12	1L	0.18	0/4939	0.47	2/6718 (0.0%)
13	1M	0.17	0/3713	0.39	0/5063
14	1N	0.17	0/2765	0.44	0/3758
15	1O	0.15	0/2650	0.40	0/3588
16	1P	0.15	0/2828	0.44	0/3834
17	1Q	0.20	0/1070	0.54	0/1446
18	1R	0.16	0/755	0.48	0/1018
19	1S	0.21	0/711	0.65	0/956
20	1T	0.17	0/701	0.52	0/946
20	1U	0.18	0/706	0.52	0/954
21	1V	0.19	0/946	0.57	1/1281 (0.1%)
22	1W	0.24	0/995	0.68	0/1340
23	1X	0.14	0/1436	0.36	0/1938
24	1Y	0.11	0/1037	0.28	0/1404
25	1Z	0.28	1/1199 (0.1%)	0.63	3/1617 (0.2%)
26	1a	0.22	0/577	0.57	3/777 (0.4%)
27	1b	0.16	0/664	0.45	0/912
28	1c	0.15	0/430	0.48	0/581
29	1d	0.16	0/1024	0.41	0/1383
30	1e	0.14	0/836	0.38	0/1118
31	1f	0.18	0/499	0.50	0/673

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	1g	0.18	0/858	0.49	0/1165
33	1h	0.14	0/1184	0.35	0/1603
34	1i	0.19	0/1131	0.49	1/1541 (0.1%)
35	1j	0.15	0/627	0.41	0/858
36	1k	0.16	0/668	0.46	0/903
37	1l	0.17	0/1365	0.47	0/1867
38	1m	0.14	0/1092	0.35	0/1481
39	1n	0.13	0/1549	0.35	0/2098
40	1o	0.14	0/1069	0.38	0/1430
41	1p	0.14	0/1481	0.36	0/1997
42	1q	0.19	0/1253	0.48	0/1704
43	1r	0.22	0/782	0.58	1/1057 (0.1%)
44	1s	0.24	0/394	0.61	1/533 (0.2%)
All	All	0.17	1/68147 (0.0%)	0.45	12/92402 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1Z	26	PRO	CG-CD	-5.49	1.32	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1Z	26	PRO	CA-N-CD	-13.09	93.67	112.00
12	1L	474	PRO	CA-N-CD	-9.75	98.35	112.00
25	1Z	26	PRO	N-CD-CG	-8.53	90.41	103.20
44	1s	73	PRO	CA-N-CD	-6.96	102.25	112.00
25	1Z	26	PRO	CA-CB-CG	-6.24	92.64	104.50
21	1V	112	LYS	CA-CB-CG	6.24	126.57	114.10
34	1i	35	PRO	CA-N-CD	-5.90	103.74	112.00
26	1a	2	TRP	CA-C-N	-5.46	112.49	122.38
26	1a	2	TRP	C-N-CA	-5.46	112.49	122.38
26	1a	2	TRP	N-CA-C	5.34	118.61	112.57
43	1r	63	MET	CB-CG-SD	5.29	128.58	112.70
12	1L	350	LEU	CA-CB-CG	5.20	134.48	116.30

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	85	0
2	1B	1242	0	1249	84	0
3	1C	1740	0	1691	129	0
4	1D	3452	0	3389	191	0
5	1E	1658	0	1662	126	0
6	1F	3325	0	3288	230	0
7	1G	5362	0	5389	301	0
8	1H	2504	0	2602	168	0
9	1I	1412	0	1365	107	0
10	1J	1339	0	1337	90	0
11	1K	750	0	798	60	0
12	1L	4818	0	4956	275	0
13	1M	3632	0	3836	186	0
14	1N	2712	0	2873	157	0
15	1O	2590	0	2555	126	0
16	1P	2751	0	2776	141	0
17	1Q	1047	0	1042	80	0
18	1R	741	0	704	47	0
19	1S	700	0	719	65	0
20	1T	689	0	687	64	0
20	1U	694	0	691	59	0
21	1V	927	0	972	72	0
22	1W	971	0	975	90	0
23	1X	1398	0	1378	63	0
24	1Y	1016	0	1020	22	0
25	1Z	1168	0	1161	73	0
26	1a	562	0	557	48	0
27	1b	643	0	645	34	0
28	1c	417	0	425	11	0
29	1d	996	0	990	36	0
30	1e	816	0	823	42	0
31	1f	487	0	496	23	0
32	1g	835	0	795	45	0
33	1h	1151	0	1164	56	0
34	1i	1100	0	1106	57	0
35	1j	601	0	546	45	0
36	1k	649	0	626	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	1l	1310	0	1204	67	0
38	1m	1062	0	1075	49	0
39	1n	1495	0	1434	82	0
40	1o	1045	0	1018	62	0
41	1p	1449	0	1416	67	0
42	1q	1212	0	1173	66	0
43	1r	767	0	791	53	0
44	1s	382	0	351	33	0
45	1A	47	0	71	7	0
45	1L	88	0	127	5	0
45	1N	51	0	82	6	0
45	1Y	82	0	118	7	0
46	1B	8	0	0	1	0
46	1F	8	0	0	1	0
46	1G	16	0	0	2	0
46	1I	16	0	0	1	0
47	1E	4	0	0	2	0
47	1G	4	0	0	3	0
48	1F	31	0	19	3	0
49	1G	1	0	0	0	0
50	1I	98	0	149	13	0
50	1J	35	0	44	0	0
50	1L	44	0	65	1	0
50	1f	46	0	69	3	0
51	1N	77	0	98	4	0
51	1q	61	0	64	14	0
52	1O	32	0	12	3	0
53	1O	1	0	0	0	0
54	1P	48	0	26	6	0
55	1R	1	0	0	0	0
56	1W	37	0	0	1	0
56	1n	37	0	0	0	0
57	1Y	51	0	78	8	0
58	1l	15	0	27	1	0
All	All	67472	0	67749	3373	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 25.

All (3373) 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)
5:1E:153:MET:HE1	47:1E:301:FES:S2	2.06	0.95
7:1G:283:MET:HB3	7:1G:560:ILE:HB	1.49	0.95
14:1N:128:LEU:HD11	14:1N:213:LEU:HD13	1.50	0.92
26:1a:2:TRP:HZ2	43:1r:7:ILE:HG21	1.33	0.91
12:1L:35:TYR:HH	34:1i:73:HIS:HE2	0.93	0.91
2:1B:62:MET:HB2	2:1B:153:ALA:HB1	1.54	0.90
7:1G:19:MET:H	7:1G:19:MET:HE3	1.35	0.90
16:1P:113:ILE:HD12	16:1P:114:PRO:HD3	1.52	0.89
4:1D:149:ASN:HD22	4:1D:370:PRO:HB2	1.37	0.89
3:1C:204:GLU:HA	17:1Q:50:ASN:HD22	1.39	0.87
7:1G:377:ILE:HA	7:1G:450:MET:HB3	1.58	0.86
20:1U:70:LEU:HD12	20:1U:76:ILE:HD13	1.56	0.85
9:1I:32:ARG:NH1	50:1I:204:PC1:O31	2.10	0.85
3:1C:114:LEU:HB3	22:1W:77:ARG:HD2	1.60	0.84
21:1V:54:LYS:HD2	21:1V:71:LEU:HB3	1.60	0.84
7:1G:276:ARG:HB2	7:1G:680:ALA:HB1	1.60	0.83
14:1N:313:MET:H	14:1N:313:MET:HE2	1.43	0.83
26:1a:17:PHE:HE2	26:1a:21:MET:HE2	1.44	0.82
4:1D:163:ALA:H	8:1H:278:PRO:HA	1.44	0.82
17:1Q:58:GLU:OE2	17:1Q:58:GLU:N	2.12	0.82
3:1C:66:ASP:HB2	21:1V:89:LEU:HD12	1.61	0.81
36:1k:18:TYR:HE1	36:1k:21:TRP:HB2	1.46	0.81
37:1l:54:SER:HA	37:1l:84:TYR:HB3	1.64	0.80
12:1L:276:MET:HA	12:1L:279:CYS:HB2	1.64	0.80
7:1G:30:CYS:HB3	7:1G:35:MET:HB3	1.64	0.80
12:1L:298:ILE:H	12:1L:298:ILE:HD12	1.47	0.79
20:1U:29:LYS:HE2	20:1U:40:LEU:HD12	1.64	0.79
16:1P:171:ILE:HG12	54:1P:501:NDP:H42N	1.65	0.78
20:1U:37:MET:HE3	20:1U:37:MET:H	1.49	0.78
29:1d:17:GLU:N	29:1d:17:GLU:OE2	2.16	0.78
4:1D:404:LYS:HE2	4:1D:404:LYS:HA	1.64	0.78
4:1D:162:GLY:HA3	8:1H:279:ARG:H	1.48	0.78
10:1J:17:PHE:HB3	11:1K:14:ILE:HD11	1.66	0.78
19:1S:74:LYS:HE2	19:1S:74:LYS:HA	1.65	0.78
6:1F:365:CYS:HB2	46:1F:502:SF4:S2	2.23	0.77
25:1Z:5:LYS:HA	25:1Z:5:LYS:HE3	1.66	0.77
13:1M:129:THR:HG21	13:1M:235:LEU:HD11	1.66	0.77
23:1X:43:MET:HE3	27:1b:52:TYR:HE2	1.50	0.77
6:1F:403:THR:HG21	6:1F:408:GLY:HA3	1.66	0.77
13:1M:208:PRO:HG3	13:1M:216:LEU:HD22	1.66	0.77
1:1A:52:SER:OG	1:1A:53:MET:N	2.17	0.77
4:1D:115:GLU:HG3	4:1D:194:ILE:HB	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:37:GLU:HG3	19:1S:38:LYS:HD3	1.67	0.77
6:1F:343:ILE:HD11	6:1F:425:GLU:HG2	1.64	0.76
21:1V:91:ARG:HH21	21:1V:92:LYS:HD3	1.50	0.76
7:1G:168:GLY:HA2	7:1G:396:ARG:HH21	1.51	0.76
23:1X:72:GLN:OE1	23:1X:72:GLN:N	2.18	0.76
5:1E:143:GLU:HG3	6:1F:349:ARG:HH22	1.50	0.76
5:1E:190:ARG:HH21	5:1E:193:CYS:HA	1.49	0.76
38:1m:122:GLN:HB3	38:1m:125:ASN:HB3	1.68	0.76
7:1G:47:SER:OG	7:1G:48:VAL:N	2.18	0.76
9:1I:64:GLU:OE2	9:1I:157:ASN:ND2	2.19	0.76
10:1J:99:MET:H	10:1J:99:MET:HE3	1.49	0.76
41:1p:78:GLU:HG3	41:1p:79:LYS:HG2	1.66	0.76
9:1I:84:GLU:N	9:1I:84:GLU:OE1	2.17	0.76
4:1D:148:LEU:HD22	4:1D:177:MET:HE2	1.68	0.75
6:1F:250:ASN:HB3	6:1F:272:MET:HE1	1.69	0.75
4:1D:183:ARG:HE	4:1D:207:LEU:HD23	1.51	0.75
7:1G:673:MET:HA	7:1G:673:MET:HE3	1.66	0.75
7:1G:512:GLU:HA	7:1G:515:ARG:HE	1.52	0.75
4:1D:109:VAL:HG21	4:1D:152:MET:HG2	1.67	0.75
7:1G:59:ILE:HG22	7:1G:62:ALA:HB2	1.67	0.75
18:1R:68:HIS:CD2	18:1R:87:CYS:SG	2.79	0.75
23:1X:110:VAL:O	23:1X:116:TRP:N	2.20	0.75
7:1G:488:LYS:NZ	7:1G:639:ALA:O	2.15	0.74
7:1G:534:ARG:HD2	7:1G:537:LEU:HD11	1.69	0.74
4:1D:269:LEU:HB2	4:1D:368:GLU:HB2	1.69	0.74
23:1X:34:GLN:N	23:1X:34:GLN:OE1	2.20	0.74
19:1S:17:GLU:HB2	19:1S:67:ARG:HB3	1.69	0.74
34:1i:52:ASP:HB2	34:1i:57:LYS:HE3	1.68	0.74
13:1M:114:GLU:HG3	13:1M:117:LEU:H	1.51	0.74
42:1q:133:LYS:HE2	42:1q:133:LYS:HA	1.69	0.74
7:1G:216:THR:O	7:1G:243:ARG:NH2	2.21	0.74
18:1R:59:CYS:SG	18:1R:84:CYS:HB2	2.28	0.74
11:1K:91:GLN:OE1	11:1K:91:GLN:N	2.20	0.73
8:1H:102:VAL:HG21	8:1H:154:LEU:HD21	1.70	0.73
7:1G:45:ARG:HH22	7:1G:261:GLU:HG2	1.53	0.73
12:1L:432:LEU:HD21	36:1k:65:ALA:HB2	1.71	0.73
16:1P:240:ASP:HA	16:1P:243:GLN:HE22	1.52	0.73
19:1S:57:CYS:SG	19:1S:58:SER:N	2.62	0.73
20:1U:32:VAL:HG22	20:1U:74:GLN:HB2	1.70	0.73
24:1Y:43:LYS:NZ	45:1Y:202:3PE:O31	2.22	0.73
29:1d:99:GLU:OE2	29:1d:99:GLU:N	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:38:GLU:OE1	8:1H:126:LYS:NZ	2.21	0.73
5:1E:87:TYR:HD1	6:1F:181:ALA:HB3	1.52	0.73
22:1W:54:ILE:HG12	22:1W:107:PHE:HE1	1.52	0.73
32:1g:66:PHE:HA	32:1g:70:LEU:HD12	1.70	0.73
43:1r:107:LYS:HE2	43:1r:107:LYS:H	1.53	0.73
4:1D:233:ARG:NH2	9:1I:23:GLN:O	2.21	0.73
3:1C:183:VAL:O	22:1W:101:THR:OG1	2.07	0.72
19:1S:88:ARG:NE	19:1S:88:ARG:O	2.23	0.72
6:1F:137:TYR:HD2	6:1F:192:LEU:HG	1.54	0.72
8:1H:63:PRO:HG2	8:1H:66:SER:HB3	1.70	0.72
17:1Q:90:GLU:OE1	17:1Q:90:GLU:N	2.23	0.72
2:1B:139:ILE:HG22	2:1B:140:VAL:HG13	1.70	0.72
9:1I:70:TYR:HE1	18:1R:87:CYS:HA	1.55	0.72
5:1E:78:MET:HE1	7:1G:185:THR:HA	1.71	0.72
29:1d:46:ASN:HB3	29:1d:51:ARG:HB2	1.72	0.72
22:1W:89:GLU:OE1	22:1W:89:GLU:N	2.22	0.72
14:1N:120:GLN:HE21	14:1N:177:LYS:HE2	1.52	0.72
1:1A:48:ARG:HH12	10:1J:80:PRO:HD3	1.55	0.71
1:1A:70:ALA:HB2	10:1J:59:ILE:HG21	1.72	0.71
6:1F:82:MET:HB3	6:1F:211:ALA:HB1	1.70	0.71
6:1F:139:ARG:NH2	6:1F:186:CYS:SG	2.63	0.71
16:1P:54:TYR:HA	16:1P:57:MET:HG2	1.72	0.71
25:1Z:90:ASN:ND2	25:1Z:123:GLU:O	2.23	0.71
1:1A:90:MET:HA	1:1A:90:MET:HE3	1.73	0.71
4:1D:424:VAL:HG23	4:1D:427:GLU:HB3	1.72	0.71
7:1G:118:ASP:OD2	17:1Q:46:GLN:NE2	2.22	0.71
21:1V:15:VAL:HA	21:1V:77:GLU:HG2	1.72	0.71
7:1G:38:PRO:HG2	7:1G:90:ARG:HD3	1.71	0.71
22:1W:42:GLU:N	22:1W:42:GLU:OE2	2.22	0.71
3:1C:93:VAL:HG22	3:1C:108:LYS:HG3	1.71	0.71
4:1D:393:ALA:HB3	4:1D:396:PHE:HB2	1.72	0.71
9:1I:138:GLU:OE1	9:1I:138:GLU:N	2.24	0.71
14:1N:265:MET:HA	14:1N:265:MET:HE3	1.72	0.71
43:1r:32:LYS:O	43:1r:35:GLN:NE2	2.24	0.71
13:1M:72:LEU:HA	13:1M:75:LEU:HD12	1.71	0.71
16:1P:46:ILE:HG22	16:1P:48:PRO:HD3	1.73	0.71
4:1D:19:MET:H	4:1D:19:MET:HE3	1.56	0.71
7:1G:285:ARG:NH1	7:1G:289:GLY:O	2.24	0.71
9:1I:98:PRO:HA	9:1I:104:ARG:HG2	1.72	0.71
12:1L:359:MET:N	12:1L:359:MET:SD	2.63	0.71
13:1M:30:HIS:HA	13:1M:33:LEU:HB2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:48:HIS:O	22:1W:51:GLN:NE2	2.24	0.70
4:1D:228:MET:HE2	4:1D:228:MET:HA	1.72	0.70
5:1E:96:GLY:HA2	5:1E:135:LYS:HG2	1.73	0.70
13:1M:46:GLY:HA2	32:1g:84:ARG:HA	1.73	0.70
16:1P:66:GLY:HA3	17:1Q:69:LEU:HD21	1.73	0.70
36:1k:38:ARG:HH21	36:1k:40:LEU:HB2	1.54	0.70
14:1N:45:MET:HE2	14:1N:45:MET:HA	1.73	0.70
11:1K:2:PRO:HD3	30:1e:72:MET:HE1	1.73	0.70
7:1G:329:VAL:HG23	7:1G:505:LEU:HD21	1.74	0.70
12:1L:387:THR:OG1	12:1L:461:SER:O	2.10	0.70
14:1N:95:MET:HE1	14:1N:145:ILE:HD12	1.73	0.70
17:1Q:27:GLU:N	17:1Q:27:GLU:OE2	2.24	0.70
20:1U:22:TYR:HE1	36:1k:43:PRO:HB2	1.57	0.70
29:1d:94:VAL:HG23	29:1d:95:LYS:HD3	1.72	0.70
12:1L:161:ARG:HG3	12:1L:164:ALA:H	1.56	0.70
7:1G:358:LEU:HA	19:1S:54:ILE:HD11	1.73	0.70
41:1p:162:MET:HA	41:1p:165:GLU:HB3	1.73	0.70
4:1D:410:MET:HE2	4:1D:410:MET:H	1.56	0.70
6:1F:255:LEU:HA	6:1F:269:GLU:HA	1.74	0.70
14:1N:194:LEU:HD23	14:1N:201:THR:HG21	1.72	0.70
7:1G:349:PHE:H	7:1G:509:PRO:HB2	1.56	0.69
9:1I:19:ASP:HB3	50:1I:204:PC1:H131	1.72	0.69
6:1F:91:LYS:HG3	6:1F:219:PRO:HB2	1.74	0.69
7:1G:704:CYS:HB2	9:1I:104:ARG:H	1.57	0.69
8:1H:31:MET:HG3	9:1I:37:THR:HB	1.74	0.69
12:1L:400:ASN:HD21	12:1L:486:MET:HB2	1.56	0.69
42:1q:60:ARG:HH12	42:1q:95:ASP:HA	1.55	0.69
3:1C:65:ARG:NH1	3:1C:123:VAL:O	2.24	0.69
14:1N:327:PRO:HA	29:1d:44:ILE:HD11	1.74	0.69
5:1E:149:VAL:HB	6:1F:257:ASN:HD21	1.56	0.69
7:1G:315:VAL:HG12	7:1G:521:VAL:HB	1.74	0.69
17:1Q:16:LYS:HE2	17:1Q:97:GLU:HB2	1.74	0.69
4:1D:152:MET:HA	4:1D:152:MET:HE2	1.75	0.69
12:1L:147:VAL:HG22	12:1L:252:MET:HE2	1.74	0.69
13:1M:1:FME:HG3	13:1M:2:LEU:HD22	1.74	0.69
36:1k:40:LEU:HD12	36:1k:41:ARG:H	1.55	0.69
14:1N:294:MET:HA	14:1N:294:MET:HE3	1.75	0.69
32:1g:85:MET:H	32:1g:85:MET:HE2	1.56	0.69
34:1i:107:ASP:OD2	40:1o:70:ARG:NH2	2.26	0.69
9:1I:108:ARG:NH2	17:1Q:70:MET:O	2.22	0.69
22:1W:62:LYS:HG2	22:1W:107:PHE:HE2	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:43:HIS:HB3	7:1G:46:LEU:HB3	1.73	0.68
12:1L:203:MET:HE2	12:1L:203:MET:HA	1.74	0.68
13:1M:307:TRP:NE1	38:1m:127:SER:OG	2.26	0.68
7:1G:588:THR:HG21	17:1Q:63:GLU:HA	1.75	0.68
12:1L:129:MET:O	12:1L:133:THR:OG1	2.09	0.68
16:1P:41:MET:HE3	16:1P:41:MET:H	1.58	0.68
16:1P:317:VAL:HG13	16:1P:318:LEU:HD22	1.75	0.68
21:1V:34:LEU:O	21:1V:44:ARG:NH2	2.25	0.68
1:1A:109:LYS:N	1:1A:109:LYS:HE2	2.08	0.68
14:1N:207:ILE:HG22	14:1N:211:MET:HE1	1.74	0.68
18:1R:19:ASP:O	18:1R:25:ARG:NH2	2.26	0.68
4:1D:418:ILE:HG23	4:1D:423:ILE:HD11	1.75	0.68
15:1O:150:GLU:OE2	15:1O:150:GLU:N	2.22	0.68
34:1i:112:THR:OG1	34:1i:114:GLU:OE1	2.11	0.68
6:1F:298:ILE:HB	6:1F:335:ILE:HB	1.76	0.68
13:1M:36:LEU:HD21	50:1f:101:PC1:H371	1.75	0.68
20:1T:52:MET:HA	20:1T:52:MET:HE2	1.75	0.68
43:1r:92:LYS:HE2	43:1r:92:LYS:HA	1.74	0.68
1:1A:1:FME:HE2	25:1Z:134:LEU:HD11	1.74	0.68
1:1A:33:LYS:O	2:1B:81:ARG:NH2	2.27	0.68
3:1C:39:GLN:HB3	3:1C:51:PHE:HB2	1.76	0.67
25:1Z:26:PRO:HD2	25:1Z:26:PRO:O	1.93	0.67
42:1q:9:ARG:HD3	51:1q:201:CDL:HA31	1.74	0.67
5:1E:39:PRO:HA	44:1s:65:GLN:HB3	1.76	0.67
7:1G:362:TYR:OH	19:1S:55:ARG:NH2	2.27	0.67
13:1M:231:LEU:HA	13:1M:235:LEU:HB2	1.76	0.67
14:1N:284:MET:HG3	57:1Y:201:PGT:H242	1.76	0.67
2:1B:54:CYS:HB3	4:1D:108:TYR:HB2	1.76	0.67
5:1E:209:PRO:HA	6:1F:40:GLY:HA2	1.75	0.67
8:1H:25:ARG:NH2	8:1H:51:ASP:OD2	2.28	0.67
39:1n:34:ASP:OD1	39:1n:35:LYS:N	2.28	0.67
5:1E:164:LEU:HD11	5:1E:169:ILE:HG12	1.77	0.67
7:1G:181:MET:HA	7:1G:181:MET:HE3	1.77	0.67
16:1P:270:PHE:HD2	16:1P:278:TRP:HB2	1.60	0.67
21:1V:57:MET:O	21:1V:61:GLU:N	2.27	0.67
42:1q:122:GLN:OE1	42:1q:122:GLN:N	2.20	0.67
6:1F:258:ILE:HA	6:1F:334:VAL:HG22	1.77	0.67
7:1G:164:SER:OG	7:1G:165:GLU:OE1	2.13	0.67
4:1D:407:LYS:HE2	4:1D:407:LYS:HA	1.77	0.67
6:1F:224:ASN:ND2	48:1F:501:FMN:O2	2.28	0.67
22:1W:24:ASP:OD1	22:1W:25:MET:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:20:ARG:NE	6:1F:269:GLU:O	2.28	0.67
6:1F:302:SER:HB3	6:1F:350:LEU:HD21	1.76	0.67
17:1Q:10:LEU:HD21	22:1W:16:SER:HB2	1.77	0.67
21:1V:19:PRO:HG2	21:1V:64:VAL:HG11	1.76	0.67
8:1H:209:SER:HB3	8:1H:213:VAL:HA	1.77	0.66
12:1L:324:LEU:HB3	12:1L:395:ILE:HD11	1.78	0.66
26:1a:17:PHE:CE2	26:1a:21:MET:HE2	2.30	0.66
30:1e:31:ARG:HH22	30:1e:68:ARG:HE	1.43	0.66
39:1n:61:GLN:HA	39:1n:64:ARG:HG2	1.77	0.66
13:1M:361:MET:O	13:1M:365:THR:OG1	2.12	0.66
7:1G:10:GLU:HB3	7:1G:75:LYS:HE2	1.78	0.66
25:1Z:97:ILE:HG23	25:1Z:98:MET:HE3	1.78	0.66
12:1L:560:THR:HA	12:1L:564:LYS:HB2	1.77	0.66
7:1G:194:GLU:HG2	7:1G:195:LEU:HD22	1.77	0.66
32:1g:113:PHE:H	41:1p:158:GLN:HE22	1.43	0.66
35:1j:36:ILE:HG23	35:1j:37:LEU:HD12	1.78	0.66
1:1A:32:GLU:OE1	1:1A:32:GLU:N	2.29	0.66
8:1H:184:MET:HA	8:1H:184:MET:HE3	1.77	0.66
11:1K:42:ILE:O	11:1K:45:THR:OG1	2.12	0.66
13:1M:222:GLU:OE1	13:1M:222:GLU:N	2.28	0.66
20:1T:47:GLN:NE2	20:1T:67:ALA:O	2.27	0.66
6:1F:378:ARG:HB3	6:1F:383:ASP:HB3	1.77	0.66
13:1M:98:MET:HE1	45:1N:401:3PE:H3D1	1.77	0.66
6:1F:255:LEU:HG	6:1F:269:GLU:HG3	1.77	0.66
7:1G:66:VAL:HB	7:1G:71:MET:HG3	1.78	0.66
8:1H:149:ILE:HG21	8:1H:185:TRP:HB2	1.78	0.66
9:1I:156:ASN:OD1	18:1R:36:ASN:ND2	2.29	0.66
4:1D:107:ASP:HB3	4:1D:114:ASN:HD21	1.61	0.65
10:1J:127:ILE:HG21	11:1K:2:PRO:HG3	1.78	0.65
5:1E:86:PHE:O	7:1G:177:ARG:NH2	2.29	0.65
7:1G:504:ASP:OD1	19:1S:55:ARG:NH2	2.29	0.65
12:1L:90:ILE:H	12:1L:90:ILE:HD12	1.61	0.65
14:1N:339:MET:HE2	14:1N:339:MET:HA	1.79	0.65
16:1P:312:LEU:HG	16:1P:313:LYS:HD2	1.78	0.65
19:1S:24:GLN:HB3	19:1S:25:ARG:HH11	1.60	0.65
20:1T:29:LYS:HD2	20:1T:40:LEU:HA	1.77	0.65
8:1H:206:GLU:HG2	8:1H:207:LEU:HD23	1.78	0.65
16:1P:292:MET:HE2	16:1P:292:MET:H	1.61	0.65
42:1q:53:LYS:HE2	42:1q:53:LYS:HA	1.78	0.65
12:1L:97:THR:HG21	12:1L:125:LEU:HD11	1.77	0.65
13:1M:11:LEU:HD22	13:1M:100:ILE:HG21	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:191:SER:HB2	57:1Y:201:PGT:H31	1.78	0.65
14:1N:308:THR:HG22	14:1N:310:ASN:H	1.61	0.65
23:1X:36:ASP:OD1	23:1X:37:LYS:N	2.29	0.65
19:1S:78:LEU:HB2	19:1S:81:PHE:HD2	1.60	0.65
1:1A:33:LYS:HA	2:1B:106:GLN:HA	1.77	0.65
20:1T:12:LYS:HE2	20:1T:32:VAL:HG23	1.78	0.65
20:1T:20:LYS:HD3	20:1T:27:PRO:HB3	1.79	0.65
35:1j:26:GLU:O	35:1j:30:ALA:N	2.24	0.65
4:1D:55:HIS:HE2	8:1H:127:TYR:HH	1.43	0.65
7:1G:254:MET:HA	7:1G:254:MET:HE2	1.79	0.65
8:1H:186:PHE:O	8:1H:189:THR:OG1	2.14	0.65
10:1J:71:THR:HG21	11:1K:75:LEU:HD12	1.76	0.65
21:1V:22:ARG:HD2	21:1V:25:ILE:HD11	1.79	0.65
23:1X:18:LYS:HA	26:1a:54:ILE:HD11	1.79	0.65
2:1B:102:LYS:O	2:1B:106:GLN:NE2	2.30	0.65
7:1G:37:ILE:HD12	7:1G:38:PRO:HD2	1.79	0.65
11:1K:73:LEU:HD11	14:1N:38:LEU:HA	1.78	0.65
12:1L:156:GLY:O	13:1M:416:ARG:NH2	2.29	0.65
2:1B:69:MET:HB2	2:1B:74:VAL:HG22	1.79	0.65
5:1E:86:PHE:HD1	6:1F:200:GLN:HB2	1.61	0.65
7:1G:366:THR:H	7:1G:491:ASN:HD21	1.44	0.65
8:1H:293:PHE:O	8:1H:297:THR:OG1	2.14	0.65
23:1X:170:THR:OG1	23:1X:171:MET:SD	2.51	0.65
3:1C:180:VAL:HG21	3:1C:182:ARG:HH21	1.61	0.64
7:1G:385:ARG:HG3	7:1G:415:LEU:HA	1.79	0.64
8:1H:143:GLU:OE2	8:1H:143:GLU:N	2.24	0.64
9:1I:31:VAL:HG21	50:1I:204:PC1:H241	1.79	0.64
12:1L:150:MET:HA	12:1L:150:MET:HE3	1.78	0.64
20:1U:34:SER:HB2	20:1U:40:LEU:HD21	1.79	0.64
7:1G:121:MET:HE2	7:1G:121:MET:HA	1.79	0.64
11:1K:94:ASN:HD22	12:1L:583:LEU:HD11	1.62	0.64
14:1N:95:MET:HE2	14:1N:95:MET:HA	1.79	0.64
21:1V:57:MET:N	21:1V:57:MET:SD	2.70	0.64
24:1Y:43:LYS:NZ	45:1Y:202:3PE:O11	2.29	0.64
40:1o:38:MET:HE3	40:1o:39:VAL:H	1.61	0.64
12:1L:213:LEU:HB3	12:1L:273:VAL:HG11	1.79	0.64
16:1P:81:ILE:H	16:1P:81:ILE:HD12	1.62	0.64
32:1g:100:ARG:HG2	32:1g:107:LEU:HA	1.79	0.64
44:1s:72:SER:OG	44:1s:75:HIS:ND1	2.23	0.64
4:1D:414:VAL:HA	4:1D:417:ILE:HD12	1.79	0.64
10:1J:122:LEU:HD12	30:1e:72:MET:HG2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:2:HIS:HB3	16:1P:5:LEU:HD23	1.79	0.64
17:1Q:124:TRP:HZ3	44:1s:68:SER:HA	1.62	0.64
1:1A:34:THR:OG1	8:1H:62:ARG:O	2.14	0.64
4:1D:259:MET:HA	4:1D:259:MET:HE3	1.78	0.64
12:1L:61:MET:HA	12:1L:61:MET:HE3	1.79	0.64
37:1l:141:GLU:HA	41:1p:122:GLN:HG2	1.79	0.64
2:1B:89:ALA:HA	2:1B:116:MET:HB3	1.79	0.64
8:1H:85:MET:HB3	8:1H:233:MET:HG3	1.78	0.64
12:1L:216:LEU:HD22	12:1L:259:LEU:HD11	1.80	0.64
13:1M:219:ALA:HB1	13:1M:231:LEU:HD11	1.79	0.64
20:1U:37:MET:H	20:1U:37:MET:CE	2.10	0.64
21:1V:112:LYS:O	21:1V:112:LYS:HD3	1.98	0.64
42:1q:106:ARG:HB2	42:1q:109:ILE:HG13	1.80	0.64
9:1I:65:HIS:HA	9:1I:133:GLU:HA	1.78	0.64
7:1G:572:THR:OG1	7:1G:620:ARG:NH2	2.30	0.64
19:1S:64:LEU:HB3	19:1S:76:VAL:H	1.63	0.64
6:1F:428:GLU:OE1	6:1F:432:GLN:NE2	2.31	0.64
38:1m:94:ILE:HD11	38:1m:98:PHE:HD2	1.63	0.64
39:1n:150:THR:HG22	39:1n:152:ALA:H	1.63	0.64
1:1A:109:LYS:HE2	1:1A:109:LYS:H	1.62	0.63
3:1C:50:ILE:HB	3:1C:107:VAL:HG12	1.79	0.63
6:1F:29:HIS:HA	44:1s:39:ARG:HE	1.62	0.63
7:1G:94:MET:HE1	7:1G:119:GLN:HB3	1.79	0.63
8:1H:170:GLU:OE1	23:1X:97:ARG:NH2	2.30	0.63
12:1L:401:MET:HE1	37:1l:126:GLN:HG2	1.79	0.63
13:1M:270:ILE:O	13:1M:274:SER:OG	2.16	0.63
20:1U:47:GLN:NE2	20:1U:71:MET:SD	2.71	0.63
1:1A:98:LEU:HD12	8:1H:298:LEU:HD11	1.81	0.63
4:1D:149:ASN:HD21	4:1D:371:LYS:HE2	1.63	0.63
4:1D:390:LYS:HD2	4:1D:430:ARG:HH22	1.63	0.63
16:1P:113:ILE:HD12	16:1P:114:PRO:CD	2.28	0.63
25:1Z:108:GLU:HB2	30:1e:74:ARG:HH12	1.63	0.63
37:1l:115:MET:HA	37:1l:118:VAL:HG13	1.79	0.63
9:1I:7:MET:HA	9:1I:7:MET:HE3	1.80	0.63
16:1P:115:HIS:HB2	16:1P:155:GLU:HG3	1.79	0.63
22:1W:68:MET:HA	22:1W:68:MET:HE3	1.79	0.63
39:1n:145:PRO:O	39:1n:149:ARG:NH2	2.31	0.63
5:1E:111:ARG:HH12	6:1F:265:PRO:HG3	1.63	0.63
12:1L:503:GLU:O	12:1L:507:THR:OG1	2.16	0.63
4:1D:241:ASP:OD2	4:1D:290:ARG:NH2	2.32	0.63
7:1G:688:VAL:O	7:1G:692:THR:OG1	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:17:MET:HG2	31:1f:11:TRP:HZ2	1.64	0.63
13:1M:418:LYS:HD3	39:1n:94:GLU:OE2	1.98	0.63
23:1X:46:ARG:NH1	25:1Z:76:GLN:OE1	2.32	0.63
7:1G:41:CYS:HB3	7:1G:52:CYS:HB3	1.80	0.63
31:1f:38:ARG:HD3	31:1f:54:VAL:HG13	1.80	0.63
2:1B:125:TYR:HB2	9:1I:117:ILE:HG21	1.81	0.63
4:1D:221:ARG:HA	4:1D:224:GLU:HG2	1.81	0.63
12:1L:108:MET:HB3	12:1L:114:ILE:HD11	1.80	0.63
42:1q:14:VAL:HA	42:1q:23:TYR:HD2	1.64	0.63
5:1E:101:GLN:HB2	5:1E:155:GLN:HB3	1.81	0.63
15:1O:13:ARG:HB2	15:1O:16:ARG:HD3	1.81	0.63
18:1R:59:CYS:O	18:1R:68:HIS:NE2	2.31	0.63
37:1l:129:GLY:O	40:1o:97:ARG:NH2	2.32	0.63
4:1D:326:ASP:OD1	7:1G:127:ARG:NH2	2.32	0.63
6:1F:59:GLU:HG2	6:1F:235:CYS:HA	1.80	0.63
13:1M:294:MET:HA	13:1M:294:MET:HE3	1.80	0.63
25:1Z:127:LEU:HD13	30:1e:97:HIS:CE1	2.34	0.63
40:1o:67:LYS:O	40:1o:67:LYS:NZ	2.29	0.63
4:1D:55:HIS:HE1	8:1H:206:GLU:HA	1.64	0.62
6:1F:112:ARG:O	6:1F:148:ASN:ND2	2.28	0.62
12:1L:102:GLU:HA	12:1L:105:MET:HE3	1.79	0.62
12:1L:550:SER:HB3	13:1M:275:ILE:HG23	1.80	0.62
13:1M:278:ARG:HB3	13:1M:278:ARG:HH11	1.62	0.62
14:1N:314:LYS:HZ2	15:1O:271:ASN:HA	1.63	0.62
21:1V:34:LEU:HD11	21:1V:44:ARG:HA	1.81	0.62
23:1X:22:SER:HB3	23:1X:88:ILE:HG22	1.81	0.62
33:1h:30:LEU:HD12	33:1h:34:ILE:HG23	1.81	0.62
37:1l:25:LYS:HE2	37:1l:25:LYS:N	2.14	0.62
39:1n:67:GLU:OE2	39:1n:67:GLU:N	2.26	0.62
12:1L:314:MET:HA	12:1L:317:ILE:HG22	1.81	0.62
20:1T:37:MET:HE3	20:1T:37:MET:H	1.62	0.62
7:1G:185:THR:HG21	7:1G:189:LYS:HB2	1.81	0.62
15:1O:147:GLN:NE2	15:1O:281:GLU:OE2	2.33	0.62
20:1T:43:ASP:H	20:1T:46:ASP:HB2	1.64	0.62
27:1b:62:MET:SD	27:1b:62:MET:N	2.72	0.62
1:1A:73:LEU:O	8:1H:160:TYR:OH	2.15	0.62
6:1F:218:CYS:HB3	17:1Q:124:TRP:CD1	2.34	0.62
15:1O:168:VAL:HG13	15:1O:219:GLU:HB2	1.80	0.62
17:1Q:90:GLU:HA	17:1Q:93:VAL:HG22	1.80	0.62
27:1b:12:TRP:HD1	27:1b:19:VAL:HG11	1.64	0.62
39:1n:83:GLU:CD	39:1n:83:GLU:H	2.07	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:102:GLU:HA	40:1o:105:ARG:HB3	1.80	0.62
5:1E:108:CYS:SG	5:1E:152:PRO:HA	2.40	0.62
6:1F:76:GLY:O	6:1F:80:SER:OG	2.18	0.62
7:1G:64:LYS:HZ2	7:1G:66:VAL:HA	1.64	0.62
23:1X:56:LEU:HD21	25:1Z:84:LEU:HD21	1.82	0.62
10:1J:12:ILE:H	10:1J:12:ILE:HD12	1.65	0.62
13:1M:203:PHE:HB2	13:1M:243:MET:HE2	1.80	0.62
14:1N:88:LYS:HG2	14:1N:148:SER:HB2	1.80	0.62
25:1Z:127:LEU:HD13	30:1e:97:HIS:HE1	1.64	0.62
35:1j:26:GLU:N	35:1j:26:GLU:OE2	2.32	0.62
3:1C:35:LYS:HE3	21:1V:98:PRO:HA	1.80	0.62
25:1Z:23:ARG:HH21	43:1r:112:LEU:HD11	1.65	0.62
19:1S:42:GLU:OE1	19:1S:42:GLU:N	2.32	0.62
26:1a:2:TRP:CZ2	43:1r:7:ILE:HG21	2.25	0.62
4:1D:193:TYR:HE1	4:1D:201:GLN:H	1.46	0.61
4:1D:398:HIS:O	4:1D:421:GLN:NE2	2.33	0.61
7:1G:364:LEU:HB2	7:1G:577:GLU:HA	1.80	0.61
12:1L:62:ILE:HD12	41:1p:114:GLN:HB2	1.81	0.61
16:1P:322:ARG:NH1	16:1P:329:SER:O	2.33	0.61
22:1W:34:GLU:HA	22:1W:37:ARG:HG3	1.82	0.61
38:1m:52:ASP:HB3	38:1m:55:ARG:HB2	1.81	0.61
41:1p:10:PRO:HD2	41:1p:108:ARG:HD2	1.81	0.61
19:1S:61:GLN:HE22	19:1S:63:LYS:HG3	1.64	0.61
25:1Z:99:LYS:N	25:1Z:99:LYS:HD2	2.15	0.61
2:1B:48:MET:HE3	2:1B:78:ALA:HA	1.81	0.61
7:1G:453:LEU:HD11	7:1G:458:LEU:HG	1.81	0.61
13:1M:396:MET:HE2	13:1M:396:MET:HA	1.82	0.61
4:1D:151:ILE:O	4:1D:155:THR:OG1	2.14	0.61
6:1F:299:PRO:HD3	6:1F:306:LEU:HA	1.81	0.61
13:1M:204:MET:SD	13:1M:243:MET:HE1	2.40	0.61
15:1O:164:LEU:HB2	15:1O:248:TRP:CZ3	2.36	0.61
34:1i:26:GLU:OE2	34:1i:26:GLU:N	2.31	0.61
3:1C:82:ASP:O	4:1D:387:TYR:OH	2.19	0.61
9:1I:65:HIS:HD2	9:1I:111:ILE:HG21	1.65	0.61
16:1P:283:LYS:HA	16:1P:286:ARG:HB2	1.82	0.61
23:1X:129:LYS:NZ	27:1b:65:VAL:O	2.30	0.61
1:1A:1:FME:N	1:1A:4:MET:HE1	2.15	0.61
4:1D:425:PHE:HA	4:1D:428:VAL:HG12	1.81	0.61
6:1F:351:ILE:HD11	6:1F:372:MET:HB3	1.83	0.61
7:1G:249:ARG:HD2	7:1G:251:LEU:HD21	1.81	0.61
7:1G:665:GLN:NE2	7:1G:670:ASP:O	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:59:ARG:HD3	27:1b:81:LYS:HA	1.83	0.61
5:1E:52:ASP:OD2	5:1E:56:ARG:NH2	2.33	0.61
6:1F:56:ILE:H	6:1F:56:ILE:HD12	1.65	0.61
7:1G:359:ARG:NH2	7:1G:629:ASN:OD1	2.34	0.61
57:1Y:201:PGT:O4P	57:1Y:201:PGT:O6	2.16	0.61
4:1D:261:ARG:NH1	4:1D:268:ASP:OD2	2.33	0.61
10:1J:146:LEU:HA	11:1K:58:MET:HE1	1.82	0.61
12:1L:434:LYS:HZ1	36:1k:52:TYR:HA	1.66	0.61
16:1P:57:MET:HA	16:1P:57:MET:HE3	1.82	0.61
16:1P:319:ARG:NH2	22:1W:53:ASP:OD1	2.34	0.61
20:1T:37:MET:SD	20:1T:38:LYS:NZ	2.74	0.61
35:1j:54:PRO:HB2	35:1j:59:TRP:HZ2	1.64	0.61
12:1L:309:GLN:O	12:1L:313:MET:HG2	2.01	0.61
12:1L:401:MET:HA	12:1L:401:MET:HE3	1.83	0.61
22:1W:47:VAL:HA	22:1W:52:LEU:HD23	1.82	0.61
4:1D:55:HIS:NE2	8:1H:127:TYR:OH	2.30	0.61
4:1D:107:ASP:H	4:1D:114:ASN:HD21	1.48	0.61
16:1P:235:ARG:NH2	16:1P:291:ASP:OD1	2.34	0.61
32:1g:94:GLU:OE2	41:1p:9:TYR:OH	2.13	0.61
1:1A:38:GLU:HG3	1:1A:43:PRO:HG3	1.83	0.60
5:1E:174:ASP:HA	5:1E:177:LYS:HE3	1.82	0.60
6:1F:150:GLN:HE22	6:1F:177:VAL:HG11	1.66	0.60
7:1G:534:ARG:HA	7:1G:537:LEU:HD21	1.82	0.60
10:1J:4:TYR:HB2	10:1J:7:PHE:HB2	1.82	0.60
22:1W:34:GLU:N	22:1W:34:GLU:OE2	2.33	0.60
35:1j:69:ASP:OD1	40:1o:117:ARG:NH1	2.34	0.60
37:1l:60:PRO:HG3	37:1l:70:ARG:HH12	1.65	0.60
4:1D:58:ALA:HB1	4:1D:62:LEU:HB3	1.83	0.60
7:1G:609:MET:SD	7:1G:609:MET:N	2.69	0.60
20:1U:28:GLU:OE1	20:1U:28:GLU:N	2.34	0.60
29:1d:106:LYS:HA	29:1d:106:LYS:HE3	1.83	0.60
35:1j:64:LEU:HD21	40:1o:102:GLU:HG3	1.83	0.60
6:1F:54:ASP:N	6:1F:54:ASP:OD1	2.34	0.60
6:1F:93:LEU:HD22	6:1F:94:VAL:H	1.66	0.60
45:1L:701:3PE:H231	37:1l:88:ARG:HG2	1.83	0.60
14:1N:44:LEU:HB3	14:1N:122:ILE:HG21	1.83	0.60
15:1O:189:PRO:HA	15:1O:192:MET:HG2	1.84	0.60
20:1T:51:ILE:O	20:1T:54:MET:HE3	2.01	0.60
23:1X:46:ARG:NH2	33:1h:142:ASP:OD1	2.33	0.60
25:1Z:48:TRP:O	25:1Z:52:LYS:NZ	2.27	0.60
26:1a:64:LYS:HD2	26:1a:68:ASN:HD21	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:45:PHE:HA	34:1i:48:LYS:HZ3	1.67	0.60
5:1E:30:ARG:HA	44:1s:56:VAL:HG12	1.83	0.60
9:1I:68:ARG:HD2	9:1I:165:ILE:HD13	1.82	0.60
39:1n:67:GLU:HA	39:1n:70:PHE:HB3	1.82	0.60
5:1E:162:GLU:OE2	6:1F:108:ARG:NH2	2.34	0.60
13:1M:359:TRP:O	13:1M:363:SER:OG	2.19	0.60
17:1Q:55:TRP:HB2	17:1Q:86:PHE:HB2	1.84	0.60
26:1a:3:PHE:HE1	51:1q:201:CDL:HA21	1.66	0.60
4:1D:107:ASP:H	4:1D:114:ASN:ND2	2.00	0.60
4:1D:339:LYS:HB3	18:1R:69:PRO:HA	1.83	0.60
12:1L:94:LEU:HA	12:1L:97:THR:HG22	1.84	0.60
14:1N:237:MET:O	14:1N:237:MET:HG2	2.02	0.60
16:1P:200:THR:O	16:1P:238:LEU:N	2.32	0.60
1:1A:54:LYS:NZ	1:1A:115:GLU:O	2.32	0.60
3:1C:22:LEU:HD12	3:1C:48:LEU:HB2	1.84	0.60
3:1C:94:TYR:HB2	3:1C:107:VAL:HG22	1.83	0.60
8:1H:90:PRO:HG3	8:1H:240:ILE:HG12	1.83	0.60
19:1S:87:THR:HA	19:1S:90:LEU:HG	1.83	0.60
21:1V:91:ARG:NH2	21:1V:92:LYS:HA	2.16	0.60
34:1i:10:ARG:HB2	39:1n:155:PRO:HB3	1.84	0.60
39:1n:64:ARG:NH1	39:1n:64:ARG:HA	2.17	0.60
3:1C:53:HIS:NE2	17:1Q:6:GLN:OE1	2.32	0.60
5:1E:24:THR:N	5:1E:27:ASN:OD1	2.35	0.60
7:1G:451:VAL:HG12	7:1G:489:VAL:HG12	1.82	0.60
16:1P:19:ILE:HD12	16:1P:218:ILE:HG21	1.83	0.60
22:1W:44:PRO:HD3	22:1W:60:ARG:HH21	1.66	0.60
22:1W:62:LYS:HZ2	22:1W:107:PHE:HD2	1.48	0.60
45:1A:201:3PE:H292	8:1H:295:PRO:HB3	1.82	0.60
3:1C:155:TYR:HE2	22:1W:97:TRP:HB3	1.67	0.60
6:1F:297:VAL:HG22	6:1F:336:VAL:HA	1.83	0.60
50:1I:204:PC1:H121	25:1Z:35:MET:HE1	1.83	0.60
11:1K:40:LEU:HD22	14:1N:71:MET:HG3	1.82	0.60
12:1L:295:GLN:O	12:1L:425:ARG:NH1	2.35	0.60
16:1P:160:PHE:HB3	16:1P:163:ALA:HB2	1.83	0.60
20:1T:31:SER:N	20:1T:34:SER:OG	2.31	0.60
33:1h:64:TRP:CE2	33:1h:77:ARG:HD3	2.36	0.60
4:1D:256:SER:HB2	4:1D:373:GLU:HB3	1.83	0.60
5:1E:60:TRP:CD1	5:1E:62:PRO:HD3	2.37	0.60
12:1L:61:MET:HB2	12:1L:82:MET:HB2	1.82	0.60
13:1M:190:TRP:HA	13:1M:193:ILE:HD13	1.82	0.60
18:1R:60:ASP:OD2	18:1R:62:GLY:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:1g:112:CYS:SG	32:1g:113:PHE:N	2.75	0.60
3:1C:210:ARG:NH2	7:1G:34:GLY:O	2.35	0.59
17:1Q:124:TRP:O	44:1s:68:SER:OG	2.19	0.59
20:1T:66:ASP:O	20:1T:69:LYS:HG3	2.02	0.59
7:1G:379:LEU:HB2	7:1G:408:LEU:HD23	1.84	0.59
7:1G:675:ASP:OD1	7:1G:676:SER:N	2.34	0.59
12:1L:82:MET:HE1	12:1L:133:THR:HB	1.83	0.59
16:1P:30:LEU:HD11	16:1P:94:LEU:HD22	1.84	0.59
17:1Q:57:MET:HE2	17:1Q:57:MET:HA	1.84	0.59
17:1Q:66:GLU:N	17:1Q:66:GLU:OE2	2.36	0.59
20:1T:51:ILE:HA	20:1T:54:MET:HG3	1.84	0.59
4:1D:19:MET:H	4:1D:19:MET:CE	2.15	0.59
4:1D:88:GLU:OE2	4:1D:430:ARG:NH2	2.32	0.59
7:1G:107:ILE:HG22	9:1I:78:ILE:HD13	1.84	0.59
7:1G:114:CYS:HB3	7:1G:117:GLN:HG3	1.84	0.59
15:1O:312:VAL:HG11	28:1c:2:PHE:HB2	1.84	0.59
16:1P:157:ARG:NH1	16:1P:163:ALA:O	2.34	0.59
23:1X:52:PRO:HB3	25:1Z:80:ASP:OD1	2.02	0.59
26:1a:32:GLY:O	26:1a:34:LYS:NZ	2.35	0.59
32:1g:61:VAL:HG13	32:1g:62:PHE:HD1	1.66	0.59
5:1E:192:SER:OG	6:1F:26:TYR:O	2.21	0.59
12:1L:173:LEU:HD12	13:1M:405:LEU:HD11	1.83	0.59
14:1N:272:LYS:HG2	33:1h:108:LEU:HD11	1.85	0.59
22:1W:22:SER:OG	22:1W:31:ARG:NH2	2.35	0.59
23:1X:12:LEU:HD13	25:1Z:85:GLN:HB2	1.84	0.59
34:1i:54:ALA:HB3	34:1i:57:LYS:NZ	2.17	0.59
35:1j:69:ASP:OD2	40:1o:113:ARG:NH1	2.36	0.59
38:1m:51:ASN:HD22	39:1n:165:LEU:HD22	1.67	0.59
38:1m:51:ASN:O	39:1n:128:ARG:NH2	2.35	0.59
12:1L:501:ALA:O	12:1L:505:ASN:ND2	2.33	0.59
13:1M:107:ILE:O	13:1M:111:THR:OG1	2.19	0.59
3:1C:175:ARG:NH2	3:1C:186:GLU:OE1	2.34	0.59
4:1D:231:ASN:HD21	25:1Z:25:LEU:HD11	1.68	0.59
15:1O:97:GLN:OE1	52:1O:401:GTP:N2	2.33	0.59
16:1P:245:ILE:HA	16:1P:248:VAL:HG12	1.83	0.59
27:1b:64:ASP:OD1	27:1b:65:VAL:N	2.35	0.59
3:1C:86:ARG:NH1	3:1C:91:GLU:OE1	2.36	0.59
4:1D:246:THR:HB	21:1V:12:GLY:HA3	1.83	0.59
5:1E:123:LYS:NZ	5:1E:170:GLU:O	2.36	0.59
9:1I:43:ARG:HG2	43:1r:11:ARG:HE	1.67	0.59
14:1N:230:LEU:HD11	14:1N:244:MET:HE1	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:207:LYS:HA	15:1O:211:LEU:HD12	1.85	0.59
15:1O:223:TYR:HB3	15:1O:227:GLU:HB2	1.85	0.59
18:1R:93:GLN:HB3	18:1R:96:HIS:HA	1.85	0.59
21:1V:37:ILE:HG13	21:1V:38:PRO:HD2	1.84	0.59
33:1h:55:ILE:HD12	33:1h:56:PRO:HD2	1.83	0.59
37:1l:98:TRP:HA	37:1l:101:MET:HB2	1.85	0.59
1:1A:99:ALA:HB1	45:1A:201:3PE:H2B2	1.83	0.59
12:1L:63:ILE:HG22	34:1i:96:VAL:HG13	1.82	0.59
36:1k:35:LEU:HD12	36:1k:40:LEU:HB3	1.85	0.59
4:1D:303:GLU:O	4:1D:307:SER:OG	2.20	0.59
5:1E:148:CYS:N	6:1F:105:CYS:SG	2.75	0.59
6:1F:99:GLU:HG2	6:1F:104:THR:HB	1.83	0.59
6:1F:189:GLU:HG3	6:1F:222:VAL:HG21	1.85	0.59
13:1M:6:ILE:H	13:1M:6:ILE:HD12	1.68	0.59
13:1M:237:LYS:NZ	13:1M:316:MET:O	2.35	0.59
23:1X:21:SER:HB2	26:1a:47:LEU:HD12	1.83	0.59
39:1n:83:GLU:OE1	39:1n:83:GLU:N	2.33	0.59
1:1A:3:ILE:O	1:1A:6:THR:OG1	2.19	0.59
2:1B:165:ARG:NH1	42:1q:77:VAL:O	2.36	0.59
13:1M:93:LYS:O	13:1M:97:THR:OG1	2.20	0.59
14:1N:49:ASN:OD1	14:1N:52:ALA:N	2.34	0.59
15:1O:28:ASP:OD1	15:1O:29:GLY:N	2.35	0.59
15:1O:265:ASN:HD22	15:1O:268:GLU:H	1.50	0.59
29:1d:2:MET:HE2	29:1d:2:MET:N	2.18	0.59
42:1q:95:ASP:OD2	43:1r:33:ARG:N	2.36	0.59
10:1J:157:THR:HG21	11:1K:62:ILE:HD12	1.84	0.58
12:1L:4:PHE:HB2	12:1L:53:MET:HE3	1.85	0.58
12:1L:42:TYR:OH	34:1i:66:HIS:ND1	2.34	0.58
13:1M:84:LEU:O	13:1M:92:LYS:NZ	2.27	0.58
16:1P:197:GLY:HA2	16:1P:288:HIS:HE1	1.68	0.58
31:1f:3:VAL:HA	31:1f:6:ILE:HG13	1.84	0.58
37:1l:14:PRO:HB3	37:1l:19:GLU:HG2	1.84	0.58
42:1q:6:VAL:HG12	51:1q:201:CDL:HA61	1.85	0.58
3:1C:33:LEU:HA	21:1V:98:PRO:HB2	1.84	0.58
6:1F:294:LEU:HA	6:1F:338:ASP:HA	1.86	0.58
7:1G:318:ILE:HG12	7:1G:522:LEU:HD11	1.84	0.58
7:1G:666:LEU:HD12	7:1G:667:THR:HG22	1.85	0.58
10:1J:121:GLY:HA2	11:1K:3:LEU:HB2	1.85	0.58
12:1L:315:VAL:HG12	12:1L:399:VAL:HG11	1.84	0.58
12:1L:341:MET:O	12:1L:345:SER:OG	2.20	0.58
14:1N:1:FME:HE3	14:1N:46:LYS:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:24:GLN:HB3	19:1S:25:ARG:NH1	2.18	0.58
35:1j:28:PHE:HA	35:1j:31:THR:HG22	1.84	0.58
37:1l:5:THR:OG1	37:1l:6:LYS:N	2.35	0.58
9:1I:151:LYS:HD2	9:1I:155:LEU:HD23	1.85	0.58
9:1I:172:ASP:OD2	9:1I:176:ARG:NH2	2.35	0.58
13:1M:277:LEU:HD21	13:1M:405:LEU:HB3	1.85	0.58
16:1P:200:THR:HB	16:1P:238:LEU:HB2	1.83	0.58
25:1Z:58:ARG:NH2	27:1b:48:THR:OG1	2.36	0.58
41:1p:116:GLU:OE2	41:1p:123:ASN:ND2	2.37	0.58
4:1D:246:THR:HA	21:1V:11:VAL:HG13	1.86	0.58
10:1J:38:GLY:HA2	10:1J:57:PHE:HE1	1.67	0.58
12:1L:121:LEU:HD22	12:1L:246:LEU:HD23	1.86	0.58
12:1L:129:MET:N	12:1L:129:MET:SD	2.77	0.58
22:1W:91:GLU:HA	22:1W:94:ILE:HG12	1.85	0.58
36:1k:40:LEU:HD12	36:1k:41:ARG:N	2.18	0.58
44:1s:71:GLN:HE22	44:1s:75:HIS:CE1	2.21	0.58
6:1F:375:VAL:HA	6:1F:378:ARG:HD3	1.83	0.58
8:1H:181:LEU:HA	8:1H:184:MET:HB2	1.85	0.58
12:1L:111:ASP:OD2	39:1n:96:TYR:OH	2.21	0.58
12:1L:362:LEU:HD12	12:1L:366:MET:HE2	1.85	0.58
14:1N:97:MET:HA	14:1N:97:MET:HE2	1.85	0.58
16:1P:238:LEU:HD21	16:1P:287:VAL:HG12	1.86	0.58
40:1o:47:ASP:OD1	40:1o:47:ASP:N	2.35	0.58
3:1C:118:GLU:HA	3:1C:143:ALA:HB3	1.86	0.58
3:1C:189:GLU:OE1	16:1P:14:SER:N	2.35	0.58
4:1D:290:ARG:N	4:1D:295:ASP:OD2	2.37	0.58
7:1G:550:GLY:HA2	7:1G:554:ALA:HB3	1.84	0.58
11:1K:59:MET:HG3	11:1K:60:PRO:HD3	1.85	0.58
12:1L:206:ASN:OD1	12:1L:206:ASN:N	2.36	0.58
13:1M:269:MET:O	13:1M:273:SER:OG	2.22	0.58
38:1m:1:SER:OG	38:1m:4:LYS:NZ	2.36	0.58
39:1n:70:PHE:O	39:1n:74:GLN:N	2.36	0.58
39:1n:137:LYS:O	39:1n:137:LYS:NZ	2.34	0.58
2:1B:39:TRP:HA	2:1B:42:ARG:HH11	1.69	0.58
3:1C:16:ASP:HA	3:1C:19:HIS:HB3	1.85	0.58
7:1G:366:THR:OG1	7:1G:450:MET:HE1	2.03	0.58
7:1G:430:GLN:NE2	7:1G:431:ASP:OD1	2.37	0.58
11:1K:37:MET:HG2	11:1K:67:ALA:HB1	1.86	0.58
5:1E:46:ALA:HB3	5:1E:73:LEU:HD11	1.85	0.58
5:1E:78:MET:HA	5:1E:81:TYR:CD2	2.39	0.58
6:1F:212:ASP:OD2	6:1F:212:ASP:N	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:534:ARG:NH1	7:1G:556:MET:O	2.36	0.58
8:1H:274:ARG:NE	8:1H:274:ARG:O	2.37	0.58
11:1K:8:ILE:H	11:1K:8:ILE:HD12	1.69	0.58
15:1O:165:PRO:HG3	15:1O:217:LYS:HD2	1.86	0.58
22:1W:51:GLN:O	22:1W:100:ARG:NH2	2.37	0.58
3:1C:40:VAL:HG12	43:1r:69:MET:HE3	1.85	0.58
3:1C:133:GLU:OE1	3:1C:133:GLU:N	2.31	0.58
12:1L:90:ILE:O	12:1L:94:LEU:HG	2.03	0.58
12:1L:364:LYS:NZ	36:1k:59:ASN:OD1	2.37	0.58
16:1P:243:GLN:N	16:1P:243:GLN:OE1	2.36	0.58
20:1U:26:ASP:OD1	20:1U:29:LYS:NZ	2.25	0.58
23:1X:63:ASN:ND2	25:1Z:78:GLU:OE2	2.36	0.58
27:1b:81:LYS:H	27:1b:81:LYS:HD2	1.67	0.58
33:1h:34:ILE:HG12	33:1h:35:PRO:HD3	1.84	0.58
37:1l:13:TYR:CE1	37:1l:39:ASP:HB2	2.38	0.58
1:1A:98:LEU:HD12	8:1H:298:LEU:HD21	1.86	0.58
3:1C:61:LEU:HB3	3:1C:123:VAL:HG11	1.86	0.58
5:1E:153:MET:HG2	5:1E:162:GLU:HG3	1.85	0.58
12:1L:340:PHE:O	12:1L:344:GLY:N	2.34	0.58
14:1N:329:MET:HA	14:1N:329:MET:HE3	1.86	0.58
16:1P:144:ARG:HD2	16:1P:147:ARG:HD2	1.85	0.58
1:1A:8:LEU:O	1:1A:12:THR:HG23	2.04	0.57
5:1E:121:GLN:HE21	5:1E:127:LYS:HA	1.68	0.57
6:1F:150:GLN:HA	6:1F:153:ILE:HB	1.85	0.57
12:1L:7:LEU:HA	12:1L:10:THR:HG22	1.85	0.57
15:1O:116:LEU:HD23	15:1O:260:ARG:HG3	1.86	0.57
21:1V:93:MET:HG2	21:1V:96:TRP:HD1	1.69	0.57
22:1W:27:GLU:HA	22:1W:30:ARG:HB3	1.84	0.57
22:1W:111:GLU:N	22:1W:111:GLU:OE2	2.32	0.57
3:1C:43:SER:OG	3:1C:44:CYS:N	2.37	0.57
4:1D:133:ARG:NH2	4:1D:202:ASP:OD1	2.37	0.57
5:1E:110:LEU:HD21	6:1F:337:MET:HB2	1.86	0.57
6:1F:272:MET:HE2	6:1F:318:ASP:HA	1.85	0.57
21:1V:13:LEU:HD11	21:1V:78:GLU:HB3	1.85	0.57
7:1G:348:VAL:HG13	7:1G:510:GLY:HA3	1.86	0.57
8:1H:136:VAL:O	8:1H:140:ILE:HG13	2.03	0.57
12:1L:298:ILE:HG13	12:1L:356:ILE:HD13	1.85	0.57
22:1W:91:GLU:OE2	22:1W:91:GLU:N	2.34	0.57
12:1L:142:ILE:HD13	13:1M:370:PRO:HB2	1.87	0.57
42:1q:29:ARG:NH2	42:1q:65:THR:O	2.37	0.57
7:1G:194:GLU:OE1	7:1G:385:ARG:NH2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:35:LYS:HD3	9:1I:45:PRO:HG3	1.85	0.57
9:1I:65:HIS:CD2	9:1I:111:ILE:HG21	2.39	0.57
12:1L:295:GLN:HB2	12:1L:301:ILE:HD12	1.87	0.57
14:1N:95:MET:O	14:1N:99:THR:OG1	2.23	0.57
20:1T:80:ILE:HG22	20:1T:84:LYS:HE3	1.86	0.57
26:1a:42:SER:O	26:1a:46:ASN:ND2	2.38	0.57
33:1h:134:ASP:O	33:1h:138:LYS:NZ	2.37	0.57
39:1n:30:CYS:O	39:1n:32:HIS:N	2.36	0.57
3:1C:87:GLN:OE1	3:1C:87:GLN:N	2.27	0.57
4:1D:283:PHE:HA	4:1D:309:ARG:HH21	1.70	0.57
5:1E:67:ASN:OD1	5:1E:81:TYR:OH	2.17	0.57
9:1I:65:HIS:ND1	9:1I:133:GLU:HB2	2.19	0.57
15:1O:184:GLN:N	15:1O:184:GLN:OE1	2.37	0.57
17:1Q:34:LYS:HA	17:1Q:102:SER:HB2	1.85	0.57
20:1T:37:MET:H	20:1T:37:MET:CE	2.16	0.57
1:1A:106:TRP:NE1	45:1A:201:3PE:O12	2.35	0.57
2:1B:92:LEU:HD11	2:1B:100:LEU:HG	1.85	0.57
4:1D:65:VAL:HG23	4:1D:77:ASP:HB3	1.86	0.57
7:1G:665:GLN:HA	7:1G:670:ASP:HB2	1.86	0.57
19:1S:88:ARG:HE	19:1S:88:ARG:C	2.13	0.57
21:1V:72:GLN:N	21:1V:72:GLN:OE1	2.38	0.57
39:1n:178:MET:HE3	39:1n:178:MET:H	1.69	0.57
7:1G:53:ARG:N	47:1G:803:FES:S1	2.76	0.57
7:1G:326:GLU:OE2	7:1G:620:ARG:NH2	2.36	0.57
8:1H:143:GLU:HA	8:1H:146:LEU:HB2	1.85	0.57
8:1H:253:GLU:HA	26:1a:21:MET:HE1	1.87	0.57
14:1N:179:MET:HE3	14:1N:179:MET:HA	1.85	0.57
15:1O:219:GLU:HG3	15:1O:241:LEU:HG	1.85	0.57
15:1O:318:TRP:O	29:1d:58:LEU:N	2.30	0.57
19:1S:39:ARG:NH2	19:1S:83:ALA:O	2.37	0.57
20:1T:17:TYR:HA	20:1T:20:LYS:NZ	2.20	0.57
22:1W:70:ASN:HD22	22:1W:82:LEU:HG	1.70	0.57
23:1X:69:PHE:HA	23:1X:72:GLN:HE22	1.70	0.57
37:1l:33:ASP:OD1	37:1l:33:ASP:N	2.36	0.57
40:1o:14:LYS:HE2	40:1o:112:LYS:HE3	1.85	0.57
42:1q:66:THR:HG23	42:1q:74:PHE:HB2	1.87	0.57
6:1F:15:LEU:HD23	6:1F:20:ARG:HG2	1.87	0.57
13:1M:388:TRP:O	38:1m:108:ARG:NH1	2.38	0.57
16:1P:176:ASP:OD1	16:1P:180:ASN:ND2	2.38	0.57
19:1S:14:GLY:O	19:1S:69:ALA:N	2.38	0.57
27:1b:29:ILE:HG23	27:1b:30:ILE:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
43:1r:39:LYS:HE3	43:1r:39:LYS:HA	1.87	0.57
8:1H:135:ALA:O	8:1H:139:THR:OG1	2.20	0.57
9:1I:108:ARG:NH1	9:1I:110:ASP:OD2	2.38	0.57
12:1L:532:ILE:HD11	37:1I:101:MET:HB3	1.87	0.57
16:1P:167:LYS:NZ	16:1P:228:PHE:O	2.27	0.57
20:1U:25:ILE:HD11	20:1U:42:LEU:HD23	1.87	0.57
23:1X:72:GLN:HA	23:1X:75:ARG:HE	1.70	0.57
30:1e:46:ILE:HD12	30:1e:50:ARG:HH21	1.70	0.57
32:1g:87:GLU:OE1	32:1g:87:GLU:N	2.38	0.57
1:1A:56:PHE:HZ	11:1K:75:LEU:HB3	1.69	0.56
5:1E:51:LEU:HD21	5:1E:84:ALA:HB2	1.87	0.56
7:1G:615:THR:OG1	7:1G:618:GLN:NE2	2.38	0.56
16:1P:132:ILE:HG22	16:1P:166:ILE:HB	1.86	0.56
16:1P:134:HIS:HB2	16:1P:149:LYS:HE3	1.86	0.56
3:1C:68:THR:HA	21:1V:82:GLN:NE2	2.19	0.56
5:1E:148:CYS:SG	6:1F:103:GLY:N	2.78	0.56
7:1G:201:ASP:HA	17:1Q:45:MET:HB3	1.86	0.56
7:1G:575:ASN:ND2	7:1G:577:GLU:OE2	2.38	0.56
10:1J:103:MET:HG2	11:1K:10:MET:HE1	1.87	0.56
14:1N:123:SER:OG	14:1N:125:GLN:OE1	2.23	0.56
40:1o:27:ASP:N	40:1o:27:ASP:OD1	2.37	0.56
6:1F:19:ASP:HA	6:1F:241:TRP:HZ2	1.71	0.56
6:1F:60:VAL:HA	6:1F:63:SER:HB3	1.86	0.56
7:1G:27:LEU:HD21	7:1G:55:CYS:HB2	1.88	0.56
8:1H:126:LYS:O	8:1H:130:ILE:HG13	2.05	0.56
8:1H:205:SER:OG	8:1H:279:ARG:NH1	2.38	0.56
9:1I:70:TYR:CE1	18:1R:87:CYS:HA	2.39	0.56
10:1J:118:LYS:HZ2	11:1K:1:FME:HCN	1.70	0.56
12:1L:276:MET:SD	12:1L:276:MET:N	2.72	0.56
13:1M:367:LEU:HD11	13:1M:408:LEU:HD21	1.87	0.56
13:1M:403:THR:HA	13:1M:406:TYR:CE2	2.40	0.56
15:1O:204:ASN:OD1	15:1O:204:ASN:N	2.39	0.56
20:1T:12:LYS:HE3	20:1T:16:LEU:HD11	1.87	0.56
20:1T:56:ASP:OD1	20:1T:56:ASP:N	2.33	0.56
26:1a:4:GLU:N	26:1a:4:GLU:OE1	2.38	0.56
32:1g:80:LEU:HD22	32:1g:81:PRO:HD2	1.87	0.56
32:1g:114:ASP:OD2	32:1g:116:ASN:ND2	2.38	0.56
2:1B:95:LYS:HE3	3:1C:155:TYR:CE1	2.40	0.56
7:1G:399:TRP:O	17:1Q:127:ARG:NH1	2.23	0.56
50:1I:204:PC1:H12	25:1Z:28:ARG:HG3	1.88	0.56
12:1L:136:ASN:HA	12:1L:197:ASP:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:284:ILE:HG22	32:1g:27:GLN:HB2	1.87	0.56
29:1d:58:LEU:HA	29:1d:61:GLN:HE21	1.69	0.56
3:1C:63:PHE:HA	21:1V:89:LEU:HD11	1.86	0.56
3:1C:209:TYR:CD1	4:1D:360:PRO:HD2	2.41	0.56
4:1D:148:LEU:O	4:1D:174:ARG:NH1	2.38	0.56
4:1D:162:GLY:HA3	8:1H:279:ARG:N	2.18	0.56
6:1F:45:THR:HG1	6:1F:167:CYS:HG	1.54	0.56
16:1P:38:LEU:O	16:1P:43:SER:OG	2.24	0.56
22:1W:70:ASN:OD1	22:1W:70:ASN:N	2.36	0.56
2:1B:150:PRO:HG3	4:1D:189:MET:HG3	1.86	0.56
7:1G:383:ASN:H	7:1G:387:GLU:HG2	1.70	0.56
7:1G:617:ASP:HA	7:1G:620:ARG:HG3	1.87	0.56
9:1I:49:ASN:O	9:1I:53:GLU:N	2.36	0.56
11:1K:47:ILE:HG12	14:1N:79:LEU:HD13	1.88	0.56
15:1O:204:ASN:HB2	15:1O:208:LYS:HE3	1.86	0.56
17:1Q:104:ASP:N	17:1Q:104:ASP:OD1	2.38	0.56
19:1S:42:GLU:O	19:1S:46:ALA:N	2.38	0.56
34:1i:103:ILE:HG22	41:1p:17:PRO:HB3	1.87	0.56
38:1m:51:ASN:OD1	39:1n:168:HIS:ND1	2.27	0.56
39:1n:138:GLN:NE2	39:1n:155:PRO:O	2.39	0.56
7:1G:185:THR:O	7:1G:187:ILE:N	2.39	0.56
7:1G:306:MET:HE2	7:1G:306:MET:N	2.19	0.56
7:1G:407:ALA:HB1	7:1G:422:LEU:HD11	1.87	0.56
8:1H:199:ASP:OD2	8:1H:279:ARG:NH2	2.29	0.56
14:1N:80:TYR:HA	30:1e:67:LEU:HD21	1.87	0.56
14:1N:207:ILE:O	14:1N:210:THR:OG1	2.22	0.56
16:1P:19:ILE:HG23	16:1P:43:SER:HB3	1.86	0.56
16:1P:64:ASP:HB3	16:1P:67:GLN:HG2	1.88	0.56
17:1Q:124:TRP:CZ3	44:1s:68:SER:HA	2.40	0.56
21:1V:39:LYS:HA	21:1V:44:ARG:HD2	1.88	0.56
36:1k:20:GLN:N	36:1k:20:GLN:OE1	2.38	0.56
42:1q:6:VAL:HA	42:1q:9:ARG:HD2	1.87	0.56
5:1E:18:ASP:N	5:1E:18:ASP:OD1	2.37	0.56
6:1F:218:CYS:HB3	17:1Q:124:TRP:NE1	2.21	0.56
7:1G:332:LYS:HD3	7:1G:343:LEU:HD13	1.88	0.56
7:1G:444:LYS:NZ	7:1G:476:ASN:O	2.37	0.56
8:1H:80:SER:O	8:1H:84:THR:OG1	2.24	0.56
8:1H:169:GLN:NE2	8:1H:240:ILE:O	2.38	0.56
17:1Q:91:ASP:OD1	17:1Q:91:ASP:N	2.32	0.56
20:1T:18:VAL:HA	20:1T:21:LEU:HB2	1.87	0.56
23:1X:146:ARG:NE	30:1e:41:GLU:OE1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:1a:1:MET:SD	26:1a:1:MET:N	2.79	0.56
43:1r:102:ARG:HE	43:1r:103:TRP:N	2.04	0.56
5:1E:100:ILE:HG13	5:1E:156:ILE:HD12	1.87	0.56
11:1K:48:ILE:HD13	11:1K:56:ALA:HB1	1.88	0.56
12:1L:3:PRO:HB2	12:1L:7:LEU:HD23	1.87	0.56
16:1P:92:ILE:HD11	16:1P:218:ILE:HD11	1.86	0.56
18:1R:63:GLY:O	18:1R:67:GLY:N	2.39	0.56
21:1V:85:ASN:O	21:1V:89:LEU:N	2.31	0.56
22:1W:18:LYS:HE2	22:1W:18:LYS:N	2.21	0.56
1:1A:73:LEU:HD13	8:1H:151:LEU:HD21	1.87	0.56
7:1G:58:GLU:OE2	7:1G:83:SER:OG	2.21	0.56
7:1G:218:ARG:HG3	9:1I:81:LYS:HB2	1.87	0.56
13:1M:168:GLN:NE2	33:1h:104:ARG:HD2	2.21	0.56
13:1M:334:TYR:O	13:1M:338:HIS:N	2.38	0.56
20:1U:70:LEU:HD11	20:1U:79:TYR:HB3	1.87	0.56
23:1X:68:ASP:N	23:1X:68:ASP:OD2	2.37	0.56
31:1f:28:ARG:O	31:1f:57:LYS:NZ	2.39	0.56
34:1i:100:LYS:NZ	41:1p:116:GLU:OE1	2.38	0.56
40:1o:16:PRO:HB3	40:1o:104:GLU:HG2	1.88	0.56
5:1E:95:VAL:HG21	5:1E:99:HIS:CD2	2.40	0.55
8:1H:20:LEU:HA	26:1a:12:MET:HE1	1.87	0.55
12:1L:176:ARG:HA	12:1L:179:ASP:HB2	1.87	0.55
12:1L:432:LEU:HD13	36:1k:62:PHE:HA	1.88	0.55
14:1N:202:ILE:O	14:1N:206:LEU:HD12	2.06	0.55
22:1W:66:MET:O	56:1W:201:EHZ:O1	2.23	0.55
33:1h:7:ARG:NH2	34:1i:28:SER:O	2.39	0.55
38:1m:16:THR:HG23	38:1m:17:LEU:HD12	1.88	0.55
1:1A:73:LEU:HA	8:1H:151:LEU:HD11	1.88	0.55
2:1B:62:MET:CE	2:1B:69:MET:HE3	2.36	0.55
4:1D:164:MET:O	4:1D:167:PHE:HB3	2.06	0.55
6:1F:392:LEU:HD12	6:1F:395:ILE:HD11	1.88	0.55
7:1G:45:ARG:NH1	7:1G:261:GLU:OE1	2.39	0.55
7:1G:601:ARG:NH1	7:1G:601:ARG:O	2.39	0.55
35:1j:37:LEU:HB2	36:1k:77:PHE:HE1	1.71	0.55
44:1s:63:MET:HE2	44:1s:63:MET:N	2.20	0.55
7:1G:9:ILE:HD11	7:1G:75:LYS:HB2	1.87	0.55
14:1N:330:ILE:HD12	14:1N:331:VAL:N	2.21	0.55
22:1W:52:LEU:HB3	22:1W:104:MET:HE1	1.88	0.55
39:1n:154:PRO:HB2	39:1n:157:ARG:HH22	1.72	0.55
3:1C:149:ARG:HA	22:1W:88:MET:HE2	1.88	0.55
6:1F:89:ARG:HE	6:1F:218:CYS:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:95:VAL:HG22	6:1F:228:VAL:HG11	1.87	0.55
11:1K:59:MET:HG2	14:1N:84:TRP:CH2	2.41	0.55
17:1Q:11:ILE:HG22	22:1W:23:ARG:HD2	1.89	0.55
18:1R:37:GLU:H	18:1R:37:GLU:CD	2.13	0.55
19:1S:81:PHE:HD1	19:1S:82:SER:H	1.54	0.55
20:1U:21:LEU:HD11	36:1k:47:ASN:HA	1.88	0.55
3:1C:179:GLU:OE2	16:1P:40:ARG:NH2	2.40	0.55
4:1D:170:MET:HE1	4:1D:221:ARG:HB3	1.88	0.55
13:1M:328:CYS:SG	13:1M:436:LEU:HD21	2.46	0.55
20:1U:69:LYS:HZ2	34:1i:2:GLY:C	2.14	0.55
37:1l:18:GLU:H	37:1l:18:GLU:CD	2.14	0.55
37:1l:54:SER:N	37:1l:57:GLU:OE1	2.40	0.55
12:1L:573:MET:HB2	14:1N:167:TRP:CZ2	2.42	0.55
4:1D:410:MET:HE2	4:1D:410:MET:N	2.21	0.55
7:1G:11:VAL:HG23	7:1G:77:TRP:H	1.72	0.55
8:1H:179:TRP:HE1	25:1Z:43:LEU:HG	1.71	0.55
8:1H:189:THR:O	8:1H:193:THR:OG1	2.22	0.55
13:1M:193:ILE:H	13:1M:193:ILE:HD12	1.71	0.55
15:1O:140:ARG:HA	15:1O:140:ARG:HH11	1.72	0.55
34:1i:63:THR:O	34:1i:67:SER:OG	2.19	0.55
38:1m:113:LYS:O	38:1m:113:LYS:NZ	2.40	0.55
3:1C:127:ALA:HB1	3:1C:131:GLU:OE2	2.07	0.55
6:1F:66:ARG:NH2	6:1F:249:ARG:O	2.36	0.55
8:1H:215:TYR:HE2	8:1H:219:PRO:HB2	1.72	0.55
10:1J:173:ARG:HH12	15:1O:254:ARG:HG2	1.72	0.55
15:1O:157:LYS:HE2	15:1O:157:LYS:H	1.72	0.55
16:1P:294:LEU:HD23	16:1P:294:LEU:H	1.72	0.55
30:1e:85:LEU:HD21	30:1e:91:TYR:HB3	1.89	0.55
32:1g:77:VAL:HA	32:1g:80:LEU:HG	1.88	0.55
40:1o:98:MET:HE3	40:1o:98:MET:H	1.72	0.55
7:1G:228:ILE:HD12	7:1G:237:ASN:HA	1.89	0.55
12:1L:88:MET:HE2	12:1L:330:CYS:SG	2.47	0.55
12:1L:160:GLY:HA3	39:1n:94:GLU:OE1	2.07	0.55
13:1M:423:ILE:HG22	38:1m:58:VAL:HB	1.89	0.55
23:1X:76:HIS:O	23:1X:78:ALA:N	2.40	0.55
30:1e:29:PRO:HB3	33:1h:138:LYS:HG2	1.89	0.55
7:1G:372:GLU:OE1	7:1G:372:GLU:N	2.37	0.55
13:1M:47:GLU:HB3	41:1p:92:ARG:HE	1.72	0.55
15:1O:291:ARG:NH2	32:1g:29:ASP:OD1	2.38	0.55
16:1P:157:ARG:NH2	16:1P:227:THR:OG1	2.38	0.55
1:1A:1:FME:O1	1:1A:2:ASN:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:162:GLN:OE1	42:1q:116:ASN:ND2	2.40	0.54
7:1G:74:MET:N	7:1G:74:MET:HE3	2.22	0.54
12:1L:71:LEU:N	12:1L:74:VAL:O	2.33	0.54
13:1M:40:SER:O	33:1h:80:TYR:OH	2.21	0.54
14:1N:26:TRP:HB3	14:1N:74:ILE:HD13	1.89	0.54
14:1N:106:LEU:HD11	14:1N:139:LEU:HD13	1.88	0.54
16:1P:108:ASP:HA	16:1P:112:LYS:HG3	1.89	0.54
20:1U:36:PHE:HA	20:1U:40:LEU:HD23	1.89	0.54
5:1E:93:LYS:HG3	5:1E:94:PRO:HD2	1.90	0.54
6:1F:146:ALA:O	6:1F:149:LEU:HD23	2.07	0.54
7:1G:379:LEU:HA	7:1G:452:VAL:HG13	1.89	0.54
12:1L:294:THR:O	12:1L:524:ASN:ND2	2.38	0.54
14:1N:85:THR:OG1	14:1N:87:THR:OG1	2.25	0.54
16:1P:268:ARG:HD3	16:1P:281:ARG:NH2	2.22	0.54
19:1S:74:LYS:HD3	19:1S:75:ASN:H	1.72	0.54
20:1T:6:LEU:HD23	20:1T:84:LYS:HE2	1.88	0.54
41:1p:26:PRO:HB2	41:1p:31:TYR:HE2	1.72	0.54
4:1D:111:MET:N	4:1D:111:MET:SD	2.81	0.54
6:1F:154:ARG:NH2	44:1s:57:GLU:O	2.32	0.54
7:1G:36:GLN:HG3	7:1G:39:ARG:HH21	1.73	0.54
7:1G:60:GLU:O	7:1G:61:LYS:HG3	2.08	0.54
12:1L:86:SER:OG	12:1L:262:ARG:NH2	2.41	0.54
13:1M:425:ASN:HD22	38:1m:57:GLY:HA2	1.73	0.54
14:1N:263:LYS:O	14:1N:267:ILE:HG12	2.07	0.54
15:1O:25:ILE:O	15:1O:123:VAL:HA	2.07	0.54
19:1S:23:CYS:HB2	19:1S:60:VAL:H	1.72	0.54
37:1l:114:PHE:HD2	37:1l:115:MET:HE2	1.72	0.54
41:1p:70:VAL:O	41:1p:90:GLN:NE2	2.39	0.54
44:1s:73:PRO:HD2	44:1s:74:ARG:H	1.72	0.54
3:1C:63:PHE:HD1	21:1V:89:LEU:HD11	1.71	0.54
4:1D:49:LEU:HB3	4:1D:66:MET:SD	2.47	0.54
5:1E:9:HIS:CE1	5:1E:63:ILE:HB	2.42	0.54
5:1E:190:ARG:NH2	5:1E:193:CYS:HA	2.20	0.54
6:1F:208:PRO:HD2	17:1Q:118:TYR:HD2	1.72	0.54
7:1G:206:GLY:N	46:1G:801:SF4:S1	2.73	0.54
12:1L:481:THR:HG22	40:1o:91:HIS:CD2	2.42	0.54
14:1N:162:ILE:HA	14:1N:185:ALA:HA	1.90	0.54
14:1N:267:ILE:O	14:1N:271:THR:OG1	2.17	0.54
16:1P:138:ASP:HB3	16:1P:141:SER:HB3	1.89	0.54
16:1P:171:ILE:H	54:1P:501:NDP:H71N	1.54	0.54
42:1q:78:ASP:OD1	42:1q:79:GLY:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:168:PHE:HB2	8:1H:32:GLN:HB3	1.89	0.54
5:1E:108:CYS:HB3	5:1E:113:SER:HG	1.73	0.54
6:1F:118:LEU:HD11	6:1F:136:ILE:HD12	1.89	0.54
6:1F:120:GLU:OE2	6:1F:236:ARG:NH1	2.40	0.54
7:1G:109:ASP:HB2	7:1G:209:THR:HG21	1.89	0.54
7:1G:145:LEU:HD23	7:1G:145:LEU:H	1.73	0.54
13:1M:73:LEU:HD21	13:1M:100:ILE:HG22	1.90	0.54
13:1M:183:SER:O	41:1p:152:ARG:NH2	2.35	0.54
14:1N:170:LEU:HD12	14:1N:292:PHE:HD2	1.71	0.54
16:1P:335:LYS:HD2	16:1P:335:LYS:C	2.33	0.54
25:1Z:68:ARG:HD3	25:1Z:69:ILE:HD13	1.89	0.54
32:1g:85:MET:HE2	32:1g:85:MET:N	2.21	0.54
34:1i:111:GLU:OE1	34:1i:111:GLU:N	2.33	0.54
35:1j:10:ARG:HH12	35:1j:16:GLN:HG2	1.72	0.54
8:1H:26:LYS:NZ	26:1a:4:GLU:O	2.38	0.54
8:1H:281:ARG:HB3	8:1H:284:GLN:HG3	1.89	0.54
9:1I:84:GLU:H	9:1I:84:GLU:CD	2.13	0.54
10:1J:153:LEU:O	10:1J:157:THR:OG1	2.22	0.54
12:1L:111:ASP:HB3	12:1L:114:ILE:HD13	1.90	0.54
12:1L:545:SER:O	12:1L:550:SER:OG	2.25	0.54
16:1P:86:GLU:HB2	16:1P:87:HIS:CE1	2.42	0.54
38:1m:53:PRO:HG3	39:1n:128:ARG:HE	1.72	0.54
4:1D:103:PHE:HB3	4:1D:114:ASN:HB3	1.90	0.54
7:1G:248:MET:N	7:1G:248:MET:SD	2.81	0.54
26:1a:3:PHE:CZ	51:1q:201:CDL:HA4	2.42	0.54
6:1F:101:GLU:HB2	6:1F:184:TYR:OH	2.07	0.54
8:1H:137:ALA:O	8:1H:141:SER:OG	2.26	0.54
10:1J:163:ILE:HG13	14:1N:12:THR:HG21	1.89	0.54
12:1L:576:MET:HE3	45:1Y:202:3PE:H31	1.90	0.54
13:1M:1:FME:SD	13:1M:52:PHE:HB3	2.47	0.54
14:1N:17:THR:HG23	14:1N:137:ALA:HB2	1.90	0.54
51:1N:402:CDL:H751	51:1N:402:CDL:H611	1.89	0.54
15:1O:173:ASP:N	15:1O:223:TYR:O	2.32	0.54
20:1T:48:VAL:HA	20:1T:51:ILE:HD11	1.89	0.54
22:1W:54:ILE:HG12	22:1W:107:PHE:CE1	2.40	0.54
23:1X:142:HIS:ND1	25:1Z:114:THR:OG1	2.40	0.54
32:1g:35:GLU:N	32:1g:35:GLU:OE2	2.40	0.54
32:1g:72:LEU:H	32:1g:72:LEU:HD12	1.73	0.54
3:1C:133:GLU:HA	3:1C:136:ASP:HB2	1.90	0.54
5:1E:55:GLN:NE2	5:1E:89:MET:O	2.40	0.54
5:1E:154:VAL:HG23	5:1E:161:TYR:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:129:LEU:HD13	51:1N:402:CDL:H532	1.88	0.54
19:1S:68:TYR:N	19:1S:72:GLN:O	2.39	0.54
7:1G:252:PRO:HB3	7:1G:263:ILE:HG23	1.89	0.54
10:1J:129:ASP:OD2	10:1J:130:THR:N	2.41	0.54
12:1L:135:ASN:ND2	12:1L:199:GLN:OE1	2.41	0.54
12:1L:188:TRP:CD2	12:1L:212:PRO:HG3	2.43	0.54
14:1N:190:MET:HE1	14:1N:205:LEU:HA	1.90	0.54
16:1P:41:MET:HE3	16:1P:41:MET:N	2.23	0.54
20:1U:32:VAL:O	20:1U:74:GLN:N	2.41	0.54
25:1Z:27:ARG:NH2	25:1Z:28:ARG:O	2.38	0.54
6:1F:164:LYS:HB3	44:1s:63:MET:SD	2.49	0.53
7:1G:36:GLN:HE22	17:1Q:49:VAL:HG13	1.72	0.53
7:1G:331:LEU:HD21	7:1G:525:LEU:HD22	1.89	0.53
12:1L:323:HIS:CE1	12:1L:475:MET:HE1	2.43	0.53
13:1M:72:LEU:HD23	13:1M:75:LEU:HD12	1.90	0.53
16:1P:57:MET:O	16:1P:60:ARG:HG2	2.08	0.53
21:1V:1:ALA:N	21:1V:63:ASP:OD1	2.42	0.53
23:1X:171:MET:SD	23:1X:171:MET:N	2.81	0.53
2:1B:30:VAL:HG22	2:1B:173:LEU:HB3	1.91	0.53
6:1F:89:ARG:NE	6:1F:217:GLY:O	2.41	0.53
7:1G:99:ALA:O	7:1G:134:LYS:NZ	2.33	0.53
7:1G:386:PHE:HB3	7:1G:671:PHE:HB2	1.90	0.53
8:1H:233:MET:HE3	8:1H:233:MET:C	2.32	0.53
29:1d:72:GLY:O	29:1d:76:LEU:HD23	2.09	0.53
33:1h:95:GLN:HB2	41:1p:82:LEU:HD21	1.90	0.53
1:1A:93:PHE:CE2	1:1A:97:LEU:HD22	2.42	0.53
2:1B:25:ARG:HG3	2:1B:27:GLU:H	1.73	0.53
3:1C:58:ILE:H	3:1C:58:ILE:HD12	1.73	0.53
3:1C:131:GLU:HA	3:1C:134:ILE:HG22	1.90	0.53
7:1G:12:PHE:HA	7:1G:17:SER:HA	1.91	0.53
7:1G:190:MET:N	7:1G:190:MET:HE3	2.23	0.53
7:1G:521:VAL:HG13	7:1G:542:PHE:HB3	1.89	0.53
16:1P:81:ILE:HG21	16:1P:117:ILE:HG22	1.91	0.53
20:1U:61:GLU:OE1	39:1n:81:PHE:HB2	2.09	0.53
21:1V:30:ILE:H	21:1V:30:ILE:HD12	1.73	0.53
30:1e:36:GLU:HB2	30:1e:62:PHE:CE1	2.42	0.53
35:1j:60:THR:OG1	35:1j:61:ASP:N	2.41	0.53
1:1A:71:LEU:HD22	10:1J:146:LEU:HD21	1.91	0.53
3:1C:137:MET:HE1	3:1C:153:THR:HG23	1.90	0.53
4:1D:202:ASP:OD1	4:1D:203:LEU:N	2.41	0.53
6:1F:41:ASP:OD1	6:1F:42:TRP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:134:ALA:N	6:1F:174:ASP:O	2.38	0.53
7:1G:276:ARG:HA	42:1q:135:GLN:NE2	2.23	0.53
10:1J:17:PHE:HA	10:1J:20:PHE:CE2	2.43	0.53
12:1L:440:LEU:HD22	20:1U:14:ARG:HH12	1.73	0.53
12:1L:482:MET:HG2	12:1L:487:LYS:HG3	1.90	0.53
22:1W:114:ARG:HD3	22:1W:115:PRO:HD3	1.90	0.53
26:1a:67:GLU:CD	26:1a:67:GLU:H	2.17	0.53
36:1k:18:TYR:CE1	36:1k:21:TRP:HB2	2.36	0.53
37:1l:50:LEU:HD12	37:1l:78:HIS:HA	1.90	0.53
4:1D:350:LYS:NZ	7:1G:118:ASP:OD1	2.30	0.53
9:1I:164:GLU:OE2	42:1q:87:HIS:ND1	2.37	0.53
10:1J:45:LEU:HD23	10:1J:50:SER:HA	1.91	0.53
13:1M:207:MET:HG2	13:1M:298:ILE:HD11	1.89	0.53
20:1T:51:ILE:HD12	20:1T:52:MET:N	2.22	0.53
20:1T:75:GLU:OE1	20:1T:75:GLU:N	2.41	0.53
43:1r:32:LYS:HZ2	43:1r:35:GLN:HA	1.74	0.53
1:1A:53:MET:SD	10:1J:172:THR:OG1	2.67	0.53
5:1E:40:GLU:HA	5:1E:43:LYS:HE2	1.90	0.53
6:1F:343:ILE:HD12	6:1F:344:VAL:N	2.24	0.53
7:1G:283:MET:HE2	7:1G:283:MET:HA	1.89	0.53
10:1J:98:MET:HA	10:1J:98:MET:HE3	1.89	0.53
12:1L:83:ASP:OD1	12:1L:84:TYR:N	2.42	0.53
12:1L:240:PRO:HD2	12:1L:243:VAL:HG21	1.89	0.53
13:1M:313:THR:HA	13:1M:316:MET:HB2	1.91	0.53
15:1O:176:VAL:HA	15:1O:179:ILE:HD12	1.90	0.53
34:1i:105:PRO:HD2	40:1o:63:ILE:HD11	1.91	0.53
44:1s:62:ARG:C	44:1s:63:MET:HE2	2.34	0.53
1:1A:70:ALA:HA	1:1A:73:LEU:HD23	1.89	0.53
15:1O:35:LYS:HE3	15:1O:126:ARG:HG3	1.90	0.53
17:1Q:95:PHE:HA	17:1Q:98:LYS:HD3	1.91	0.53
30:1e:82:ARG:HD2	30:1e:86:ILE:HG12	1.91	0.53
35:1j:61:ASP:HB3	35:1j:66:ILE:HB	1.90	0.53
2:1B:47:PRO:HA	2:1B:85:VAL:O	2.09	0.53
4:1D:37:ASP:CG	11:1K:95:LEU:HD11	2.34	0.53
9:1I:145:GLU:OE2	16:1P:66:GLY:N	2.38	0.53
9:1I:162:GLU:HB3	42:1q:109:ILE:HG12	1.89	0.53
12:1L:310:LEU:HA	12:1L:313:MET:CG	2.39	0.53
13:1M:16:TRP:O	13:1M:93:LYS:NZ	2.38	0.53
15:1O:261:MET:HA	15:1O:261:MET:HE2	1.90	0.53
38:1m:44:ARG:HH22	39:1n:143:THR:HG23	1.74	0.53
6:1F:142:PHE:HB3	6:1F:145:GLU:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:690:ALA:HB2	7:1G:698:VAL:HG11	1.91	0.53
8:1H:134:ARG:HH21	8:1H:200:LEU:HD13	1.74	0.53
8:1H:202:GLU:HA	8:1H:210:GLY:HA3	1.90	0.53
12:1L:54:PHE:O	12:1L:58:GLY:N	2.41	0.53
12:1L:63:ILE:HD11	12:1L:80:PHE:HD2	1.73	0.53
12:1L:542:LEU:HD21	37:1L:88:ARG:HD3	1.90	0.53
13:1M:215:TRP:O	13:1M:219:ALA:N	2.38	0.53
13:1M:325:MET:HE2	13:1M:440:HIS:HB3	1.91	0.53
19:1S:39:ARG:HH22	19:1S:87:THR:HB	1.73	0.53
21:1V:30:ILE:HA	21:1V:33:VAL:HG22	1.90	0.53
3:1C:116:PRO:HG3	22:1W:20:ILE:HG13	1.91	0.53
4:1D:2:ARG:HE	32:1g:31:ASP:HA	1.72	0.53
4:1D:4:TRP:CG	13:1M:140:THR:HG1	2.27	0.53
5:1E:190:ARG:HE	5:1E:193:CYS:HA	1.74	0.53
6:1F:123:LEU:HB3	6:1F:162:ILE:HD13	1.91	0.53
6:1F:171:TYR:CE2	6:1F:173:PHE:HB2	2.44	0.53
2:1B:93:THR:HG23	2:1B:96:MET:H	1.73	0.52
7:1G:585:VAL:O	17:1Q:61:THR:OG1	2.27	0.52
13:1M:61:LEU:HB2	13:1M:457:PRO:HD3	1.91	0.52
14:1N:147:GLN:HB3	33:1h:125:TYR:CZ	2.44	0.52
14:1N:316:GLN:HA	15:1O:302:ARG:HH21	1.73	0.52
15:1O:24:VAL:O	15:1O:24:VAL:HG12	2.09	0.52
22:1W:17:VAL:HG21	22:1W:77:ARG:CZ	2.39	0.52
6:1F:20:ARG:NH2	6:1F:270:GLU:OE1	2.42	0.52
6:1F:145:GLU:OE1	6:1F:145:GLU:N	2.37	0.52
8:1H:63:PRO:O	8:1H:66:SER:OG	2.24	0.52
12:1L:500:LEU:HD23	12:1L:500:LEU:H	1.73	0.52
13:1M:47:GLU:OE1	13:1M:47:GLU:N	2.41	0.52
13:1M:196:TRP:HZ2	13:1M:254:THR:HG23	1.75	0.52
14:1N:30:TRP:NE1	14:1N:34:GLU:OE2	2.43	0.52
16:1P:79:ASP:HB3	16:1P:82:ARG:HH22	1.74	0.52
20:1T:19:LEU:HD23	20:1T:25:ILE:HG21	1.91	0.52
26:1a:3:PHE:HA	26:1a:6:LEU:HD23	1.91	0.52
36:1k:22:LYS:N	36:1k:22:LYS:HE2	2.24	0.52
36:1k:35:LEU:O	36:1k:39:GLY:N	2.40	0.52
38:1m:4:LYS:HE2	38:1m:4:LYS:N	2.23	0.52
1:1A:51:PHE:HB2	1:1A:55:PHE:CE2	2.45	0.52
4:1D:209:ASP:OD1	25:1Z:16:TYR:OH	2.26	0.52
6:1F:276:LEU:HD23	6:1F:276:LEU:H	1.73	0.52
10:1J:86:ASN:HB3	10:1J:89:VAL:HG22	1.92	0.52
12:1L:345:SER:O	12:1L:349:SER:OG	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:1N:262:PRO:O	14:1N:266:ILE:HG12	2.09	0.52
14:1N:329:MET:HE1	51:1N:402:CDL:H802	1.91	0.52
16:1P:111:VAL:C	16:1P:114:PRO:HD2	2.35	0.52
18:1R:59:CYS:SG	18:1R:84:CYS:HB3	2.45	0.52
31:1f:49:ARG:NE	31:1f:52:GLU:OE1	2.42	0.52
33:1h:62:GLU:OE1	33:1h:63:HIS:N	2.42	0.52
43:1r:63:MET:HA	43:1r:63:MET:HE3	1.90	0.52
4:1D:284:ASP:OD2	4:1D:306:GLN:NE2	2.38	0.52
20:1T:46:ASP:OD1	22:1W:64:ARG:NH2	2.42	0.52
20:1U:69:LYS:NZ	34:1i:2:GLY:O	2.39	0.52
25:1Z:38:VAL:O	25:1Z:42:THR:HG23	2.09	0.52
40:1o:64:GLN:OE1	40:1o:64:GLN:N	2.43	0.52
41:1p:162:MET:HE3	41:1p:162:MET:H	1.74	0.52
4:1D:4:TRP:CD1	13:1M:140:THR:HA	2.44	0.52
5:1E:184:PRO:HD2	44:1s:44:HIS:CD2	2.45	0.52
7:1G:444:LYS:HA	7:1G:477:ILE:HD13	1.91	0.52
12:1L:350:LEU:O	12:1L:350:LEU:HD23	2.09	0.52
12:1L:514:LYS:NZ	45:1L:703:3PE:O12	2.32	0.52
13:1M:71:TRP:CZ3	32:1g:69:VAL:HG11	2.44	0.52
13:1M:310:MET:HE3	13:1M:459:TYR:HA	1.91	0.52
15:1O:134:PHE:O	15:1O:138:MET:HG3	2.09	0.52
23:1X:121:LEU:HD13	25:1Z:62:ILE:HD11	1.91	0.52
36:1k:21:TRP:C	36:1k:22:LYS:HE2	2.33	0.52
41:1p:58:ASN:N	41:1p:58:ASN:OD1	2.41	0.52
3:1C:180:VAL:HG13	3:1C:182:ARG:HB3	1.91	0.52
4:1D:279:ASP:OD1	4:1D:279:ASP:N	2.40	0.52
7:1G:108:CYS:O	7:1G:218:ARG:NH1	2.32	0.52
9:1I:92:ILE:HG12	9:1I:111:ILE:HG12	1.90	0.52
10:1J:86:ASN:OD1	10:1J:87:LYS:N	2.41	0.52
21:1V:64:VAL:HB	21:1V:76:ILE:HG13	1.92	0.52
23:1X:24:LEU:HB3	25:1Z:71:LEU:HD11	1.90	0.52
3:1C:50:ILE:HG22	3:1C:52:ILE:HG22	1.91	0.52
6:1F:106:LYS:HB2	6:1F:255:LEU:HD22	1.90	0.52
6:1F:262:VAL:HA	6:1F:287:VAL:HA	1.91	0.52
7:1G:365:ASN:HB2	7:1G:488:LYS:HB3	1.90	0.52
8:1H:20:LEU:HD22	8:1H:232:ILE:HD11	1.92	0.52
12:1L:524:ASN:ND2	39:1n:77:GLN:OE1	2.43	0.52
13:1M:399:ASN:O	13:1M:403:THR:OG1	2.27	0.52
14:1N:120:GLN:O	14:1N:176:ARG:NH2	2.42	0.52
15:1O:136:GLU:OE1	15:1O:140:ARG:NH2	2.43	0.52
35:1j:12:ARG:HH11	36:1k:50:TRP:CD1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:55:CYS:HB3	2:1B:116:MET:HG3	1.92	0.52
3:1C:111:THR:HG22	3:1C:112:ASP:O	2.10	0.52
5:1E:32:GLU:O	5:1E:36:LYS:HG2	2.10	0.52
6:1F:184:TYR:CE2	48:1F:501:FMN:H6	2.45	0.52
6:1F:189:GLU:O	6:1F:193:ILE:HG12	2.09	0.52
13:1M:278:ARG:HH12	38:1m:71:ARG:NH1	2.07	0.52
13:1M:307:TRP:HE1	38:1m:127:SER:HG	1.58	0.52
13:1M:434:ASN:HB3	33:1h:21:PHE:CE2	2.45	0.52
14:1N:139:LEU:HD23	14:1N:205:LEU:HD22	1.92	0.52
21:1V:88:SER:O	21:1V:92:LYS:HG2	2.10	0.52
26:1a:57:VAL:HG13	26:1a:59:ARG:HG2	1.92	0.52
39:1n:139:LEU:O	39:1n:143:THR:OG1	2.21	0.52
1:1A:17:LEU:HB3	8:1H:222:MET:HE1	1.91	0.52
1:1A:42:ASP:HB2	22:1W:99:GLN:HE22	1.75	0.52
1:1A:44:MET:HB3	22:1W:96:VAL:HG11	1.92	0.52
7:1G:380:VAL:HG13	7:1G:409:ILE:HD11	1.91	0.52
11:1K:16:LEU:HA	11:1K:36:MET:HE3	1.92	0.52
12:1L:293:ILE:HD12	12:1L:294:THR:HG23	1.91	0.52
12:1L:331:MET:N	12:1L:331:MET:SD	2.82	0.52
17:1Q:55:TRP:NE1	17:1Q:108:ARG:HH22	2.07	0.52
34:1i:41:PRO:HA	34:1i:44:GLN:HE22	1.75	0.52
37:1l:17:PRO:HA	37:1l:20:ARG:HB2	1.91	0.52
51:1q:201:CDL:HB32	51:1q:201:CDL:OB9	2.10	0.52
1:1A:46:SER:OG	8:1H:126:LYS:HD3	2.09	0.52
4:1D:366:ALA:HB1	4:1D:373:GLU:OE2	2.09	0.52
7:1G:382:THR:HB	7:1G:454:GLY:HA3	1.92	0.52
7:1G:536:ASP:OD1	7:1G:536:ASP:N	2.42	0.52
8:1H:307:LEU:HA	8:1H:310:MET:SD	2.50	0.52
12:1L:359:MET:HB2	12:1L:430:ALA:HA	1.92	0.52
14:1N:8:THR:O	14:1N:12:THR:HG23	2.10	0.52
19:1S:19:ARG:HB2	19:1S:65:TRP:HB2	1.91	0.52
19:1S:63:LYS:NZ	19:1S:75:ASN:HB2	2.25	0.52
20:1U:72:CYS:O	20:1U:76:ILE:N	2.37	0.52
28:1c:43:LYS:HE3	28:1c:49:GLU:HB2	1.92	0.52
32:1g:40:LYS:HA	32:1g:40:LYS:HE2	1.91	0.52
34:1i:34:LEU:HD23	34:1i:34:LEU:H	1.74	0.52
3:1C:13:PRO:HD3	4:1D:129:GLN:HG2	1.92	0.51
3:1C:35:LYS:HD2	3:1C:36:TYR:CE1	2.45	0.51
5:1E:201:SER:C	5:1E:202:LEU:HD23	2.36	0.51
6:1F:205:LEU:HB2	17:1Q:118:TYR:CZ	2.45	0.51
7:1G:108:CYS:SG	7:1G:206:GLY:HA3	2.50	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:523:PHE:HA	7:1G:544:ILE:HG22	1.92	0.51
7:1G:648:LEU:HD13	19:1S:44:LYS:HG2	1.91	0.51
10:1J:110:GLU:HG2	10:1J:112:GLU:H	1.73	0.51
11:1K:4:VAL:O	11:1K:8:ILE:HD12	2.11	0.51
12:1L:324:LEU:HD21	12:1L:476:THR:HG21	1.91	0.51
12:1L:356:ILE:HD11	12:1L:430:ALA:HB2	1.92	0.51
13:1M:393:ILE:HA	13:1M:396:MET:HB2	1.91	0.51
17:1Q:36:ARG:NE	17:1Q:38:PHE:HD1	2.09	0.51
20:1U:6:LEU:CD1	20:1U:11:ILE:HD11	2.41	0.51
22:1W:101:THR:O	22:1W:105:ARG:NH1	2.43	0.51
25:1Z:95:ALA:HB2	25:1Z:106:VAL:HG11	1.91	0.51
41:1p:84:MET:HE1	41:1p:152:ARG:HD2	1.92	0.51
2:1B:95:LYS:HE3	3:1C:155:TYR:HE1	1.73	0.51
4:1D:343:GLU:O	4:1D:347:HIS:ND1	2.42	0.51
6:1F:15:LEU:O	6:1F:20:ARG:NH1	2.43	0.51
9:1I:86:VAL:HG11	9:1I:125:ALA:HB2	1.92	0.51
10:1J:59:ILE:HD13	11:1K:64:LEU:HD11	1.92	0.51
10:1J:71:THR:OG1	11:1K:27:MET:SD	2.66	0.51
14:1N:154:MET:HE1	14:1N:191:THR:HB	1.91	0.51
15:1O:153:ASN:HB3	15:1O:157:LYS:NZ	2.25	0.51
16:1P:3:HIS:CD2	42:1q:132:LYS:HD2	2.45	0.51
23:1X:38:PRO:HG3	23:1X:65:CYS:SG	2.50	0.51
4:1D:126:LEU:HD13	4:1D:330:VAL:HG21	1.92	0.51
5:1E:36:LYS:HE3	44:1s:62:ARG:HG3	1.92	0.51
5:1E:121:GLN:NE2	5:1E:127:LYS:HA	2.26	0.51
13:1M:237:LYS:HG2	13:1M:316:MET:CE	2.40	0.51
19:1S:92:ASN:OD1	19:1S:92:ASN:N	2.42	0.51
21:1V:18:THR:O	21:1V:18:THR:OG1	2.25	0.51
36:1k:20:GLN:HG2	36:1k:21:TRP:CD1	2.44	0.51
6:1F:19:ASP:HA	6:1F:241:TRP:CZ2	2.45	0.51
8:1H:5:ASN:HB2	26:1a:26:ILE:HD13	1.92	0.51
8:1H:91:MET:O	8:1H:93:TYR:N	2.44	0.51
12:1L:395:ILE:O	12:1L:399:VAL:HG22	2.10	0.51
16:1P:24:PHE:CZ	16:1P:81:ILE:HG23	2.46	0.51
38:1m:36:LEU:HD22	39:1n:150:THR:HA	1.93	0.51
40:1o:38:MET:HE3	40:1o:39:VAL:N	2.26	0.51
5:1E:55:GLN:NE2	5:1E:91:ASN:OD1	2.44	0.51
7:1G:147:LYS:N	7:1G:209:THR:O	2.35	0.51
8:1H:112:ALA:O	8:1H:115:SER:OG	2.27	0.51
12:1L:183:VAL:HG11	13:1M:400:MET:HE1	1.93	0.51
13:1M:158:LEU:HD13	14:1N:283:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:201:VAL:N	16:1P:290:SER:OG	2.35	0.51
17:1Q:56:LYS:HB3	17:1Q:58:GLU:OE2	2.10	0.51
28:1c:28:TRP:NE1	29:1d:66:THR:HG22	2.24	0.51
33:1h:41:THR:O	33:1h:45:VAL:HG22	2.10	0.51
33:1h:94:LEU:HB3	41:1p:81:ILE:HD13	1.93	0.51
2:1B:154:GLU:OE1	2:1B:154:GLU:N	2.43	0.51
4:1D:88:GLU:HA	4:1D:91:ILE:HD12	1.91	0.51
6:1F:105:CYS:N	6:1F:257:ASN:OD1	2.43	0.51
7:1G:141:ASN:OD1	7:1G:141:ASN:N	2.42	0.51
7:1G:190:MET:HB2	7:1G:192:MET:HE1	1.93	0.51
12:1L:458:LEU:HD23	35:1j:28:PHE:CD2	2.46	0.51
12:1L:573:MET:HB2	14:1N:167:TRP:CE2	2.46	0.51
22:1W:40:TYR:CE2	22:1W:60:ARG:HD2	2.46	0.51
37:1l:126:GLN:HE21	40:1o:1:GLY:H1	1.57	0.51
42:1q:78:ASP:H	42:1q:81:MET:HE1	1.76	0.51
2:1B:81:ARG:HE	8:1H:61:LEU:HD11	1.75	0.51
2:1B:104:TYR:CE1	2:1B:111:ARG:HD2	2.45	0.51
3:1C:36:TYR:HE2	3:1C:59:PRO:HG2	1.75	0.51
3:1C:129:TRP:HH2	4:1D:78:PRO:HB2	1.74	0.51
4:1D:177:MET:HA	4:1D:180:PHE:CD2	2.46	0.51
5:1E:104:THR:HG22	6:1F:349:ARG:HE	1.74	0.51
7:1G:10:GLU:OE2	7:1G:17:SER:OG	2.26	0.51
7:1G:174:THR:O	7:1G:174:THR:OG1	2.27	0.51
12:1L:488:MET:HE1	35:1j:47:VAL:O	2.11	0.51
13:1M:88:THR:O	13:1M:92:LYS:HG3	2.10	0.51
16:1P:97:ARG:HH21	54:1P:501:NDP:H51A	1.74	0.51
20:1U:17:TYR:OH	36:1k:16:PRO:O	2.15	0.51
21:1V:91:ARG:NH2	21:1V:92:LYS:HD3	2.22	0.51
22:1W:23:ARG:NE	22:1W:23:ARG:O	2.43	0.51
22:1W:66:MET:HA	22:1W:69:LYS:HZ2	1.75	0.51
36:1k:48:GLU:OE1	39:1n:33:ARG:NE	2.39	0.51
37:1l:15:LYS:HD3	37:1l:15:LYS:N	2.26	0.51
39:1n:96:TYR:HB2	39:1n:177:PRO:HG2	1.93	0.51
42:1q:69:ASN:OD1	42:1q:112:ASN:ND2	2.43	0.51
3:1C:87:GLN:H	3:1C:87:GLN:CD	2.17	0.51
7:1G:599:ILE:HG22	22:1W:122:PHE:HZ	1.74	0.51
9:1I:99:ARG:H	9:1I:104:ARG:HG2	1.76	0.51
12:1L:330:CYS:HB2	12:1L:331:MET:SD	2.51	0.51
13:1M:450:ASN:OD1	13:1M:452:LYS:NZ	2.44	0.51
15:1O:226:ARG:HA	15:1O:226:ARG:CZ	2.41	0.51
16:1P:46:ILE:HG21	16:1P:84:VAL:HB	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:1S:24:GLN:HB3	19:1S:25:ARG:HD2	1.92	0.51
19:1S:64:LEU:HD22	19:1S:65:TRP:H	1.76	0.51
22:1W:62:LYS:HD2	22:1W:66:MET:SD	2.50	0.51
26:1a:2:TRP:CZ2	43:1r:7:ILE:HD13	2.46	0.51
26:1a:58:ASN:O	26:1a:58:ASN:ND2	2.43	0.51
37:1l:58:ARG:NH1	37:1l:70:ARG:O	2.44	0.51
39:1n:25:HIS:CE1	39:1n:78:PRO:HB3	2.46	0.51
39:1n:136:VAL:O	39:1n:140:GLN:NE2	2.44	0.51
41:1p:31:TYR:O	41:1p:35:ILE:HG22	2.11	0.51
43:1r:47:LYS:NZ	43:1r:50:ASN:O	2.44	0.51
2:1B:95:LYS:NZ	3:1C:153:THR:O	2.43	0.51
5:1E:152:PRO:O	5:1E:164:LEU:HB3	2.11	0.51
6:1F:149:LEU:O	6:1F:153:ILE:N	2.40	0.51
7:1G:418:ARG:HE	44:1s:75:HIS:HA	1.75	0.51
8:1H:167:THR:HA	8:1H:170:GLU:HG3	1.93	0.51
12:1L:486:MET:HE2	12:1L:486:MET:C	2.35	0.51
13:1M:141:GLU:HG2	13:1M:222:GLU:HG2	1.93	0.51
13:1M:428:ALA:N	39:1n:105:ASP:OD1	2.38	0.51
15:1O:70:ASP:O	15:1O:74:SER:N	2.44	0.51
16:1P:36:ASN:O	16:1P:40:ARG:NH1	2.44	0.51
19:1S:24:GLN:HE22	19:1S:58:SER:HA	1.76	0.51
23:1X:3:ILE:HD11	25:1Z:105:LYS:NZ	2.26	0.51
25:1Z:130:ASN:OD1	25:1Z:131:GLU:N	2.44	0.51
34:1i:123:PRO:HG2	34:1i:125:GLN:HE22	1.76	0.51
42:1q:67:GLU:OE2	42:1q:70:GLY:N	2.39	0.51
3:1C:32:ILE:HD13	3:1C:63:PHE:CZ	2.46	0.51
4:1D:322:GLU:CD	43:1r:44:PRO:HD3	2.36	0.51
5:1E:60:TRP:NE1	5:1E:62:PRO:HD3	2.26	0.51
7:1G:632:ARG:NH2	19:1S:57:CYS:SG	2.81	0.51
16:1P:27:THR:OG1	54:1P:501:NDP:O1X	2.29	0.51
29:1d:105:ASP:O	29:1d:107:LYS:NZ	2.44	0.51
30:1e:16:TRP:CE3	30:1e:17:MET:HB3	2.46	0.51
31:1f:11:TRP:O	31:1f:14:ILE:HG22	2.11	0.51
33:1h:14:SER:OG	39:1n:110:GLU:OE1	2.29	0.51
1:1A:17:LEU:HB3	8:1H:222:MET:CE	2.41	0.50
1:1A:41:PHE:HB3	4:1D:50:ASN:HD22	1.76	0.50
2:1B:113:VAL:HG13	2:1B:142:VAL:HA	1.93	0.50
3:1C:20:LYS:HD3	3:1C:21:GLN:N	2.26	0.50
5:1E:23:PHE:HB3	5:1E:27:ASN:HB2	1.91	0.50
5:1E:173:ILE:HA	5:1E:176:LEU:HB2	1.93	0.50
6:1F:79:TRP:O	6:1F:83:ASN:ND2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:365:ASN:N	7:1G:491:ASN:OD1	2.43	0.50
7:1G:403:ASP:HA	17:1Q:127:ARG:HH22	1.75	0.50
8:1H:314:ILE:HD12	8:1H:314:ILE:O	2.11	0.50
9:1I:64:GLU:HB2	9:1I:139:PHE:CE1	2.46	0.50
14:1N:268:GLN:HG3	23:1X:167:PHE:HZ	1.76	0.50
15:1O:182:ARG:HA	15:1O:185:LYS:HD2	1.92	0.50
21:1V:57:MET:HG3	21:1V:70:GLN:HB3	1.93	0.50
22:1W:43:VAL:HG21	22:1W:60:ARG:HD3	1.92	0.50
22:1W:92:GLU:HA	22:1W:97:TRP:HE3	1.76	0.50
25:1Z:43:LEU:O	25:1Z:46:GLY:N	2.45	0.50
25:1Z:101:VAL:HG11	25:1Z:104:TRP:HE3	1.74	0.50
28:1c:13:ASP:O	28:1c:17:VAL:HG12	2.12	0.50
32:1g:111:ASN:HA	41:1p:161:ARG:HH22	1.76	0.50
33:1h:127:THR:OG1	33:1h:128:ILE:N	2.45	0.50
39:1n:18:LEU:HD13	39:1n:21:ARG:HH22	1.77	0.50
1:1A:106:TRP:CZ2	8:1H:291:LYS:HD2	2.47	0.50
4:1D:95:THR:HA	4:1D:385:ARG:HG2	1.93	0.50
5:1E:48:LEU:HB3	5:1E:49:PRO:HD3	1.92	0.50
5:1E:87:TYR:CD1	6:1F:181:ALA:HB3	2.40	0.50
6:1F:253:THR:OG1	6:1F:254:LYS:N	2.44	0.50
7:1G:40:PHE:HE1	7:1G:115:ASP:HB3	1.76	0.50
7:1G:357:ASP:CG	19:1S:52:ILE:H	2.20	0.50
7:1G:409:ILE:HG23	7:1G:422:LEU:HD13	1.93	0.50
7:1G:702:SER:OG	9:1I:104:ARG:NE	2.44	0.50
9:1I:110:ASP:HB3	17:1Q:70:MET:HE1	1.93	0.50
10:1J:129:ASP:HB2	30:1e:31:ARG:HD2	1.92	0.50
20:1U:21:LEU:O	36:1k:46:ARG:NH1	2.45	0.50
26:1a:28:LYS:HG2	26:1a:33:GLY:HA2	1.93	0.50
28:1c:28:TRP:O	28:1c:32:ILE:HD12	2.10	0.50
4:1D:125:LEU:HD11	4:1D:363:THR:HB	1.93	0.50
5:1E:112:ASN:O	5:1E:115:SER:OG	2.28	0.50
6:1F:108:ARG:HG2	6:1F:112:ARG:HH12	1.76	0.50
6:1F:154:ARG:NH1	44:1s:57:GLU:HG3	2.25	0.50
7:1G:298:ASP:HB2	7:1G:302:ARG:HH22	1.75	0.50
50:1I:204:PC1:H122	25:1Z:30:LEU:O	2.12	0.50
12:1L:81:LYS:HD3	12:1L:83:ASP:HB2	1.94	0.50
13:1M:121:LEU:HA	13:1M:124:ALA:HB3	1.92	0.50
18:1R:56:VAL:C	18:1R:57:ILE:HD12	2.36	0.50
19:1S:78:LEU:HD12	19:1S:78:LEU:O	2.12	0.50
22:1W:99:GLN:OE1	22:1W:99:GLN:HA	2.10	0.50
29:1d:57:GLY:O	29:1d:61:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:1f:2:ASN:OD1	31:1f:5:GLN:HB3	2.11	0.50
34:1i:120:LYS:HE3	40:1o:39:VAL:HG23	1.91	0.50
37:1l:13:TYR:HD2	37:1l:14:PRO:N	2.10	0.50
37:1l:63:ASP:OD1	37:1l:63:ASP:N	2.39	0.50
38:1m:45:GLU:OE1	38:1m:45:GLU:N	2.45	0.50
3:1C:137:MET:HB3	3:1C:162:PHE:HB2	1.92	0.50
4:1D:180:PHE:O	4:1D:184:VAL:HG22	2.11	0.50
6:1F:363:THR:HG23	6:1F:364:PRO:HD3	1.92	0.50
12:1L:33:PRO:HB3	12:1L:118:PHE:CZ	2.46	0.50
12:1L:371:THR:O	12:1L:375:ILE:HD12	2.12	0.50
13:1M:51:ASN:HA	13:1M:57:PHE:HB2	1.94	0.50
16:1P:279:THR:HA	16:1P:283:LYS:HD2	1.92	0.50
20:1U:21:LEU:HD21	36:1k:47:ASN:N	2.27	0.50
31:1f:2:ASN:OD1	31:1f:6:ILE:HG23	2.12	0.50
39:1n:69:GLU:O	39:1n:73:GLY:N	2.37	0.50
42:1q:132:LYS:HE2	42:1q:134:ILE:O	2.12	0.50
1:1A:80:GLN:HE22	8:1H:314:ILE:HD13	1.76	0.50
2:1B:44:SER:OG	8:1H:51:ASP:OD1	2.27	0.50
2:1B:112:TYR:CZ	2:1B:167:ILE:HD11	2.46	0.50
4:1D:238:ARG:HD2	8:1H:281:ARG:HB2	1.93	0.50
5:1E:101:GLN:HB3	5:1E:142:VAL:HG21	1.93	0.50
6:1F:280:ILE:HB	6:1F:287:VAL:HG13	1.94	0.50
6:1F:312:CYS:HA	6:1F:315:VAL:HG12	1.93	0.50
6:1F:337:MET:HE1	6:1F:343:ILE:HA	1.94	0.50
7:1G:349:PHE:HD1	7:1G:350:PRO:HD2	1.76	0.50
7:1G:617:ASP:OD2	7:1G:617:ASP:N	2.45	0.50
12:1L:415:ALA:O	12:1L:419:THR:N	2.44	0.50
13:1M:258:ALA:HA	13:1M:302:MET:HE1	1.92	0.50
13:1M:422:HIS:O	38:1m:55:ARG:NH1	2.43	0.50
15:1O:285:GLY:HA3	32:1g:28:GLU:HG2	1.93	0.50
19:1S:23:CYS:HA	19:1S:57:CYS:O	2.11	0.50
20:1T:36:PHE:HA	20:1T:40:LEU:HB2	1.92	0.50
33:1h:94:LEU:HD13	41:1p:81:ILE:HB	1.92	0.50
43:1r:47:LYS:HG2	43:1r:51:ASN:HD22	1.75	0.50
3:1C:114:LEU:HD21	17:1Q:17:LEU:HD11	1.94	0.50
6:1F:253:THR:HA	6:1F:272:MET:HB3	1.92	0.50
6:1F:255:LEU:HD12	6:1F:255:LEU:H	1.76	0.50
6:1F:315:VAL:HG13	6:1F:317:MET:HE1	1.94	0.50
7:1G:366:THR:OG1	7:1G:491:ASN:ND2	2.45	0.50
7:1G:545:TYR:HB3	7:1G:560:ILE:HD13	1.93	0.50
7:1G:704:CYS:HB2	9:1I:104:ARG:N	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:1J:150:GLY:HA3	11:1K:58:MET:HE1	1.93	0.50
12:1L:302:VAL:O	12:1L:306:THR:HG23	2.11	0.50
16:1P:315:ILE:HG12	16:1P:331:MET:HB3	1.92	0.50
17:1Q:30:ILE:HD11	17:1Q:99:ASN:O	2.11	0.50
20:1U:11:ILE:HG22	20:1U:77:VAL:HG22	1.93	0.50
21:1V:63:ASP:OD2	21:1V:66:LYS:N	2.37	0.50
37:1l:12:PRO:O	37:1l:46:ASP:HB3	2.11	0.50
4:1D:170:MET:HE2	4:1D:170:MET:HA	1.94	0.50
7:1G:396:ARG:HG2	7:1G:417:TYR:HD2	1.75	0.50
8:1H:65:THR:OG1	8:1H:124:ASN:OD1	2.29	0.50
9:1I:13:ASP:OD1	9:1I:16:SER:N	2.27	0.50
14:1N:174:GLN:HE22	14:1N:226:THR:HB	1.75	0.50
16:1P:167:LYS:HE3	16:1P:227:THR:HG22	1.94	0.50
17:1Q:57:MET:HG2	17:1Q:84:LEU:HD23	1.93	0.50
17:1Q:67:ASN:HB3	17:1Q:72:TRP:H	1.77	0.50
23:1X:126:LYS:HD2	27:1b:66:PRO:HG3	1.93	0.50
32:1g:101:GLU:N	32:1g:101:GLU:OE2	2.45	0.50
34:1i:46:TRP:CH2	34:1i:61:TYR:HA	2.47	0.50
37:1l:132:GLN:OE1	37:1l:155:HIS:ND1	2.45	0.50
42:1q:68:MET:HE2	42:1q:68:MET:HA	1.94	0.50
3:1C:49:GLU:OE2	3:1C:106:ARG:NH2	2.41	0.50
5:1E:200:THR:HG21	6:1F:283:HIS:HA	1.94	0.50
6:1F:276:LEU:HA	6:1F:279:LEU:HD23	1.94	0.50
7:1G:227:SER:O	7:1G:253:ARG:NH2	2.45	0.50
9:1I:106:THR:HG23	9:1I:151:LYS:HE3	1.93	0.50
13:1M:192:ASN:HA	13:1M:195:MET:HB3	1.94	0.50
14:1N:118:VAL:O	14:1N:122:ILE:HG13	2.12	0.50
16:1P:81:ILE:HG12	16:1P:117:ILE:HG22	1.94	0.50
16:1P:196:LEU:HB3	16:1P:198:LYS:HG2	1.94	0.50
20:1U:12:LYS:O	20:1U:16:LEU:HG	2.12	0.50
22:1W:105:ARG:O	22:1W:108:HIS:ND1	2.44	0.50
36:1k:71:LYS:H	36:1k:71:LYS:HD3	1.76	0.50
3:1C:155:TYR:HB2	22:1W:102:HIS:CE1	2.46	0.50
3:1C:168:LEU:HD22	4:1D:93:TYR:CD2	2.47	0.50
4:1D:29:LYS:HD2	4:1D:30:PRO:HD2	1.93	0.50
6:1F:65:LEU:HD23	6:1F:242:PHE:HZ	1.76	0.50
12:1L:84:TYR:HA	12:1L:87:VAL:HG12	1.94	0.50
12:1L:144:TRP:CH2	12:1L:256:GLY:HA2	2.46	0.50
12:1L:539:TYR:HE2	38:1m:9:ARG:HH21	1.60	0.50
20:1U:37:MET:HE3	20:1U:37:MET:N	2.23	0.50
34:1i:119:MET:HE2	34:1i:122:PHE:HE1	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:67:TYR:CZ	2:1B:154:GLU:HB3	2.46	0.49
3:1C:158:GLU:CD	17:1Q:24:GLY:HA3	2.36	0.49
3:1C:203:TRP:CZ3	7:1G:36:GLN:HG2	2.46	0.49
5:1E:96:GLY:O	5:1E:98:TYR:N	2.45	0.49
7:1G:46:LEU:HD21	7:1G:161:ARG:HB2	1.93	0.49
7:1G:422:LEU:H	7:1G:422:LEU:HD12	1.76	0.49
10:1J:115:ILE:O	10:1J:117:PHE:N	2.43	0.49
10:1J:167:VAL:O	10:1J:171:ILE:HG22	2.10	0.49
12:1L:604:TYR:CD2	14:1N:153:LEU:HD23	2.47	0.49
15:1O:124:LEU:HD11	15:1O:127:SER:HA	1.93	0.49
15:1O:183:ILE:HA	15:1O:186:LYS:HG2	1.94	0.49
57:1Y:201:PGT:H131	57:1Y:201:PGT:H361	1.93	0.49
31:1f:53:GLU:OE2	31:1f:53:GLU:N	2.38	0.49
35:1j:10:ARG:HH22	35:1j:16:GLN:HB3	1.76	0.49
37:1l:58:ARG:O	37:1l:70:ARG:NH2	2.45	0.49
39:1n:43:MET:HE3	39:1n:43:MET:C	2.37	0.49
41:1p:72:ASP:OD1	41:1p:74:THR:HG22	2.12	0.49
43:1r:4:THR:O	43:1r:8:GLN:HG3	2.11	0.49
2:1B:99:ALA:O	2:1B:103:VAL:HG23	2.12	0.49
6:1F:68:ARG:HB3	6:1F:254:LYS:HZ1	1.77	0.49
6:1F:403:THR:OG1	6:1F:405:CYS:O	2.25	0.49
15:1O:104:ARG:HG3	15:1O:128:ILE:HG22	1.93	0.49
18:1R:19:ASP:OD2	18:1R:22:ASP:HB2	2.12	0.49
20:1U:82:ASP:N	20:1U:82:ASP:OD1	2.45	0.49
23:1X:76:HIS:ND1	23:1X:113:LYS:HE2	2.27	0.49
2:1B:54:CYS:HB3	4:1D:108:TYR:CB	2.42	0.49
2:1B:63:ALA:HB2	2:1B:69:MET:HE1	1.94	0.49
6:1F:145:GLU:HA	6:1F:148:ASN:HB2	1.95	0.49
7:1G:347:GLU:HB2	7:1G:499:GLN:CD	2.37	0.49
11:1K:59:MET:HA	11:1K:62:ILE:HB	1.94	0.49
12:1L:81:LYS:HB2	12:1L:135:ASN:HD22	1.76	0.49
12:1L:86:SER:O	12:1L:89:PHE:N	2.44	0.49
12:1L:535:ARG:NH1	37:1l:90:ASP:OD2	2.46	0.49
45:1L:701:3PE:H112	45:1L:701:3PE:H11	1.95	0.49
14:1N:270:MET:HG3	14:1N:279:PRO:HG3	1.93	0.49
26:1a:51:ASP:HA	26:1a:54:ILE:HG22	1.94	0.49
39:1n:60:THR:HA	39:1n:63:LEU:HG	1.94	0.49
41:1p:103:ASN:O	41:1p:107:GLU:HG2	2.13	0.49
42:1q:29:ARG:NH1	42:1q:64:TYR:O	2.45	0.49
1:1A:84:LEU:HD13	27:1b:42:ILE:HG22	1.93	0.49
5:1E:109:MET:HA	5:1E:113:SER:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:42:GLU:O	22:1W:46:THR:HG23	2.12	0.49
22:1W:66:MET:SD	22:1W:66:MET:N	2.85	0.49
26:1a:65:GLY:N	26:1a:67:GLU:OE2	2.44	0.49
33:1h:56:PRO:HG2	33:1h:59:TYR:HD2	1.78	0.49
34:1i:41:PRO:HA	34:1i:44:GLN:NE2	2.28	0.49
35:1j:19:ARG:HD2	35:1j:23:ILE:HG23	1.93	0.49
36:1k:26:THR:O	36:1k:28:LEU:N	2.45	0.49
38:1m:112:GLU:OE2	38:1m:113:LYS:N	2.44	0.49
1:1A:18:VAL:HG21	8:1H:76:ILE:HD11	1.95	0.49
3:1C:58:ILE:O	3:1C:62:THR:OG1	2.29	0.49
3:1C:72:PHE:O	3:1C:124:TYR:OH	2.29	0.49
4:1D:143:GLU:OE2	4:1D:278:TYR:OH	2.30	0.49
7:1G:241:SER:OG	7:1G:249:ARG:O	2.26	0.49
7:1G:324:ASP:HB3	7:1G:571:ALA:HB1	1.95	0.49
7:1G:460:ARG:NH2	7:1G:462:ASP:OD2	2.39	0.49
7:1G:597:TRP:HE1	7:1G:616:LEU:HD23	1.76	0.49
8:1H:140:ILE:HA	8:1H:143:GLU:OE1	2.12	0.49
9:1I:43:ARG:HH11	43:1r:24:GLN:HE22	1.61	0.49
14:1N:309:ASN:ND2	14:1N:312:LYS:HE3	2.27	0.49
15:1O:175:PRO:O	15:1O:179:ILE:HG13	2.12	0.49
17:1Q:20:THR:HG21	17:1Q:30:ILE:HG12	1.93	0.49
19:1S:62:PRO:HB2	19:1S:78:LEU:HD12	1.95	0.49
20:1T:66:ASP:OD1	20:1T:66:ASP:N	2.46	0.49
24:1Y:93:GLY:HA3	24:1Y:118:GLY:HA2	1.94	0.49
24:1Y:96:GLY:O	24:1Y:99:THR:OG1	2.30	0.49
40:1o:61:TYR:HD2	40:1o:89:CYS:HB2	1.76	0.49
1:1A:31:SER:HB3	16:1P:320:ARG:HB2	1.94	0.49
4:1D:33:TRP:NE1	15:1O:154:GLU:OE2	2.46	0.49
8:1H:179:TRP:CG	8:1H:180:PRO:HD3	2.48	0.49
14:1N:156:THR:O	14:1N:160:LEU:HD22	2.12	0.49
15:1O:53:GLU:OE2	15:1O:104:ARG:NH2	2.45	0.49
15:1O:198:TYR:O	15:1O:202:ILE:HG22	2.12	0.49
17:1Q:55:TRP:HE1	17:1Q:108:ARG:HH22	1.61	0.49
22:1W:116:THR:C	22:1W:121:LYS:HZ1	2.19	0.49
41:1p:100:GLU:HA	41:1p:103:ASN:HD22	1.78	0.49
42:1q:48:TYR:CD1	42:1q:62:VAL:HG23	2.48	0.49
4:1D:66:MET:HA	4:1D:76:CYS:HA	1.95	0.49
7:1G:215:PHE:CD1	9:1I:104:ARG:HD3	2.47	0.49
7:1G:333:ASP:HB3	7:1G:611:LEU:HD11	1.94	0.49
8:1H:162:LEU:HA	8:1H:165:LEU:HD23	1.95	0.49
9:1I:141:THR:OG1	9:1I:146:GLU:OE2	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:192:MET:N	15:1O:192:MET:SD	2.85	0.49
16:1P:208:VAL:HG12	16:1P:212:LYS:NZ	2.27	0.49
20:1U:54:MET:HE2	20:1U:54:MET:N	2.28	0.49
26:1a:22:ALA:O	26:1a:26:ILE:HD12	2.12	0.49
30:1e:66:LEU:HD12	30:1e:67:LEU:HD22	1.95	0.49
2:1B:79:SER:HB3	8:1H:208:VAL:HG12	1.94	0.49
5:1E:117:LEU:O	5:1E:121:GLN:HB2	2.13	0.49
6:1F:99:GLU:OE1	6:1F:108:ARG:N	2.45	0.49
7:1G:276:ARG:NH1	7:1G:682:GLN:OE1	2.46	0.49
7:1G:475:GLN:NE2	7:1G:646:ASN:OD1	2.27	0.49
11:1K:1:FME:HG2	11:1K:2:PRO:HD2	1.94	0.49
14:1N:200:MET:HE1	14:1N:269:GLU:HB2	1.95	0.49
20:1T:37:MET:HE3	20:1T:37:MET:N	2.28	0.49
39:1n:106:TRP:CE3	39:1n:110:GLU:HB3	2.48	0.49
44:1s:47:SER:N	44:1s:50:THR:OG1	2.46	0.49
2:1B:113:VAL:CG1	2:1B:142:VAL:HA	2.43	0.49
3:1C:58:ILE:HB	3:1C:59:PRO:HD3	1.94	0.49
3:1C:90:PHE:CD2	3:1C:140:VAL:HB	2.48	0.49
4:1D:413:ASP:OD2	8:1H:281:ARG:HD3	2.13	0.49
5:1E:35:VAL:O	5:1E:43:LYS:NZ	2.33	0.49
5:1E:148:CYS:HA	5:1E:153:MET:HE1	1.95	0.49
6:1F:217:GLY:C	17:1Q:124:TRP:HD1	2.20	0.49
7:1G:54:MET:HE1	7:1G:94:MET:HE2	1.95	0.49
7:1G:539:LYS:HD3	42:1q:145:LYS:HZ3	1.78	0.49
12:1L:360:GLY:H	12:1L:362:LEU:HD23	1.78	0.49
13:1M:71:TRP:HZ3	32:1g:69:VAL:HG11	1.76	0.49
14:1N:136:LEU:O	14:1N:140:SER:OG	2.31	0.49
15:1O:223:TYR:CZ	15:1O:234:VAL:HG23	2.47	0.49
37:1l:37:TYR:CE1	37:1l:49:LYS:HD2	2.48	0.49
1:1A:87:MET:HA	10:1J:147:TYR:HB3	1.93	0.49
4:1D:75:LYS:HD2	4:1D:75:LYS:C	2.38	0.49
4:1D:176:LYS:HZ2	43:1r:26:ARG:HH11	1.60	0.49
6:1F:98:ASP:OD1	6:1F:100:GLY:N	2.45	0.49
7:1G:276:ARG:HE	42:1q:135:GLN:NE2	2.11	0.49
7:1G:318:ILE:HD12	7:1G:511:VAL:HG12	1.94	0.49
10:1J:8:ILE:O	10:1J:12:ILE:HD12	2.12	0.49
15:1O:114:HIS:O	15:1O:118:THR:OG1	2.31	0.49
23:1X:47:TRP:CZ3	33:1h:141:PRO:HG3	2.48	0.49
27:1b:31:LEU:H	27:1b:31:LEU:HD12	1.78	0.49
35:1j:19:ARG:O	35:1j:23:ILE:HG12	2.11	0.49
39:1n:9:LEU:HB3	39:1n:14:LYS:HD3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:1B:101:ARG:NH1	2:1B:105:ASP:OD2	2.41	0.48
3:1C:88:ASN:ND2	21:1V:110:GLN:OE1	2.43	0.48
6:1F:109:GLU:O	6:1F:113:HIS:ND1	2.45	0.48
6:1F:249:ARG:NH1	6:1F:249:ARG:HA	2.29	0.48
6:1F:352:GLU:HA	6:1F:373:ASN:HD21	1.78	0.48
7:1G:681:SER:OG	7:1G:684:MET:HB3	2.13	0.48
8:1H:130:ILE:HD12	8:1H:131:GLY:N	2.28	0.48
8:1H:221:ALA:O	8:1H:225:MET:N	2.31	0.48
9:1I:64:GLU:O	9:1I:134:GLY:N	2.40	0.48
11:1K:44:SER:O	11:1K:48:ILE:HG13	2.13	0.48
12:1L:536:LEU:HB3	12:1L:537:PRO:HD3	1.95	0.48
13:1M:95:TYR:HD1	13:1M:136:TRP:CD2	2.31	0.48
13:1M:116:ILE:O	13:1M:120:ILE:HG12	2.12	0.48
17:1Q:19:ILE:HG22	17:1Q:22:LEU:HD21	1.94	0.48
23:1X:129:LYS:HD3	27:1b:65:VAL:HG13	1.94	0.48
25:1Z:121:MET:HE2	25:1Z:137:THR:HG22	1.93	0.48
29:1d:89:ASP:HB2	33:1h:121:PRO:HG2	1.94	0.48
37:1l:13:TYR:HE1	37:1l:39:ASP:HB2	1.77	0.48
37:1l:85:ILE:HG22	37:1l:88:ARG:HB2	1.93	0.48
2:1B:148:GLY:CA	9:1I:118:TYR:HE1	2.25	0.48
4:1D:243:GLY:H	4:1D:409:HIS:CE1	2.30	0.48
12:1L:69:MET:C	12:1L:69:MET:HE2	2.38	0.48
12:1L:237:MET:HB3	12:1L:299:LYS:HD3	1.94	0.48
12:1L:400:ASN:ND2	12:1L:486:MET:HB2	2.24	0.48
50:1L:702:PC1:H271	13:1M:446:LEU:HD12	1.95	0.48
13:1M:192:ASN:O	13:1M:195:MET:HB3	2.13	0.48
26:1a:5:ILE:HD12	26:1a:5:ILE:H	1.78	0.48
30:1e:28:ILE:HD12	30:1e:28:ILE:O	2.14	0.48
33:1h:34:ILE:O	33:1h:38:ILE:HG12	2.13	0.48
35:1j:29:SER:O	35:1j:32:MET:HG3	2.13	0.48
41:1p:72:ASP:HB3	41:1p:90:GLN:HE21	1.76	0.48
7:1G:380:VAL:HA	7:1G:409:ILE:HD11	1.96	0.48
8:1H:61:LEU:HD12	8:1H:61:LEU:O	2.13	0.48
8:1H:105:MET:HG2	8:1H:237:PHE:CE2	2.47	0.48
10:1J:123:GLY:O	10:1J:126:VAL:HG22	2.14	0.48
10:1J:134:GLY:HA3	25:1Z:68:ARG:HH22	1.78	0.48
10:1J:170:GLU:HA	10:1J:170:GLU:OE2	2.13	0.48
12:1L:184:LEU:HD23	13:1M:393:ILE:HG21	1.94	0.48
15:1O:182:ARG:O	15:1O:185:LYS:N	2.46	0.48
17:1Q:49:VAL:C	17:1Q:51:ASN:H	2.22	0.48
20:1U:51:ILE:HD12	20:1U:52:MET:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:1W:17:VAL:HG22	22:1W:18:LYS:H	1.76	0.48
34:1i:23:LYS:HE3	34:1i:23:LYS:HA	1.96	0.48
34:1i:63:THR:O	34:1i:67:SER:N	2.46	0.48
38:1m:44:ARG:HH21	39:1n:148:PRO:HB3	1.78	0.48
39:1n:30:CYS:HB3	39:1n:35:LYS:HB3	1.94	0.48
2:1B:148:GLY:HA2	9:1I:118:TYR:HE1	1.78	0.48
6:1F:66:ARG:HA	6:1F:74:PRO:HA	1.94	0.48
6:1F:193:ILE:HD12	6:1F:204:ARG:CZ	2.42	0.48
8:1H:132:ALA:O	8:1H:136:VAL:HG12	2.14	0.48
8:1H:158:GLY:HA2	8:1H:315:PRO:HG2	1.94	0.48
9:1I:168:ASN:HD21	42:1q:93:MET:HE1	1.77	0.48
13:1M:54:LEU:HD13	33:1h:93:ILE:HG23	1.95	0.48
20:1T:26:ASP:OD2	20:1T:29:LYS:N	2.33	0.48
25:1Z:26:PRO:O	25:1Z:28:ARG:HG2	2.13	0.48
33:1h:68:LYS:HB3	41:1p:62:TYR:CZ	2.48	0.48
38:1m:125:ASN:O	41:1p:139:GLN:NE2	2.46	0.48
39:1n:116:ASP:OD1	39:1n:117:TYR:N	2.46	0.48
3:1C:211:GLN:OE1	21:1V:112:LYS:NZ	2.46	0.48
4:1D:161:ILE:HG23	8:1H:278:PRO:HB3	1.94	0.48
6:1F:125:GLY:C	6:1F:129:MET:HE2	2.39	0.48
7:1G:496:ILE:HG22	7:1G:499:GLN:HB2	1.95	0.48
12:1L:10:THR:O	12:1L:14:ILE:HG12	2.14	0.48
14:1N:258:SER:OG	14:1N:333:SER:O	2.30	0.48
16:1P:69:ILE:HD12	18:1R:26:VAL:HG13	1.95	0.48
16:1P:177:ARG:H	16:1P:180:ASN:HD21	1.62	0.48
17:1Q:35:VAL:HG22	17:1Q:59:PHE:CD2	2.48	0.48
17:1Q:62:ARG:HD3	17:1Q:62:ARG:HA	1.67	0.48
19:1S:81:PHE:CE1	19:1S:85:GLN:HB2	2.49	0.48
20:1U:6:LEU:HD12	20:1U:11:ILE:HD11	1.94	0.48
25:1Z:112:HIS:ND1	25:1Z:112:HIS:O	2.45	0.48
33:1h:12:LYS:O	39:1n:106:TRP:NE1	2.45	0.48
35:1j:37:LEU:HB2	36:1k:77:PHE:CE1	2.49	0.48
37:1l:115:MET:O	37:1l:119:GLY:N	2.44	0.48
1:1A:56:PHE:CZ	11:1K:75:LEU:HB3	2.49	0.48
2:1B:86:MET:O	2:1B:113:VAL:HA	2.13	0.48
2:1B:171:LYS:H	16:1P:52:GLU:CD	2.22	0.48
3:1C:50:ILE:O	3:1C:107:VAL:HA	2.14	0.48
3:1C:76:ALA:HB3	3:1C:95:ASN:HB3	1.94	0.48
4:1D:171:PHE:HA	4:1D:174:ARG:HB2	1.95	0.48
4:1D:282:GLU:HG2	4:1D:313:GLN:HE22	1.79	0.48
5:1E:31:ILE:HA	5:1E:34:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:249:ARG:HA	6:1F:249:ARG:CZ	2.44	0.48
7:1G:528:ASP:OD2	7:1G:545:TYR:OH	2.22	0.48
8:1H:314:ILE:HD12	25:1Z:58:ARG:HD3	1.94	0.48
9:1I:57:LEU:O	43:1r:33:ARG:NH2	2.47	0.48
12:1L:4:PHE:CE2	12:1L:61:MET:HG2	2.49	0.48
12:1L:72:GLN:OE1	13:1M:310:MET:HE1	2.14	0.48
12:1L:142:ILE:HD11	13:1M:371:PRO:HB3	1.96	0.48
12:1L:226:GLN:O	12:1L:230:HIS:N	2.47	0.48
12:1L:306:THR:O	12:1L:310:LEU:HD12	2.13	0.48
13:1M:307:TRP:NE1	38:1m:127:SER:HG	2.10	0.48
16:1P:24:PHE:HZ	16:1P:81:ILE:HG23	1.79	0.48
16:1P:98:GLU:OE2	16:1P:145:TYR:OH	2.31	0.48
22:1W:21:PHE:HB2	22:1W:80:ASP:OD1	2.14	0.48
22:1W:96:VAL:O	22:1W:96:VAL:HG22	2.14	0.48
24:1Y:61:THR:O	24:1Y:65:ILE:HD12	2.13	0.48
26:1a:2:TRP:CZ2	51:1q:201:CDL:PB2	3.01	0.48
32:1g:57:ASN:O	32:1g:61:VAL:HG12	2.14	0.48
34:1i:56:TRP:HE3	34:1i:57:LYS:HZ2	1.61	0.48
37:1l:15:LYS:HD3	37:1l:15:LYS:H	1.78	0.48
3:1C:132:ARG:HH21	3:1C:149:ARG:HB2	1.78	0.48
4:1D:165:THR:N	4:1D:166:PRO:HD2	2.28	0.48
6:1F:30:ASP:OD1	6:1F:35:GLY:N	2.47	0.48
6:1F:127:ARG:HH21	6:1F:171:TYR:HE1	1.62	0.48
7:1G:552:VAL:O	7:1G:555:PRO:HD2	2.14	0.48
7:1G:564:ALA:C	7:1G:569:LYS:HZ1	2.22	0.48
8:1H:228:TYR:HA	8:1H:231:ILE:HG12	1.95	0.48
9:1I:32:ARG:NH2	50:1I:204:PC1:O11	2.40	0.48
9:1I:175:TYR:CE1	43:1r:38:PRO:HG3	2.49	0.48
12:1L:293:ILE:CD1	12:1L:294:THR:HG23	2.44	0.48
13:1M:25:ILE:O	13:1M:29:VAL:HG23	2.14	0.48
13:1M:70:THR:HA	13:1M:103:GLN:HE21	1.79	0.48
13:1M:220:HIS:NE2	13:1M:231:LEU:HD22	2.29	0.48
13:1M:278:ARG:NH2	37:1l:82:ASP:OD1	2.46	0.48
13:1M:369:LEU:HD12	13:1M:370:PRO:HD2	1.95	0.48
14:1N:324:LYS:HA	14:1N:324:LYS:HD2	1.68	0.48
16:1P:137:ALA:HA	16:1P:146:LEU:HB3	1.96	0.48
19:1S:16:ARG:NH2	19:1S:69:ALA:HB2	2.28	0.48
20:1T:37:MET:HE1	20:1T:71:MET:HB3	1.94	0.48
21:1V:80:ILE:HD12	21:1V:81:LEU:N	2.29	0.48
29:1d:26:LEU:HG	29:1d:27:THR:HG23	1.96	0.48
29:1d:111:GLU:OE1	32:1g:119:GLN:NE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:1e:93:PRO:HB3	30:1e:97:HIS:CD2	2.49	0.48
33:1h:91:MET:HG2	41:1p:85:PHE:CD2	2.49	0.48
34:1i:10:ARG:CZ	39:1n:153:LEU:HD22	2.43	0.48
44:1s:73:PRO:HD2	44:1s:74:ARG:N	2.28	0.48
1:1A:13:LEU:HD11	8:1H:14:LEU:HD11	1.95	0.48
45:1A:201:3PE:H3A1	27:1b:22:PHE:HB3	1.95	0.48
2:1B:93:THR:HA	2:1B:132:VAL:HA	1.95	0.48
6:1F:360:GLY:HA2	6:1F:366:ARG:HB2	1.95	0.48
8:1H:87:VAL:HG22	8:1H:88:PRO:HD3	1.95	0.48
10:1J:51:PHE:CE2	10:1J:143:ILE:HG21	2.48	0.48
12:1L:323:HIS:CD2	12:1L:475:MET:HE1	2.48	0.48
12:1L:338:MET:HE1	12:1L:458:LEU:N	2.29	0.48
13:1M:130:LEU:O	13:1M:134:THR:OG1	2.21	0.48
14:1N:87:THR:HG22	14:1N:88:LYS:H	1.79	0.48
15:1O:32:CYS:O	15:1O:182:ARG:NH1	2.47	0.48
15:1O:164:LEU:H	15:1O:164:LEU:HD12	1.79	0.48
18:1R:75:LEU:HD23	18:1R:75:LEU:HA	1.73	0.48
20:1U:27:PRO:HA	20:1U:30:LEU:HD13	1.96	0.48
32:1g:23:THR:OG1	32:1g:24:ILE:N	2.45	0.48
38:1m:44:ARG:NH2	39:1n:148:PRO:HB3	2.28	0.48
1:1A:12:THR:O	1:1A:16:LEU:HG	2.14	0.48
6:1F:121:GLY:HA2	6:1F:232:PRO:HD3	1.95	0.48
7:1G:134:LYS:HB2	18:1R:72:TYR:CD2	2.49	0.48
7:1G:166:ILE:HD12	7:1G:262:TRP:CH2	2.49	0.48
7:1G:381:GLY:O	7:1G:456:SER:OG	2.32	0.48
7:1G:628:PRO:HD3	19:1S:21:HIS:CE1	2.49	0.48
16:1P:74:ASN:O	16:1P:80:SER:OG	2.27	0.48
16:1P:203:GLN:HG2	16:1P:232:GLY:H	1.79	0.48
20:1T:12:LYS:HD2	20:1T:77:VAL:HG21	1.96	0.48
20:1U:64:ASP:OD1	39:1n:17:ARG:HG3	2.12	0.48
23:1X:97:ARG:HA	23:1X:100:ARG:HH11	1.78	0.48
40:1o:88:TYR:CZ	40:1o:92:LEU:HD11	2.48	0.48
4:1D:360:PRO:HG3	4:1D:382:GLY:HA3	1.95	0.48
6:1F:79:TRP:HH2	6:1F:228:VAL:HA	1.79	0.48
6:1F:93:LEU:O	6:1F:135:TYR:N	2.46	0.48
9:1I:128:VAL:HG12	18:1R:69:PRO:HD2	1.96	0.48
11:1K:96:LEU:HD21	14:1N:120:GLN:HB3	1.96	0.48
12:1L:237:MET:SD	12:1L:303:ALA:HB2	2.54	0.48
13:1M:424:ASN:HD21	38:1m:56:LEU:HA	1.79	0.48
15:1O:27:VAL:HG21	15:1O:39:ALA:HA	1.96	0.48
16:1P:57:MET:HE1	16:1P:60:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:1j:29:SER:OG	36:1k:68:LYS:O	2.32	0.48
40:1o:38:MET:HG2	40:1o:57:TYR:CD1	2.49	0.48
7:1G:213:TYR:O	7:1G:216:THR:OG1	2.23	0.47
7:1G:406:VAL:HG23	7:1G:419:TYR:HA	1.95	0.47
7:1G:432:ILE:HD11	7:1G:437:HIS:HD2	1.78	0.47
12:1L:306:THR:O	12:1L:309:GLN:N	2.47	0.47
14:1N:251:MET:HG2	14:1N:293:TYR:CE2	2.49	0.47
16:1P:29:PHE:CD1	16:1P:175:GLU:HG2	2.49	0.47
17:1Q:9:GLN:O	22:1W:19:PRO:HG3	2.14	0.47
18:1R:24:ARG:HB2	18:1R:24:ARG:HH11	1.78	0.47
21:1V:23:LEU:HB3	21:1V:58:VAL:HG21	1.95	0.47
23:1X:143:SER:OG	23:1X:146:ARG:NH2	2.45	0.47
31:1f:26:LEU:H	31:1f:26:LEU:HD12	1.78	0.47
34:1i:68:ILE:HD12	34:1i:69:PHE:N	2.29	0.47
39:1n:41:CYS:O	39:1n:45:ALA:N	2.44	0.47
2:1B:62:MET:HE3	2:1B:69:MET:HE3	1.96	0.47
6:1F:305:PRO:HG3	6:1F:413:TRP:HB3	1.97	0.47
6:1F:395:ILE:HA	6:1F:398:GLN:HB2	1.95	0.47
8:1H:20:LEU:HD23	8:1H:228:TYR:HD1	1.79	0.47
9:1I:65:HIS:CD2	9:1I:113:MET:HE1	2.50	0.47
12:1L:205:ASN:ND2	12:1L:207:GLU:OE2	2.47	0.47
19:1S:63:LYS:NZ	19:1S:76:VAL:O	2.46	0.47
24:1Y:40:ILE:HG23	24:1Y:45:PRO:HG3	1.96	0.47
27:1b:51:ASN:OD1	27:1b:51:ASN:N	2.47	0.47
38:1m:48:LEU:HD23	39:1n:165:LEU:HD21	1.96	0.47
40:1o:46:ASN:HA	40:1o:55:ARG:HH22	1.79	0.47
42:1q:83:PRO:HB2	42:1q:85:GLU:OE1	2.14	0.47
5:1E:199:LEU:HD12	5:1E:202:LEU:HG	1.96	0.47
6:1F:276:LEU:HD21	6:1F:312:CYS:O	2.15	0.47
7:1G:45:ARG:NH2	7:1G:260:GLU:HB3	2.29	0.47
9:1I:128:VAL:HG12	18:1R:68:HIS:HB2	1.95	0.47
12:1L:163:ASP:N	12:1L:163:ASP:OD1	2.47	0.47
13:1M:243:MET:O	13:1M:247:THR:OG1	2.20	0.47
16:1P:141:SER:OG	16:1P:146:LEU:HB2	2.15	0.47
17:1Q:39:VAL:HG11	17:1Q:108:ARG:HG3	1.96	0.47
20:1T:42:LEU:HD13	20:1T:46:ASP:HB3	1.96	0.47
20:1U:66:ASP:OD2	20:1U:66:ASP:N	2.37	0.47
20:1U:84:LYS:HB2	20:1U:84:LYS:HE2	1.61	0.47
21:1V:100:GLU:OE1	21:1V:100:GLU:N	2.47	0.47
23:1X:102:GLN:H	23:1X:102:GLN:CD	2.20	0.47
30:1e:93:PRO:HB3	30:1e:97:HIS:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:8:LEU:HD11	39:1n:174:ARG:CZ	2.44	0.47
37:1l:34:TYR:CD1	37:1l:48:PRO:HB3	2.49	0.47
39:1n:48:ASP:N	39:1n:48:ASP:OD1	2.40	0.47
1:1A:48:ARG:NH1	10:1J:80:PRO:HD3	2.25	0.47
6:1F:343:ILE:HD12	6:1F:344:VAL:H	1.78	0.47
7:1G:177:ARG:HG2	7:1G:178:GLY:N	2.29	0.47
8:1H:276:SER:C	8:1H:277:TYR:HD1	2.22	0.47
12:1L:132:VAL:HG23	12:1L:258:PHE:CZ	2.49	0.47
12:1L:143:GLY:O	12:1L:147:VAL:HG12	2.14	0.47
14:1N:187:MET:HE2	14:1N:187:MET:HA	1.95	0.47
14:1N:276:ILE:HD12	57:1Y:201:PGT:H2	1.96	0.47
16:1P:41:MET:H	16:1P:41:MET:CE	2.27	0.47
19:1S:18:ILE:HG23	19:1S:52:ILE:HG23	1.97	0.47
19:1S:30:GLN:OE1	19:1S:33:ARG:NH1	2.41	0.47
20:1U:8:LEU:HG	20:1U:88:GLU:OE1	2.14	0.47
22:1W:36:TYR:O	22:1W:40:TYR:N	2.47	0.47
23:1X:25:LYS:NZ	23:1X:94:GLN:HB2	2.29	0.47
33:1h:21:PHE:CZ	33:1h:25:MET:HE1	2.50	0.47
33:1h:32:THR:C	33:1h:35:PRO:HD2	2.39	0.47
38:1m:24:ILE:HD13	38:1m:29:ARG:HD3	1.96	0.47
38:1m:122:GLN:O	41:1p:139:GLN:NE2	2.47	0.47
41:1p:98:ASP:OD2	41:1p:141:ARG:NH1	2.48	0.47
1:1A:106:TRP:CH2	27:1b:18:LEU:HD21	2.49	0.47
2:1B:88:VAL:O	2:1B:116:MET:HB3	2.15	0.47
4:1D:200:HIS:NE2	9:1I:124:GLU:OE2	2.47	0.47
7:1G:278:ARG:HH12	7:1G:549:HIS:CD2	2.32	0.47
7:1G:358:LEU:HD23	19:1S:54:ILE:HD11	1.95	0.47
7:1G:365:ASN:HB3	7:1G:488:LYS:HZ3	1.79	0.47
7:1G:695:ILE:HD12	7:1G:696:GLN:N	2.30	0.47
8:1H:301:CYS:O	8:1H:305:ILE:HG22	2.14	0.47
14:1N:54:GLU:HB3	14:1N:58:LYS:NZ	2.29	0.47
20:1T:35:HIS:HB3	20:1T:38:LYS:HG3	1.97	0.47
20:1U:8:LEU:HA	20:1U:11:ILE:HD13	1.96	0.47
23:1X:141:TYR:O	25:1Z:115:ARG:NH1	2.42	0.47
25:1Z:51:MET:SD	25:1Z:55:ARG:NH2	2.87	0.47
26:1a:13:ALA:O	26:1a:17:PHE:HB2	2.14	0.47
32:1g:24:ILE:O	32:1g:26:LEU:N	2.47	0.47
35:1j:51:PHE:HB3	40:1o:91:HIS:CD2	2.50	0.47
41:1p:75:GLU:OE1	41:1p:75:GLU:N	2.43	0.47
42:1q:14:VAL:HA	42:1q:23:TYR:CD2	2.48	0.47
4:1D:151:ILE:HD11	4:1D:218:PHE:HZ	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:279:LEU:HA	6:1F:283:HIS:ND1	2.29	0.47
15:1O:147:GLN:NE2	15:1O:148:CYS:SG	2.87	0.47
17:1Q:59:PHE:CD1	17:1Q:79:LEU:HB3	2.50	0.47
20:1T:36:PHE:HD1	20:1T:40:LEU:HD12	1.80	0.47
29:1d:51:ARG:O	29:1d:53:VAL:N	2.43	0.47
41:1p:162:MET:H	41:1p:162:MET:CE	2.28	0.47
2:1B:90:GLY:HA2	46:1B:201:SF4:S2	2.55	0.47
2:1B:116:MET:HE1	2:1B:156:LEU:HB2	1.96	0.47
3:1C:108:LYS:HE2	3:1C:108:LYS:HB2	1.63	0.47
4:1D:255:PHE:CZ	4:1D:405:MET:HE1	2.50	0.47
5:1E:87:TYR:HB3	6:1F:181:ALA:O	2.14	0.47
5:1E:108:CYS:HB3	5:1E:113:SER:OG	2.15	0.47
5:1E:137:PHE:HZ	5:1E:176:LEU:HB3	1.80	0.47
6:1F:49:LEU:HD21	6:1F:124:VAL:HG12	1.96	0.47
6:1F:57:LEU:HD22	6:1F:80:SER:HB3	1.96	0.47
6:1F:104:THR:HG22	6:1F:106:LYS:HZ3	1.79	0.47
6:1F:134:ALA:HB3	6:1F:175:VAL:HA	1.96	0.47
7:1G:349:PHE:CE2	7:1G:362:TYR:HB3	2.50	0.47
7:1G:447:LYS:HE2	7:1G:447:LYS:N	2.30	0.47
7:1G:534:ARG:HG2	42:1q:145:LYS:HB2	1.97	0.47
8:1H:31:MET:SD	9:1I:41:LEU:HB2	2.55	0.47
8:1H:153:VAL:O	8:1H:174:MET:HE1	2.14	0.47
8:1H:186:PHE:O	8:1H:190:LEU:HD12	2.15	0.47
8:1H:233:MET:HE3	8:1H:234:MET:N	2.30	0.47
10:1J:4:TYR:O	10:1J:7:PHE:HB2	2.14	0.47
10:1J:38:GLY:HA2	10:1J:57:PHE:CE1	2.46	0.47
12:1L:483:PRO:HG3	35:1j:53:TYR:CZ	2.50	0.47
14:1N:58:LYS:O	14:1N:62:THR:HG22	2.14	0.47
14:1N:100:MET:HB3	14:1N:111:PHE:CE2	2.49	0.47
14:1N:311:MET:HE2	14:1N:311:MET:HB2	1.79	0.47
15:1O:24:VAL:O	15:1O:166:PRO:HB3	2.13	0.47
16:1P:26:ALA:HB3	16:1P:47:VAL:HG23	1.95	0.47
16:1P:172:PHE:CD2	16:1P:204:PRO:HB2	2.49	0.47
20:1T:47:GLN:HG2	20:1T:50:ILE:HD11	1.95	0.47
20:1T:58:PHE:HB2	20:1T:60:PHE:CD1	2.49	0.47
22:1W:43:VAL:HB	22:1W:60:ARG:HE	1.80	0.47
22:1W:63:VAL:O	22:1W:67:PHE:HD1	1.96	0.47
25:1Z:93:GLU:HG3	30:1e:97:HIS:CE1	2.50	0.47
25:1Z:120:MET:SD	25:1Z:121:MET:N	2.87	0.47
35:1j:33:TRP:CZ2	36:1k:67:LEU:HA	2.50	0.47
42:1q:68:MET:HG3	42:1q:115:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:12:ARG:HA	4:1D:129:GLN:HG2	1.96	0.47
3:1C:158:GLU:OE2	17:1Q:24:GLY:HA3	2.15	0.47
4:1D:423:ILE:O	4:1D:423:ILE:HD12	2.15	0.47
5:1E:159:ASN:HB2	5:1E:184:PRO:HB3	1.97	0.47
6:1F:305:PRO:HD2	6:1F:327:THR:HA	1.97	0.47
8:1H:149:ILE:HG12	8:1H:181:LEU:HD22	1.97	0.47
12:1L:71:LEU:HD12	13:1M:307:TRP:CZ2	2.50	0.47
12:1L:81:LYS:CD	12:1L:83:ASP:HB2	2.45	0.47
15:1O:226:ARG:HH21	15:1O:229:GLU:HG2	1.80	0.47
16:1P:37:HIS:O	16:1P:41:MET:HE1	2.14	0.47
16:1P:135:LEU:HB3	16:1P:169:SER:HA	1.97	0.47
16:1P:208:VAL:HG12	16:1P:212:LYS:HZ2	1.79	0.47
21:1V:52:ASN:HA	21:1V:55:LEU:HB3	1.97	0.47
3:1C:75:LEU:HB2	3:1C:124:TYR:CD2	2.49	0.47
5:1E:21:PHE:CD2	5:1E:65:ALA:HA	2.50	0.47
5:1E:143:GLU:HG2	6:1F:353:PHE:HD1	1.78	0.47
5:1E:146:GLY:HA3	6:1F:142:PHE:CZ	2.50	0.47
6:1F:243:ALA:HA	6:1F:251:SER:HB2	1.97	0.47
7:1G:50:GLY:HA2	7:1G:69:CYS:SG	2.55	0.47
7:1G:378:LEU:HD11	7:1G:439:PHE:HE1	1.80	0.47
8:1H:314:ILE:HD11	27:1b:44:ILE:HD11	1.97	0.47
9:1I:26:LEU:O	9:1I:28:THR:N	2.48	0.47
9:1I:28:THR:HB	9:1I:32:ARG:NH2	2.30	0.47
12:1L:51:LEU:HD22	12:1L:91:PRO:HG2	1.96	0.47
13:1M:14:MET:HG3	31:1f:12:VAL:HB	1.97	0.47
17:1Q:88:THR:HG23	17:1Q:90:GLU:OE1	2.15	0.47
22:1W:90:LEU:HD12	22:1W:91:GLU:H	1.80	0.47
32:1g:61:VAL:HG13	32:1g:62:PHE:CD1	2.48	0.47
33:1h:49:GLU:OE2	33:1h:69:HIS:ND1	2.34	0.47
37:1l:60:PRO:HB2	39:1n:85:PRO:HG3	1.97	0.47
51:1q:201:CDL:H162	51:1q:201:CDL:H331	1.97	0.47
4:1D:257:GLY:HA3	4:1D:372:GLY:HA2	1.96	0.47
6:1F:21:ILE:HG12	6:1F:230:VAL:HG12	1.97	0.47
6:1F:105:CYS:O	6:1F:109:GLU:HG2	2.15	0.47
7:1G:117:GLN:NE2	46:1G:801:SF4:S3	2.88	0.47
7:1G:283:MET:SD	7:1G:291:LEU:HB3	2.55	0.47
7:1G:347:GLU:OE1	7:1G:455:SER:OG	2.33	0.47
10:1J:125:TRP:HB2	25:1Z:137:THR:HG21	1.97	0.47
14:1N:109:SER:O	14:1N:112:HIS:ND1	2.39	0.47
14:1N:335:LEU:O	29:1d:37:LEU:HD21	2.14	0.47
19:1S:17:GLU:OE2	19:1S:51:PRO:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:44:LEU:H	25:1Z:44:LEU:HD12	1.79	0.47
37:1l:58:ARG:HH12	37:1l:71:LEU:HD23	1.80	0.47
37:1l:111:PHE:O	37:1l:115:MET:HE3	2.15	0.47
5:1E:42:HIS:HD2	6:1F:216:PHE:HB3	1.80	0.46
6:1F:117:LYS:H	6:1F:117:LYS:HE2	1.80	0.46
6:1F:277:LYS:HE2	6:1F:277:LYS:HB2	1.65	0.46
6:1F:317:MET:N	6:1F:317:MET:SD	2.87	0.46
8:1H:26:LYS:HA	8:1H:36:GLY:HA3	1.97	0.46
8:1H:307:LEU:HB3	8:1H:308:PRO:HD3	1.97	0.46
10:1J:78:MET:O	10:1J:79:TYR:HD2	1.98	0.46
12:1L:8:THR:HG21	12:1L:82:MET:HG3	1.97	0.46
12:1L:81:LYS:C	12:1L:82:MET:HE2	2.40	0.46
12:1L:226:GLN:HG2	12:1L:314:MET:HE1	1.96	0.46
15:1O:8:PHE:O	15:1O:13:ARG:NH1	2.43	0.46
15:1O:279:LEU:HD12	15:1O:282:ILE:H	1.79	0.46
19:1S:30:GLN:HA	19:1S:33:ARG:HB3	1.98	0.46
32:1g:110:SER:HA	41:1p:137:ALA:HB1	1.97	0.46
34:1i:9:LEU:O	34:1i:13:GLN:HG2	2.15	0.46
1:1A:97:LEU:HD12	1:1A:97:LEU:HA	1.70	0.46
4:1D:173:GLU:HA	4:1D:176:LYS:HG3	1.97	0.46
6:1F:248:GLU:C	6:1F:250:ASN:H	2.22	0.46
9:1I:143:THR:OG1	9:1I:146:GLU:OE2	2.28	0.46
10:1J:36:SER:HA	10:1J:39:VAL:HG12	1.96	0.46
12:1L:71:LEU:HD12	13:1M:307:TRP:CE2	2.50	0.46
12:1L:161:ARG:NH1	39:1n:88:THR:O	2.40	0.46
12:1L:355:ASP:OD1	12:1L:357:ARG:NE	2.41	0.46
14:1N:309:ASN:HD21	14:1N:312:LYS:HE3	1.80	0.46
16:1P:185:MET:HA	16:1P:185:MET:HE3	1.97	0.46
19:1S:23:CYS:HB3	19:1S:26:SER:OG	2.15	0.46
20:1U:47:GLN:HA	20:1U:50:ILE:HG13	1.97	0.46
21:1V:26:LEU:O	21:1V:30:ILE:HD12	2.15	0.46
23:1X:51:ASP:HB3	23:1X:54:ARG:HG2	1.97	0.46
25:1Z:120:MET:HB3	25:1Z:123:GLU:OE1	2.16	0.46
27:1b:31:LEU:HA	27:1b:34:LEU:HB2	1.97	0.46
27:1b:52:TYR:HD1	27:1b:53:PRO:N	2.12	0.46
35:1j:67:LEU:O	40:1o:110:ARG:NE	2.49	0.46
2:1B:81:ARG:HD3	8:1H:214:GLU:HA	1.97	0.46
4:1D:347:HIS:O	4:1D:351:LEU:HB2	2.16	0.46
5:1E:150:ASN:HB3	5:1E:163:ASP:H	1.79	0.46
7:1G:159:CYS:HA	7:1G:199:ILE:HD11	1.97	0.46
12:1L:226:GLN:CG	12:1L:314:MET:HE1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:310:LEU:HA	12:1L:313:MET:HG3	1.96	0.46
13:1M:421:HIS:HB3	38:1m:50:TYR:OH	2.15	0.46
14:1N:339:MET:HE1	29:1d:30:ARG:HG2	1.96	0.46
15:1O:167:HIS:HE2	15:1O:248:TRP:CD1	2.33	0.46
16:1P:278:TRP:CD1	16:1P:278:TRP:H	2.32	0.46
20:1T:81:ALA:HA	20:1T:84:LYS:HZ1	1.80	0.46
35:1j:39:ARG:O	35:1j:43:ASP:N	2.44	0.46
41:1p:136:LYS:HB3	41:1p:136:LYS:HE3	1.64	0.46
2:1B:34:ASP:HB2	2:1B:173:LEU:HB2	1.97	0.46
2:1B:95:LYS:HD3	4:1D:82:LEU:HD23	1.96	0.46
3:1C:68:THR:HA	21:1V:82:GLN:HE21	1.80	0.46
4:1D:5:GLN:NE2	14:1N:304:MET:HB2	2.31	0.46
5:1E:167:LYS:HE2	5:1E:167:LYS:HB2	1.64	0.46
6:1F:226:GLU:HA	6:1F:229:ALA:HB3	1.97	0.46
6:1F:319:PHE:HD1	6:1F:329:LEU:HB3	1.81	0.46
7:1G:38:PRO:HG3	7:1G:123:PHE:CE2	2.50	0.46
7:1G:195:LEU:HD12	7:1G:198:ASN:HD21	1.80	0.46
10:1J:105:TYR:O	10:1J:109:LYS:HG2	2.15	0.46
12:1L:69:MET:CE	12:1L:71:LEU:HD23	2.46	0.46
12:1L:291:CYS:O	12:1L:295:GLN:NE2	2.42	0.46
13:1M:367:LEU:HD21	13:1M:404:ALA:HA	1.97	0.46
15:1O:19:THR:OG1	15:1O:20:GLU:N	2.48	0.46
16:1P:186:ARG:HG3	16:1P:187:TRP:HD1	1.80	0.46
19:1S:19:ARG:N	19:1S:65:TRP:O	2.41	0.46
19:1S:32:VAL:HA	19:1S:35:PHE:HB3	1.97	0.46
20:1U:51:ILE:HD12	20:1U:52:MET:H	1.81	0.46
21:1V:91:ARG:CZ	21:1V:92:LYS:HA	2.45	0.46
22:1W:17:VAL:HG22	22:1W:18:LYS:N	2.31	0.46
25:1Z:97:ILE:HD11	30:1e:82:ARG:HA	1.96	0.46
31:1f:7:VAL:O	31:1f:11:TRP:HB3	2.16	0.46
34:1i:54:ALA:HB3	34:1i:57:LYS:HZ3	1.79	0.46
41:1p:139:GLN:O	41:1p:157:LYS:NZ	2.48	0.46
2:1B:114:VAL:HG13	2:1B:144:ILE:HG22	1.98	0.46
4:1D:66:MET:N	4:1D:66:MET:HE3	2.30	0.46
4:1D:112:MET:HG3	4:1D:194:ILE:HG12	1.98	0.46
4:1D:184:VAL:HG23	4:1D:185:SER:H	1.80	0.46
5:1E:42:HIS:CD2	6:1F:216:PHE:HB3	2.50	0.46
6:1F:275:PRO:HD3	6:1F:316:LEU:HG	1.98	0.46
7:1G:226:GLU:HA	7:1G:253:ARG:HH12	1.81	0.46
8:1H:14:LEU:HD21	8:1H:83:LEU:HD21	1.98	0.46
8:1H:54:LYS:HD3	8:1H:55:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:1H:260:VAL:O	8:1H:264:LEU:HD22	2.16	0.46
9:1I:67:LEU:O	9:1I:158:GLY:HA3	2.16	0.46
10:1J:119:PHE:CZ	11:1K:1:FME:HE2	2.51	0.46
11:1K:16:LEU:HD12	11:1K:20:LEU:HD13	1.97	0.46
12:1L:286:LEU:HD21	45:1L:703:3PE:H2D1	1.97	0.46
13:1M:114:GLU:OE2	13:1M:174:LEU:HB2	2.15	0.46
15:1O:116:LEU:HD21	15:1O:259:LEU:HD23	1.96	0.46
17:1Q:123:SER:OG	17:1Q:124:TRP:N	2.47	0.46
20:1T:17:TYR:HA	20:1T:20:LYS:HZ2	1.80	0.46
20:1U:12:LYS:HA	20:1U:15:VAL:HB	1.96	0.46
26:1a:3:PHE:CE1	51:1q:201:CDL:HA21	2.50	0.46
29:1d:73:TYR:O	29:1d:77:LYS:HG3	2.15	0.46
32:1g:63:PHE:O	32:1g:67:SER:HB3	2.15	0.46
32:1g:63:PHE:O	32:1g:68:ILE:HG13	2.15	0.46
33:1h:34:ILE:CG1	33:1h:35:PRO:HD3	2.45	0.46
44:1s:52:LEU:HA	44:1s:55:ASN:HB3	1.97	0.46
2:1B:116:MET:SD	2:1B:151:PRO:HG2	2.56	0.46
2:1B:117:GLY:O	2:1B:121:ASN:ND2	2.49	0.46
4:1D:233:ARG:NH2	9:1I:27:TRP:HA	2.31	0.46
6:1F:106:LYS:H	6:1F:106:LYS:HD2	1.80	0.46
6:1F:267:THR:O	6:1F:267:THR:OG1	2.29	0.46
6:1F:438:GLN:OE1	6:1F:438:GLN:N	2.45	0.46
7:1G:87:LYS:HB2	7:1G:87:LYS:HE3	1.79	0.46
9:1I:12:MET:HE2	9:1I:12:MET:HA	1.98	0.46
9:1I:42:PHE:HA	26:1a:2:TRP:CD1	2.50	0.46
9:1I:161:TRP:O	9:1I:165:ILE:HG13	2.15	0.46
10:1J:77:GLU:HB3	11:1K:25:HIS:CE1	2.50	0.46
12:1L:419:THR:HA	12:1L:422:TYR:CZ	2.51	0.46
12:1L:489:THR:O	12:1L:493:VAL:HG22	2.15	0.46
14:1N:7:THR:HG21	51:1N:402:CDL:H352	1.98	0.46
14:1N:73:ALA:HB2	14:1N:97:MET:HG3	1.97	0.46
16:1P:34:VAL:O	16:1P:38:LEU:N	2.42	0.46
16:1P:170:ASP:OD1	16:1P:170:ASP:N	2.48	0.46
18:1R:9:GLU:OE2	18:1R:18:TYR:HB2	2.14	0.46
20:1U:78:ASP:HB3	34:1i:15:ARG:NE	2.30	0.46
21:1V:75:GLN:OE1	21:1V:76:ILE:N	2.44	0.46
24:1Y:139:LYS:HE2	33:1h:112:ARG:HD2	1.96	0.46
27:1b:37:TYR:HD1	27:1b:40:TYR:HD2	1.63	0.46
40:1o:1:GLY:H3	40:1o:3:HIS:CD2	2.33	0.46
1:1A:25:PRO:HB2	8:1H:59:GLU:HA	1.97	0.46
1:1A:80:GLN:NE2	8:1H:314:ILE:HD13	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:106:TRP:CE3	45:1A:201:3PE:H252	2.51	0.46
4:1D:33:TRP:CG	15:1O:275:ILE:HD11	2.49	0.46
5:1E:93:LYS:HE2	5:1E:93:LYS:HB2	1.73	0.46
5:1E:171:GLU:HA	5:1E:174:ASP:HB2	1.98	0.46
6:1F:15:LEU:HB2	6:1F:271:GLU:H	1.80	0.46
6:1F:296:ALA:HA	6:1F:308:PRO:HA	1.97	0.46
7:1G:564:ALA:HB1	7:1G:568:GLU:HG2	1.98	0.46
12:1L:250:SER:HB2	12:1L:333:ALA:HA	1.98	0.46
12:1L:558:LEU:HD22	13:1M:211:GLY:HA2	1.98	0.46
13:1M:122:PHE:CZ	13:1M:206:LYS:HD2	2.51	0.46
14:1N:120:GLN:OE1	14:1N:176:ARG:NH2	2.49	0.46
15:1O:226:ARG:O	15:1O:229:GLU:HG3	2.15	0.46
20:1T:19:LEU:HD22	20:1T:30:LEU:HD23	1.97	0.46
21:1V:93:MET:HG2	21:1V:96:TRP:CD1	2.49	0.46
40:1o:3:HIS:CD2	40:1o:4:LEU:HD22	2.50	0.46
40:1o:68:CYS:O	40:1o:72:SER:HB3	2.15	0.46
43:1r:104:GLU:OE2	43:1r:107:LYS:NZ	2.47	0.46
3:1C:57:VAL:HG11	3:1C:117:ILE:HG23	1.98	0.46
3:1C:58:ILE:HD11	3:1C:118:GLU:HG3	1.97	0.46
4:1D:347:HIS:CG	7:1G:121:MET:HE1	2.51	0.46
6:1F:319:PHE:CD1	6:1F:329:LEU:HB3	2.51	0.46
6:1F:376:MET:HE3	6:1F:377:ALA:N	2.30	0.46
7:1G:323:VAL:O	7:1G:498:SER:HB3	2.16	0.46
8:1H:85:MET:HA	8:1H:85:MET:HE3	1.98	0.46
8:1H:260:VAL:O	8:1H:263:THR:HG22	2.16	0.46
12:1L:69:MET:HE1	12:1L:71:LEU:HD23	1.97	0.46
12:1L:297:ASP:HB3	12:1L:300:LYS:HG2	1.97	0.46
12:1L:554:ASP:OD1	13:1M:288:TYR:OH	2.33	0.46
12:1L:557:TRP:O	12:1L:561:ILE:HG22	2.15	0.46
12:1L:571:MET:HE3	12:1L:571:MET:HB3	1.80	0.46
15:1O:132:PHE:C	15:1O:132:PHE:CD2	2.94	0.46
16:1P:9:GLY:HA3	16:1P:15:SER:HB3	1.98	0.46
16:1P:87:HIS:HB3	18:1R:23:TYR:HA	1.96	0.46
16:1P:289:MET:HE3	16:1P:289:MET:C	2.40	0.46
19:1S:16:ARG:HG2	19:1S:67:ARG:HH21	1.80	0.46
20:1U:64:ASP:HA	20:1U:67:ALA:HB3	1.98	0.46
23:1X:30:HIS:HA	23:1X:34:GLN:HE22	1.81	0.46
25:1Z:50:MET:HE2	25:1Z:50:MET:HA	1.97	0.46
35:1j:32:MET:O	35:1j:36:ILE:HG22	2.16	0.46
38:1m:82:THR:HG23	38:1m:84:LYS:H	1.80	0.46
41:1p:76:CYS:SG	41:1p:84:MET:HG2	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:52:ASN:O	43:1r:28:GLN:NE2	2.37	0.46
2:1B:81:ARG:NH1	2:1B:106:GLN:HG3	2.30	0.46
3:1C:110:TYR:HB3	21:1V:110:GLN:NE2	2.29	0.46
3:1C:189:GLU:HG3	3:1C:189:GLU:O	2.15	0.46
5:1E:49:PRO:HA	5:1E:52:ASP:HB3	1.97	0.46
5:1E:165:THR:H	5:1E:168:ASP:HB2	1.80	0.46
6:1F:46:LYS:HE2	6:1F:168:GLY:HA3	1.98	0.46
6:1F:46:LYS:HG3	6:1F:167:CYS:O	2.16	0.46
6:1F:133:ALA:HA	6:1F:174:ASP:H	1.80	0.46
7:1G:274:LEU:HD13	7:1G:278:ARG:HH21	1.80	0.46
7:1G:427:LYS:NZ	7:1G:431:ASP:OD2	2.48	0.46
7:1G:616:LEU:O	7:1G:619:VAL:HG12	2.16	0.46
8:1H:184:MET:HE1	8:1H:293:PHE:CG	2.51	0.46
10:1J:68:PHE:HD1	11:1K:27:MET:HE1	1.81	0.46
12:1L:122:VAL:O	12:1L:126:ILE:HG12	2.15	0.46
12:1L:151:SER:HB2	12:1L:252:MET:HE3	1.97	0.46
12:1L:564:LYS:HG3	38:1m:76:TYR:CE2	2.50	0.46
13:1M:47:GLU:HB3	41:1p:92:ARG:NE	2.31	0.46
13:1M:204:MET:HE1	13:1M:209:LEU:HD13	1.97	0.46
14:1N:40:MET:O	14:1N:40:MET:HE3	2.16	0.46
14:1N:218:LEU:HD12	14:1N:326:LEU:HD21	1.97	0.46
15:1O:207:LYS:HE2	15:1O:207:LYS:HB2	1.63	0.46
17:1Q:27:GLU:O	17:1Q:30:ILE:HG22	2.15	0.46
22:1W:17:VAL:C	22:1W:18:LYS:HE2	2.41	0.46
28:1c:35:HIS:CD2	29:1d:26:LEU:HB3	2.51	0.46
44:1s:49:TYR:O	44:1s:53:ASP:N	2.46	0.46
2:1B:65:PRO:HG3	8:1H:32:GLN:O	2.15	0.46
3:1C:20:LYS:HD3	3:1C:21:GLN:H	1.81	0.46
3:1C:79:THR:HB	4:1D:390:LYS:HE3	1.98	0.46
3:1C:114:LEU:O	22:1W:20:ILE:HD12	2.16	0.46
6:1F:189:GLU:HB2	6:1F:222:VAL:HG11	1.97	0.46
6:1F:261:HIS:HB2	6:1F:337:MET:HA	1.98	0.46
7:1G:74:MET:HE1	7:1G:77:TRP:CZ3	2.50	0.46
7:1G:667:THR:OG1	7:1G:669:LYS:HG2	2.16	0.46
9:1I:78:ILE:HD11	9:1I:80:CYS:HB3	1.98	0.46
10:1J:162:LEU:O	10:1J:166:VAL:HG13	2.16	0.46
12:1L:370:THR:HA	12:1L:431:PHE:CE2	2.51	0.46
13:1M:329:LEU:HA	13:1M:437:MET:HE1	1.98	0.46
14:1N:36:ASN:OD1	14:1N:134:GLN:NE2	2.49	0.46
14:1N:275:SER:HB2	24:1Y:136:ALA:HB3	1.97	0.46
15:1O:28:ASP:OD2	15:1O:126:ARG:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:1R:55:ARG:NH2	18:1R:76:ASP:OD2	2.37	0.46
19:1S:17:GLU:HG2	19:1S:67:ARG:CZ	2.46	0.46
33:1h:13:PRO:HD3	39:1n:98:VAL:HG21	1.97	0.46
36:1k:64:GLY:HA2	36:1k:67:LEU:HD11	1.97	0.46
1:1A:13:LEU:O	1:1A:17:LEU:HB2	2.15	0.45
2:1B:59:MET:HE3	2:1B:60:MET:N	2.31	0.45
2:1B:91:THR:HG22	2:1B:119:CYS:SG	2.56	0.45
3:1C:79:THR:HB	4:1D:390:LYS:HG2	1.97	0.45
7:1G:409:ILE:HG22	7:1G:422:LEU:HB2	1.97	0.45
7:1G:539:LYS:HD3	42:1q:145:LYS:NZ	2.32	0.45
9:1I:63:GLY:H	9:1I:133:GLU:HG2	1.81	0.45
11:1K:2:PRO:HG2	11:1K:5:TYR:CD2	2.51	0.45
12:1L:4:PHE:CD2	12:1L:61:MET:HG2	2.50	0.45
12:1L:64:SER:N	34:1i:95:THR:O	2.49	0.45
13:1M:433:GLU:O	13:1M:437:MET:HG2	2.16	0.45
15:1O:32:CYS:C	15:1O:182:ARG:HH12	2.24	0.45
16:1P:196:LEU:HD13	16:1P:257:PRO:HD3	1.98	0.45
20:1T:79:TYR:CZ	20:1T:83:LYS:HD2	2.50	0.45
20:1U:83:LYS:HD2	20:1U:83:LYS:HA	1.66	0.45
21:1V:66:LYS:HB3	21:1V:66:LYS:HE2	1.78	0.45
23:1X:77:CYS:O	23:1X:80:PRO:HD2	2.15	0.45
34:1i:69:PHE:O	34:1i:73:HIS:HB2	2.16	0.45
2:1B:68:ASP:OD1	8:1H:34:ARG:HD2	2.16	0.45
3:1C:56:GLY:O	3:1C:60:VAL:HG22	2.16	0.45
4:1D:326:ASP:HB2	43:1r:44:PRO:HD2	1.99	0.45
5:1E:156:ILE:HG21	5:1E:176:LEU:HD21	1.98	0.45
6:1F:300:GLY:HA3	6:1F:329:LEU:O	2.17	0.45
6:1F:327:THR:OG1	6:1F:328:GLY:N	2.46	0.45
7:1G:314:ASP:OD1	7:1G:314:ASP:N	2.47	0.45
7:1G:357:ASP:O	19:1S:55:ARG:NH1	2.49	0.45
7:1G:568:GLU:OE1	7:1G:568:GLU:N	2.49	0.45
8:1H:206:GLU:OE1	8:1H:279:ARG:NH1	2.50	0.45
10:1J:57:PHE:HA	10:1J:61:LEU:HD23	1.97	0.45
10:1J:160:SER:O	10:1J:164:GLY:N	2.49	0.45
12:1L:73:THR:O	41:1p:106:GLN:NE2	2.50	0.45
12:1L:323:HIS:CG	12:1L:475:MET:HE1	2.52	0.45
14:1N:57:THR:O	14:1N:61:LEU:HD23	2.17	0.45
14:1N:174:GLN:O	14:1N:178:ILE:HG13	2.16	0.45
32:1g:25:ARG:C	32:1g:26:LEU:HD12	2.41	0.45
40:1o:24:PHE:HB2	40:1o:103:ARG:HH21	1.81	0.45
40:1o:98:MET:H	40:1o:98:MET:CE	2.29	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:1p:34:LYS:O	41:1p:38:LEU:HD12	2.16	0.45
2:1B:68:ASP:CG	8:1H:34:ARG:HB3	2.42	0.45
4:1D:391:ILE:O	4:1D:391:ILE:HD12	2.16	0.45
5:1E:97:LYS:HD2	5:1E:97:LYS:HA	1.67	0.45
6:1F:93:LEU:HD22	6:1F:94:VAL:N	2.31	0.45
6:1F:189:GLU:HA	6:1F:192:LEU:HB3	1.99	0.45
6:1F:199:LYS:HE2	17:1Q:132:THR:HA	1.98	0.45
7:1G:522:LEU:HB3	7:1G:543:ILE:HG13	1.97	0.45
8:1H:264:LEU:HA	8:1H:267:THR:OG1	2.17	0.45
10:1J:96:GLY:HA2	10:1J:99:MET:HE1	1.97	0.45
18:1R:60:ASP:OD2	18:1R:60:ASP:C	2.59	0.45
20:1T:65:ILE:HD12	20:1T:66:ASP:N	2.32	0.45
20:1U:52:MET:HA	20:1U:55:GLU:HB2	1.98	0.45
24:1Y:16:GLU:OE1	24:1Y:18:HIS:NE2	2.48	0.45
26:1a:28:LYS:HE3	26:1a:28:LYS:HB3	1.60	0.45
27:1b:14:LYS:H	27:1b:14:LYS:HD3	1.81	0.45
27:1b:40:TYR:HB3	27:1b:83:LEU:HD21	1.98	0.45
34:1i:24:ASP:OD2	39:1n:124:TRP:NE1	2.49	0.45
38:1m:47:LEU:HA	38:1m:50:TYR:HB3	1.99	0.45
2:1B:158:TYR:HE2	42:1q:78:ASP:OD1	2.00	0.45
3:1C:71:GLN:HE22	3:1C:100:ARG:NH1	2.14	0.45
4:1D:107:ASP:CB	4:1D:114:ASN:HD21	2.28	0.45
5:1E:34:ILE:CD1	44:1s:55:ASN:HD21	2.28	0.45
8:1H:202:GLU:HB3	8:1H:204:GLU:OE2	2.16	0.45
12:1L:331:MET:HB3	12:1L:387:THR:HG22	1.98	0.45
13:1M:329:LEU:HD12	13:1M:359:TRP:CD2	2.51	0.45
14:1N:211:MET:SD	14:1N:333:SER:OG	2.74	0.45
14:1N:300:SER:OG	14:1N:301:SER:N	2.50	0.45
15:1O:100:LEU:HD13	52:1O:401:GTP:C2	2.51	0.45
15:1O:212:PRO:O	15:1O:215:SER:OG	2.28	0.45
15:1O:246:GLY:O	15:1O:249:PRO:HD2	2.17	0.45
16:1P:50:ARG:HH21	54:1P:501:NDP:C4A	2.29	0.45
16:1P:198:LYS:HA	16:1P:237:LEU:HD21	1.97	0.45
20:1T:72:CYS:HB3	20:1T:75:GLU:OE1	2.16	0.45
24:1Y:49:LEU:HD23	24:1Y:49:LEU:H	1.81	0.45
27:1b:15:GLU:OE2	27:1b:18:LEU:N	2.49	0.45
27:1b:26:GLY:O	27:1b:30:ILE:HG12	2.16	0.45
35:1j:45:ASP:O	35:1j:50:HIS:N	2.49	0.45
40:1o:115:GLU:OE1	40:1o:116:GLN:NE2	2.50	0.45
1:1A:4:MET:O	1:1A:8:LEU:N	2.41	0.45
3:1C:83:VAL:HB	3:1C:86:ARG:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:33:TRP:CD2	15:1O:275:ILE:HD11	2.52	0.45
4:1D:71:GLU:OE1	4:1D:71:GLU:N	2.42	0.45
6:1F:28:ARG:HD3	44:1s:37:THR:O	2.15	0.45
7:1G:231:MET:N	7:1G:231:MET:HE2	2.31	0.45
8:1H:134:ARG:HG2	8:1H:282:TYR:CE2	2.51	0.45
12:1L:279:CYS:HA	37:1l:116:PHE:CZ	2.52	0.45
12:1L:296:ASN:OD1	12:1L:357:ARG:NH1	2.49	0.45
13:1M:168:GLN:HB2	13:1M:174:LEU:HD11	1.98	0.45
14:1N:88:LYS:HE3	14:1N:88:LYS:HB3	1.70	0.45
14:1N:211:MET:O	14:1N:215:MET:N	2.36	0.45
15:1O:290:ASP:O	15:1O:294:GLN:HG2	2.17	0.45
16:1P:206:TYR:O	16:1P:210:VAL:HG12	2.15	0.45
21:1V:27:TYR:HE2	21:1V:54:LYS:HB3	1.81	0.45
21:1V:71:LEU:HD22	21:1V:79:VAL:HG11	1.98	0.45
21:1V:97:LYS:HE2	21:1V:99:TRP:HZ3	1.81	0.45
26:1a:1:MET:HG3	51:1q:201:CDL:H1	1.99	0.45
28:1c:6:GLU:OE2	28:1c:7:PRO:HD2	2.16	0.45
30:1e:94:PRO:HD2	30:1e:97:HIS:CD2	2.51	0.45
31:1f:18:VAL:HA	31:1f:21:VAL:HG22	1.97	0.45
42:1q:141:SER:O	42:1q:142:THR:HB	2.17	0.45
44:1s:70:ARG:HH11	44:1s:70:ARG:HG3	1.82	0.45
4:1D:167:PHE:O	4:1D:171:PHE:HD2	1.99	0.45
4:1D:184:VAL:O	9:1I:60:ARG:NH1	2.45	0.45
4:1D:423:ILE:HD13	4:1D:425:PHE:CE1	2.52	0.45
5:1E:202:LEU:HD22	6:1F:26:TYR:CE2	2.52	0.45
7:1G:157:THR:O	7:1G:161:ARG:HG2	2.17	0.45
7:1G:278:ARG:HA	7:1G:278:ARG:HH11	1.81	0.45
11:1K:43:MET:O	11:1K:47:ILE:HD12	2.16	0.45
12:1L:483:PRO:HD2	12:1L:486:MET:SD	2.56	0.45
45:1L:701:3PE:H231	37:1l:88:ARG:HA	1.98	0.45
15:1O:8:PHE:HE1	15:1O:13:ARG:HD3	1.81	0.45
15:1O:99:TRP:O	15:1O:103:SER:OG	2.35	0.45
16:1P:209:ASP:N	16:1P:209:ASP:OD1	2.48	0.45
18:1R:21:GLY:O	18:1R:25:ARG:NH1	2.49	0.45
18:1R:32:GLN:NE2	42:1q:123:GLN:O	2.41	0.45
20:1T:47:GLN:O	20:1T:51:ILE:HG13	2.16	0.45
20:1U:9:GLU:HA	20:1U:12:LYS:HE3	1.99	0.45
32:1g:68:ILE:HD12	32:1g:69:VAL:N	2.32	0.45
34:1i:49:PHE:CZ	34:1i:57:LYS:HG3	2.52	0.45
37:1l:66:HIS:O	37:1l:70:ARG:N	2.50	0.45
42:1q:44:TYR:CD1	42:1q:68:MET:HE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:1q:48:TYR:HE2	42:1q:86:TRP:CG	2.34	0.45
42:1q:78:ASP:CG	42:1q:80:SER:H	2.25	0.45
45:1A:201:3PE:H271	27:1b:18:LEU:HD23	1.99	0.45
4:1D:90:LEU:O	4:1D:94:LYS:HG2	2.17	0.45
6:1F:257:ASN:HB3	6:1F:333:ALA:HA	1.99	0.45
7:1G:19:MET:H	7:1G:19:MET:CE	2.19	0.45
7:1G:328:LEU:O	7:1G:507:TYR:OH	2.33	0.45
9:1I:44:GLU:OE2	43:1r:25:LEU:HD23	2.16	0.45
10:1J:17:PHE:CD2	11:1K:11:ALA:HB1	2.52	0.45
12:1L:103:PHE:CE2	12:1L:242:PRO:HG3	2.52	0.45
14:1N:182:SER:HB2	14:1N:293:TYR:OH	2.17	0.45
16:1P:90:VAL:HG12	16:1P:128:LYS:HB2	1.99	0.45
16:1P:169:SER:OG	16:1P:203:GLN:O	2.32	0.45
22:1W:99:GLN:H	22:1W:102:HIS:HB2	1.81	0.45
57:1Y:201:PGT:H152	57:1Y:201:PGT:H181	1.66	0.45
25:1Z:21:TYR:OH	43:1r:108:ASP:OD2	2.33	0.45
39:1n:123:GLN:OE1	39:1n:126:ARG:NH2	2.43	0.45
39:1n:178:MET:HE3	39:1n:178:MET:N	2.31	0.45
41:1p:28:PRO:O	41:1p:32:LEU:HD22	2.17	0.45
1:1A:3:ILE:HG23	1:1A:4:MET:H	1.81	0.45
1:1A:54:LYS:HD3	1:1A:114:ALA:O	2.17	0.45
1:1A:68:GLU:HB2	1:1A:98:LEU:HD23	1.99	0.45
3:1C:195:ARG:NH2	9:1I:92:ILE:O	2.50	0.45
7:1G:24:THR:HG23	7:1G:28:GLN:HB3	1.97	0.45
8:1H:142:TYR:CZ	8:1H:289:LEU:HB2	2.52	0.45
8:1H:253:GLU:HG3	26:1a:21:MET:HE1	1.98	0.45
11:1K:27:MET:HE3	11:1K:27:MET:O	2.17	0.45
11:1K:43:MET:HA	11:1K:46:LEU:HD23	1.97	0.45
11:1K:56:ALA:C	11:1K:58:MET:N	2.75	0.45
12:1L:332:HIS:O	12:1L:336:LYS:HB3	2.17	0.45
12:1L:475:MET:HE2	12:1L:475:MET:O	2.16	0.45
13:1M:30:HIS:CD2	31:1f:16:VAL:HB	2.51	0.45
13:1M:75:LEU:HD13	13:1M:440:HIS:NE2	2.32	0.45
13:1M:190:TRP:HD1	24:1Y:126:MET:SD	2.40	0.45
13:1M:250:LEU:O	13:1M:254:THR:OG1	2.33	0.45
13:1M:286:ILE:O	13:1M:289:SER:OG	2.26	0.45
15:1O:50:HIS:HA	15:1O:123:VAL:HG13	1.99	0.45
15:1O:155:VAL:O	15:1O:159:THR:OG1	2.32	0.45
15:1O:194:ILE:HD11	15:1O:198:TYR:CD1	2.52	0.45
15:1O:318:TRP:CD1	15:1O:318:TRP:H	2.34	0.45
16:1P:71:MET:HE3	16:1P:71:MET:HB3	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:212:LYS:O	16:1P:215:ILE:HD12	2.16	0.45
16:1P:270:PHE:CD2	16:1P:278:TRP:HB2	2.46	0.45
17:1Q:93:VAL:O	17:1Q:96:ALA:N	2.50	0.45
18:1R:12:THR:OG1	18:1R:13:HIS:N	2.50	0.45
19:1S:14:GLY:O	19:1S:16:ARG:NE	2.50	0.45
22:1W:80:ASP:HA	22:1W:83:VAL:HB	1.99	0.45
23:1X:16:GLU:HA	23:1X:63:ASN:HD21	1.82	0.45
26:1a:64:LYS:NZ	26:1a:68:ASN:OD1	2.32	0.45
1:1A:103:ALA:HA	45:1A:201:3PE:H251	1.99	0.45
1:1A:111:LEU:HB2	8:1H:291:LYS:HE3	1.99	0.45
3:1C:86:ARG:NE	21:1V:110:GLN:O	2.50	0.45
4:1D:205:LEU:O	43:1r:35:GLN:HG3	2.16	0.45
7:1G:31:GLU:OE1	7:1G:31:GLU:N	2.44	0.45
7:1G:80:LEU:HD22	7:1G:83:SER:HB2	1.99	0.45
7:1G:606:ILE:HD12	7:1G:606:ILE:HA	1.87	0.45
8:1H:283:ASP:OD1	8:1H:284:GLN:N	2.50	0.45
9:1I:65:HIS:HB3	9:1I:131:ILE:HD11	1.99	0.45
13:1M:75:LEU:HA	13:1M:78:MET:HE3	1.99	0.45
13:1M:346:ARG:HE	13:1M:346:ARG:HB2	1.52	0.45
16:1P:29:PHE:HZ	16:1P:173:GLY:HA3	1.82	0.45
23:1X:95:LEU:HB3	23:1X:97:ARG:HG2	1.99	0.45
25:1Z:129:THR:HG22	30:1e:98:LEU:HA	1.98	0.45
34:1i:123:PRO:HG2	34:1i:125:GLN:NE2	2.32	0.45
37:1l:136:ASN:HA	37:1l:153:VAL:HB	1.98	0.45
1:1A:106:TRP:CH2	8:1H:291:LYS:HD2	2.52	0.45
3:1C:88:ASN:HD21	21:1V:107:PRO:HG2	1.82	0.45
7:1G:136:ALA:HB1	18:1R:74:ASN:HB2	1.99	0.45
7:1G:138:GLU:HG2	18:1R:76:ASP:HB2	1.98	0.45
12:1L:144:TRP:HH2	12:1L:256:GLY:HA2	1.80	0.45
12:1L:367:PRO:HG3	35:1j:22:LEU:HD13	1.99	0.45
13:1M:201:MET:HG2	57:1Y:201:PGT:H441	1.97	0.45
14:1N:187:MET:O	14:1N:191:THR:OG1	2.28	0.45
21:1V:77:GLU:OE1	21:1V:77:GLU:N	2.49	0.45
22:1W:84:ILE:HA	22:1W:87:LYS:HB3	1.99	0.45
25:1Z:134:LEU:HD21	25:1Z:142:TRP:HE1	1.81	0.45
27:1b:79:TRP:CD1	27:1b:79:TRP:H	2.35	0.45
35:1j:26:GLU:HA	35:1j:29:SER:HB3	1.99	0.45
35:1j:54:PRO:HB2	35:1j:59:TRP:CZ2	2.49	0.45
39:1n:65:GLN:O	39:1n:69:GLU:HG2	2.17	0.45
42:1q:85:GLU:OE1	42:1q:85:GLU:N	2.43	0.45
43:1r:40:LEU:HD13	43:1r:41:PRO:HD2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1A:29:ALA:HA	1:1A:33:LYS:HD2	1.98	0.44
2:1B:86:MET:HB2	2:1B:107:MET:HE1	1.99	0.44
3:1C:39:GLN:HE22	43:1r:67:ILE:HD11	1.82	0.44
3:1C:61:LEU:HD11	3:1C:107:VAL:HG21	2.00	0.44
4:1D:152:MET:HE1	4:1D:171:PHE:HZ	1.82	0.44
6:1F:261:HIS:HA	6:1F:288:ILE:HD12	1.99	0.44
6:1F:370:ASP:O	6:1F:374:LYS:HG2	2.16	0.44
7:1G:121:MET:C	7:1G:122:MET:HE2	2.41	0.44
7:1G:189:LYS:HE2	7:1G:189:LYS:HB3	1.83	0.44
8:1H:183:MET:HB2	9:1I:27:TRP:CH2	2.52	0.44
9:1I:54:LYS:HD3	42:1q:91:HIS:CE1	2.52	0.44
9:1I:99:ARG:HB2	9:1I:104:ARG:HA	1.99	0.44
10:1J:163:ILE:O	10:1J:167:VAL:HG12	2.17	0.44
10:1J:169:MET:HA	10:1J:172:THR:HG22	1.99	0.44
12:1L:8:THR:O	12:1L:11:THR:OG1	2.34	0.44
12:1L:88:MET:O	12:1L:91:PRO:HD2	2.16	0.44
12:1L:313:MET:SD	12:1L:328:HIS:ND1	2.90	0.44
13:1M:79:ALA:HB2	13:1M:436:LEU:HD11	1.98	0.44
13:1M:178:ILE:HD12	13:1M:178:ILE:HA	1.83	0.44
14:1N:209:ILE:HG23	14:1N:213:LEU:HD23	1.98	0.44
16:1P:113:ILE:O	16:1P:117:ILE:HG12	2.17	0.44
17:1Q:99:ASN:OD1	17:1Q:99:ASN:N	2.45	0.44
19:1S:39:ARG:HH12	19:1S:87:THR:HG21	1.82	0.44
20:1T:80:ILE:O	20:1T:84:LYS:HB3	2.17	0.44
38:1m:122:GLN:HB2	41:1p:139:GLN:HE22	1.81	0.44
41:1p:145:LEU:HD23	41:1p:145:LEU:HA	1.82	0.44
1:1A:95:LEU:HD13	8:1H:302:MET:HG3	1.99	0.44
7:1G:94:MET:CE	7:1G:119:GLN:HB3	2.47	0.44
8:1H:312:ALA:HA	27:1b:41:ALA:HB2	1.99	0.44
9:1I:54:LYS:HD3	42:1q:91:HIS:NE2	2.32	0.44
12:1L:81:LYS:HD2	12:1L:81:LYS:O	2.17	0.44
12:1L:530:PRO:O	12:1L:534:HIS:HB2	2.17	0.44
14:1N:62:THR:HG21	14:1N:114:TRP:CG	2.52	0.44
14:1N:273:ASN:OD1	24:1Y:139:LYS:N	2.45	0.44
15:1O:3:TYR:HB3	15:1O:261:MET:HE1	1.99	0.44
15:1O:144:ILE:HB	15:1O:148:CYS:SG	2.57	0.44
20:1T:49:GLU:HA	22:1W:40:TYR:HE1	1.82	0.44
20:1T:51:ILE:HD12	20:1T:52:MET:H	1.82	0.44
23:1X:10:GLU:HA	23:1X:13:LYS:HZ3	1.81	0.44
23:1X:73:ILE:HD12	23:1X:74:LYS:N	2.32	0.44
23:1X:137:PRO:HG2	23:1X:140:PRO:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1Y:38:TYR:HB3	45:1Y:202:3PE:O22	2.17	0.44
30:1e:73:LYS:HD2	30:1e:73:LYS:HA	1.66	0.44
50:1f:101:PC1:H31	50:1f:101:PC1:H322	1.41	0.44
32:1g:50:ASP:OD2	32:1g:52:ILE:HG22	2.17	0.44
34:1i:40:TRP:HB2	34:1i:43:GLU:OE1	2.18	0.44
34:1i:125:GLN:HB3	40:1o:88:TYR:HE2	1.81	0.44
42:1q:94:THR:HG22	42:1q:96:ASP:H	1.82	0.44
2:1B:63:ALA:HA	2:1B:69:MET:SD	2.57	0.44
3:1C:84:PRO:HB3	17:1Q:95:PHE:CE2	2.53	0.44
3:1C:130:TYR:HE1	4:1D:390:LYS:HZ1	1.65	0.44
4:1D:130:PRO:HA	4:1D:325:VAL:HG12	2.00	0.44
4:1D:203:LEU:HD22	4:1D:203:LEU:H	1.82	0.44
4:1D:347:HIS:NE2	7:1G:125:SER:O	2.47	0.44
4:1D:421:GLN:HB3	4:1D:423:ILE:HG23	1.99	0.44
5:1E:162:GLU:C	5:1E:186:PRO:HA	2.42	0.44
6:1F:208:PRO:HG3	17:1Q:119:GLY:HA2	1.99	0.44
7:1G:520:LYS:HB2	7:1G:520:LYS:HE2	1.86	0.44
7:1G:655:GLN:CD	7:1G:656:LEU:H	2.24	0.44
12:1L:288:THR:HG21	12:1L:307:SER:HB2	1.99	0.44
12:1L:511:LEU:O	12:1L:511:LEU:HD13	2.17	0.44
12:1L:522:PHE:HA	12:1L:528:TYR:CE1	2.52	0.44
14:1N:316:GLN:HB3	15:1O:63:THR:HG21	1.99	0.44
15:1O:300:PRO:O	28:1c:2:PHE:HE1	2.00	0.44
16:1P:147:ARG:O	16:1P:151:VAL:HG12	2.17	0.44
22:1W:62:LYS:HG2	22:1W:107:PHE:CE2	2.46	0.44
37:1l:6:LYS:HE3	37:1l:6:LYS:HA	1.98	0.44
37:1l:98:TRP:O	37:1l:101:MET:HB2	2.17	0.44
39:1n:50:HIS:ND1	39:1n:50:HIS:O	2.48	0.44
39:1n:142:GLU:OE2	39:1n:157:ARG:NH2	2.49	0.44
40:1o:7:ARG:HB2	40:1o:15:GLU:HG2	1.98	0.44
42:1q:2:GLU:O	42:1q:6:VAL:HG23	2.17	0.44
1:1A:104:TYR:HE2	1:1A:108:GLN:HG2	1.82	0.44
4:1D:362:ALA:HB1	4:1D:377:TYR:HE1	1.81	0.44
4:1D:371:LYS:HZ3	4:1D:422:ASP:HB2	1.83	0.44
5:1E:69:VAL:HG13	5:1E:73:LEU:HD23	1.99	0.44
6:1F:214:GLY:N	6:1F:218:CYS:O	2.42	0.44
9:1I:83:CYS:SG	9:1I:109:TYR:OH	2.62	0.44
12:1L:36:VAL:HG11	12:1L:118:PHE:HB3	1.99	0.44
12:1L:474:PRO:O	12:1L:474:PRO:HD2	2.17	0.44
12:1L:560:THR:O	12:1L:565:THR:OG1	2.31	0.44
13:1M:220:HIS:CD2	13:1M:231:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:22:THR:OG1	16:1P:88:SER:OG	2.30	0.44
20:1T:76:ILE:O	20:1T:80:ILE:HG13	2.18	0.44
20:1U:52:MET:HE1	39:1n:20:LYS:HA	1.99	0.44
42:1q:63:ILE:O	42:1q:63:ILE:HD12	2.17	0.44
42:1q:86:TRP:CZ3	42:1q:98:PRO:HD2	2.52	0.44
2:1B:102:LYS:HG2	2:1B:106:GLN:HE22	1.83	0.44
4:1D:169:TRP:CH2	9:1I:37:THR:HG22	2.53	0.44
6:1F:12:PHE:HB3	6:1F:271:GLU:OE1	2.17	0.44
8:1H:146:LEU:HD12	8:1H:188:SER:HB2	1.99	0.44
9:1I:152:GLU:HG2	18:1R:35:VAL:HA	1.99	0.44
12:1L:420:ALA:O	12:1L:424:THR:HG23	2.18	0.44
12:1L:458:LEU:O	12:1L:462:ILE:HG12	2.17	0.44
12:1L:483:PRO:HG3	35:1j:53:TYR:CE2	2.52	0.44
12:1L:591:PHE:CE1	14:1N:111:PHE:HA	2.53	0.44
15:1O:83:TYR:OH	52:1O:401:GTP:O3'	2.27	0.44
16:1P:20:VAL:HB	16:1P:89:ASN:H	1.83	0.44
16:1P:315:ILE:O	16:1P:319:ARG:HB2	2.17	0.44
18:1R:95:HIS:O	18:1R:95:HIS:ND1	2.48	0.44
23:1X:165:ARG:HH12	29:1d:87:ASP:CG	2.25	0.44
25:1Z:140:PHE:HB2	26:1a:45:TRP:CD1	2.52	0.44
30:1e:84:LYS:HE3	30:1e:84:LYS:HB3	1.84	0.44
31:1f:8:ARG:HD2	31:1f:8:ARG:HA	1.80	0.44
33:1h:7:ARG:HE	34:1i:27:LEU:HD12	1.81	0.44
1:1A:1:FME:HCN	25:1Z:142:TRP:CE3	2.53	0.44
2:1B:119:CYS:HA	2:1B:123:GLY:C	2.42	0.44
3:1C:41:GLN:OE1	43:1r:67:ILE:HA	2.17	0.44
3:1C:185:ALA:HB2	22:1W:105:ARG:HE	1.82	0.44
6:1F:281:GLU:HA	6:1F:286:GLY:H	1.83	0.44
6:1F:293:ASN:O	6:1F:339:ARG:HG2	2.17	0.44
7:1G:125:SER:OG	7:1G:126:ASP:N	2.51	0.44
7:1G:234:VAL:HG11	7:1G:390:LEU:HB2	1.99	0.44
7:1G:409:ILE:HD12	7:1G:409:ILE:O	2.16	0.44
7:1G:633:TYR:C	7:1G:634:ASP:OD1	2.60	0.44
8:1H:24:GLU:HA	8:1H:271:LEU:HD13	1.99	0.44
8:1H:186:PHE:CD2	50:1I:203:PC1:H2E1	2.52	0.44
8:1H:227:GLU:O	8:1H:231:ILE:HG12	2.17	0.44
9:1I:108:ARG:HG2	9:1I:110:ASP:OD1	2.18	0.44
10:1J:42:GLY:O	10:1J:46:ASN:ND2	2.41	0.44
12:1L:44:PHE:O	12:1L:48:LEU:HD22	2.17	0.44
12:1L:466:PHE:HZ	40:1o:77:LEU:HD11	1.83	0.44
12:1L:561:ILE:HG23	12:1L:562:LEU:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:1P:17:SER:HB3	16:1P:41:MET:HG2	2.00	0.44
16:1P:83:LYS:HA	16:1P:86:GLU:OE2	2.18	0.44
18:1R:60:ASP:OD2	18:1R:61:GLY:N	2.50	0.44
23:1X:90:TYR:HA	26:1a:34:LYS:HG2	2.00	0.44
30:1e:88:GLU:OE1	30:1e:88:GLU:N	2.50	0.44
1:1A:2:ASN:HB3	8:1H:2:PHE:CZ	2.53	0.44
1:1A:68:GLU:OE2	10:1J:161:LEU:HB3	2.18	0.44
4:1D:168:PHE:CB	8:1H:32:GLN:HB3	2.47	0.44
4:1D:335:ARG:HD2	9:1I:176:ARG:HD2	2.00	0.44
5:1E:106:THR:HA	5:1E:109:MET:HG3	1.99	0.44
5:1E:190:ARG:HG3	5:1E:194:GLU:O	2.18	0.44
7:1G:703:ILE:O	18:1R:85:GLY:HA2	2.17	0.44
8:1H:199:ASP:O	8:1H:203:GLY:N	2.42	0.44
10:1J:8:ILE:O	10:1J:11:THR:N	2.46	0.44
12:1L:79:SER:HB2	12:1L:135:ASN:HB3	2.00	0.44
12:1L:102:GLU:OE1	12:1L:456:ARG:NH1	2.50	0.44
12:1L:564:LYS:HD3	12:1L:564:LYS:HA	1.75	0.44
13:1M:17:MET:HG2	31:1f:11:TRP:CZ2	2.49	0.44
13:1M:231:LEU:O	13:1M:235:LEU:HB2	2.18	0.44
13:1M:278:ARG:HB3	13:1M:278:ARG:NH1	2.31	0.44
14:1N:246:VAL:HG22	45:1N:401:3PE:H3E1	2.00	0.44
14:1N:289:ASN:HA	14:1N:292:PHE:CE2	2.53	0.44
16:1P:224:LYS:H	16:1P:224:LYS:HG3	1.58	0.44
19:1S:85:GLN:O	19:1S:89:THR:OG1	2.35	0.44
20:1U:46:ASP:N	20:1U:46:ASP:OD1	2.51	0.44
22:1W:56:VAL:O	22:1W:60:ARG:HG2	2.18	0.44
23:1X:150:ASN:OD1	33:1h:124:GLN:NE2	2.50	0.44
37:1l:91:THR:HG22	38:1m:12:THR:HG22	1.99	0.44
38:1m:45:GLU:O	38:1m:49:GLN:HG3	2.17	0.44
4:1D:149:ASN:ND2	4:1D:371:LYS:HE2	2.29	0.44
4:1D:240:VAL:HG12	4:1D:294:TYR:CG	2.53	0.44
5:1E:31:ILE:HG22	5:1E:50:VAL:HG22	1.98	0.44
5:1E:97:LYS:HG3	5:1E:98:TYR:CD1	2.53	0.44
5:1E:120:ILE:HG23	5:1E:169:ILE:HG23	1.99	0.44
6:1F:96:ASN:ND2	6:1F:187:GLY:O	2.42	0.44
6:1F:398:GLN:HG2	7:1G:92:GLY:HA3	2.00	0.44
7:1G:160:ILE:HG22	7:1G:172:LEU:HB3	2.00	0.44
7:1G:460:ARG:NH1	7:1G:661:LEU:HD13	2.33	0.44
12:1L:119:LYS:HB3	12:1L:119:LYS:HE2	1.82	0.44
12:1L:250:SER:CB	12:1L:333:ALA:HA	2.48	0.44
12:1L:316:THR:HB	12:1L:395:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:573:MET:HA	12:1L:576:MET:SD	2.58	0.44
12:1L:593:ILE:HG22	12:1L:597:ILE:HD13	1.99	0.44
14:1N:102:LEU:HA	14:1N:105:LYS:HG3	1.99	0.44
15:1O:167:HIS:O	15:1O:218:CYS:HB2	2.17	0.44
18:1R:84:CYS:HB3	18:1R:87:CYS:HB2	2.00	0.44
25:1Z:120:MET:HG3	30:1e:68:ARG:HD2	1.99	0.44
34:1i:7:GLU:HA	34:1i:10:ARG:HB3	1.99	0.44
34:1i:102:ARG:NH2	40:1o:48:ALA:O	2.32	0.44
36:1k:29:GLU:N	36:1k:29:GLU:OE2	2.51	0.44
38:1m:45:GLU:HA	38:1m:48:LEU:HD12	1.98	0.44
39:1n:64:ARG:HA	39:1n:64:ARG:CZ	2.47	0.44
40:1o:61:TYR:HA	40:1o:64:GLN:HE22	1.83	0.44
40:1o:72:SER:HB2	40:1o:78:ALA:HB3	2.00	0.44
41:1p:70:VAL:HG21	41:1p:86:GLU:HB3	1.99	0.44
42:1q:88:ARG:NH2	42:1q:94:THR:OG1	2.51	0.44
2:1B:94:ASN:HB3	3:1C:174:LEU:HD11	1.99	0.44
3:1C:28:TYR:CE1	3:1C:32:ILE:HD11	2.53	0.44
3:1C:41:GLN:HE21	43:1r:65:PRO:HB2	1.83	0.44
3:1C:58:ILE:HD12	3:1C:58:ILE:N	2.32	0.44
4:1D:19:MET:SD	14:1N:171:ASN:HA	2.58	0.44
6:1F:150:GLN:NE2	6:1F:177:VAL:HG21	2.32	0.44
6:1F:185:ILE:HG21	6:1F:359:CYS:HB3	1.99	0.44
7:1G:252:PRO:HG2	17:1Q:44:ASN:OD1	2.18	0.44
7:1G:298:ASP:HB2	7:1G:302:ARG:NH2	2.33	0.44
10:1J:20:PHE:HE1	11:1K:32:CYS:HA	1.82	0.44
10:1J:109:LYS:HA	10:1J:109:LYS:HD3	1.84	0.44
10:1J:118:LYS:C	10:1J:118:LYS:HD3	2.43	0.44
12:1L:80:PHE:HB3	12:1L:82:MET:HE3	2.00	0.44
12:1L:153:LEU:HD21	13:1M:360:LEU:HD21	2.00	0.44
14:1N:88:LYS:NZ	14:1N:89:MET:O	2.50	0.44
14:1N:238:PRO:HB2	45:1N:401:3PE:C31	2.48	0.44
14:1N:304:MET:HE1	15:1O:290:ASP:HB2	1.98	0.44
14:1N:304:MET:HE3	14:1N:304:MET:HB3	1.81	0.44
14:1N:313:MET:HA	14:1N:316:GLN:OE1	2.18	0.44
15:1O:308:TYR:CZ	29:1d:51:ARG:HD3	2.53	0.44
18:1R:73:ILE:HG21	18:1R:84:CYS:HA	2.00	0.44
20:1T:67:ALA:HA	20:1T:70:LEU:HD21	2.00	0.44
20:1U:23:ASP:OD1	20:1U:23:ASP:N	2.50	0.44
21:1V:54:LYS:HD3	21:1V:57:MET:SD	2.57	0.44
22:1W:17:VAL:HG21	22:1W:77:ARG:NH2	2.33	0.44
22:1W:54:ILE:HD12	22:1W:54:ILE:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:1h:115:ARG:HB2	33:1h:123:TYR:CE2	2.53	0.44
35:1j:64:LEU:HB3	35:1j:66:ILE:HG12	1.99	0.44
43:1r:2:SER:OG	43:1r:3:ALA:N	2.51	0.44
43:1r:42:VAL:HB	43:1r:46:HIS:ND1	2.33	0.44
2:1B:144:ILE:HD13	2:1B:163:LEU:HD23	2.00	0.43
4:1D:74:ARG:N	4:1D:74:ARG:HD2	2.33	0.43
4:1D:349:PHE:O	4:1D:353:THR:HG23	2.18	0.43
4:1D:362:ALA:HB1	4:1D:377:TYR:CE1	2.52	0.43
5:1E:120:ILE:HG22	5:1E:173:ILE:HD13	1.99	0.43
5:1E:135:LYS:HE3	5:1E:135:LYS:HB3	1.79	0.43
6:1F:298:ILE:O	6:1F:334:VAL:HA	2.17	0.43
7:1G:592:LEU:HG	16:1P:6:ILE:HG23	2.00	0.43
8:1H:106:LEU:HD23	8:1H:106:LEU:HA	1.75	0.43
9:1I:57:LEU:HD12	9:1I:61:PHE:CG	2.53	0.43
9:1I:110:ASP:OD1	9:1I:110:ASP:N	2.51	0.43
12:1L:49:VAL:HG22	41:1p:32:LEU:HG	2.00	0.43
12:1L:298:ILE:HD11	12:1L:359:MET:CE	2.47	0.43
12:1L:319:ILE:HG12	12:1L:402:SER:HB3	2.00	0.43
13:1M:427:LYS:NZ	39:1n:105:ASP:HB2	2.33	0.43
14:1N:200:MET:HA	14:1N:203:LEU:HB3	1.98	0.43
15:1O:37:ARG:NH1	15:1O:41:GLU:OE2	2.49	0.43
16:1P:135:LEU:HA	16:1P:167:LYS:HB3	1.99	0.43
31:1f:37:PHE:HA	31:1f:40:LYS:HG3	2.00	0.43
39:1n:176:ARG:HB3	39:1n:178:MET:HE1	1.99	0.43
1:1A:80:GLN:OE1	8:1H:317:GLN:N	2.51	0.43
2:1B:52:LEU:HB2	2:1B:89:ALA:O	2.17	0.43
3:1C:94:TYR:HB2	3:1C:107:VAL:CG2	2.48	0.43
5:1E:155:GLN:HA	5:1E:160:TYR:HA	2.00	0.43
7:1G:192:MET:N	7:1G:192:MET:SD	2.91	0.43
7:1G:199:ILE:HD12	7:1G:199:ILE:HA	1.81	0.43
7:1G:243:ARG:HD2	7:1G:244:THR:OG1	2.18	0.43
7:1G:288:LYS:HE3	7:1G:288:LYS:HB3	1.76	0.43
9:1I:69:ARG:HD3	42:1q:108:TYR:CG	2.53	0.43
11:1K:25:HIS:ND1	11:1K:88:ASP:OD2	2.48	0.43
13:1M:335:GLU:OE1	13:1M:335:GLU:N	2.50	0.43
14:1N:157:MET:HE2	14:1N:157:MET:HB2	1.76	0.43
14:1N:276:ILE:C	14:1N:279:PRO:HD2	2.43	0.43
15:1O:32:CYS:SG	15:1O:186:LYS:HE2	2.59	0.43
17:1Q:125:ASN:OD1	17:1Q:125:ASN:N	2.52	0.43
24:1Y:84:ASP:C	24:1Y:84:ASP:OD1	2.60	0.43
25:1Z:20:ASP:OD1	25:1Z:20:ASP:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1Z:133:ILE:HD13	25:1Z:133:ILE:HA	1.81	0.43
30:1e:37:LYS:HZ2	30:1e:37:LYS:C	2.27	0.43
33:1h:54:ASP:OD2	33:1h:54:ASP:C	2.61	0.43
5:1E:162:GLU:O	5:1E:187:ARG:N	2.40	0.43
6:1F:355:LYS:HE3	6:1F:355:LYS:HB3	1.68	0.43
7:1G:39:ARG:HB2	47:1G:803:FES:S2	2.58	0.43
7:1G:55:CYS:HB3	47:1G:803:FES:S2	2.58	0.43
8:1H:288:LEU:HD11	50:1I:203:PC1:O22	2.17	0.43
9:1I:34:LEU:HD11	50:1I:203:PC1:H2B1	2.00	0.43
10:1J:26:PRO:HB2	10:1J:72:THR:HG22	2.00	0.43
12:1L:114:ILE:HD12	12:1L:114:ILE:HA	1.76	0.43
12:1L:407:TRP:O	12:1L:411:MET:HE2	2.18	0.43
13:1M:297:VAL:O	13:1M:301:ILE:HG22	2.19	0.43
15:1O:314:ASP:O	15:1O:317:ILE:HG12	2.18	0.43
17:1Q:75:THR:HG22	17:1Q:77:ASP:H	1.83	0.43
17:1Q:76:ALA:O	17:1Q:78:PRO:HD3	2.18	0.43
19:1S:55:ARG:H	19:1S:55:ARG:HD2	1.82	0.43
20:1U:81:ALA:HA	20:1U:86:VAL:HB	1.99	0.43
25:1Z:76:GLN:O	25:1Z:80:ASP:HB2	2.18	0.43
34:1i:30:ARG:HH21	39:1n:115:PRO:HG2	1.82	0.43
36:1k:81:VAL:HA	36:1k:84:GLU:HG3	2.00	0.43
37:1l:77:ILE:HD12	37:1l:77:ILE:C	2.43	0.43
40:1o:7:ARG:HD3	40:1o:15:GLU:HB2	2.00	0.43
1:1A:27:LEU:HD23	1:1A:27:LEU:H	1.84	0.43
2:1B:75:VAL:HG11	8:1H:25:ARG:HH11	1.83	0.43
2:1B:170:GLU:OE2	2:1B:170:GLU:N	2.48	0.43
4:1D:34:ASN:HD22	15:1O:158:VAL:HA	1.84	0.43
4:1D:76:CYS:SG	4:1D:403:ASP:HA	2.59	0.43
6:1F:35:GLY:O	6:1F:39:ARG:HG3	2.18	0.43
6:1F:247:ARG:NH2	6:1F:320:ASP:HB2	2.33	0.43
7:1G:378:LEU:HB2	7:1G:451:VAL:HA	2.01	0.43
7:1G:546:GLN:HG3	7:1G:599:ILE:HD11	1.99	0.43
8:1H:311:THR:O	25:1Z:55:ARG:NH1	2.52	0.43
12:1L:597:ILE:HB	12:1L:602:PHE:CE1	2.53	0.43
13:1M:277:LEU:HD23	13:1M:277:LEU:HA	1.83	0.43
13:1M:443:PRO:HA	13:1M:446:LEU:HB2	1.99	0.43
14:1N:91:ASN:HB3	14:1N:94:ALA:HB3	1.99	0.43
14:1N:161:SER:OG	14:1N:184:ILE:O	2.36	0.43
15:1O:149:VAL:HG12	15:1O:153:ASN:HD21	1.83	0.43
15:1O:285:GLY:O	15:1O:289:SER:OG	2.32	0.43
16:1P:73:TRP:HE1	16:1P:81:ILE:HG13	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1T:66:ASP:O	20:1T:70:LEU:HD23	2.18	0.43
24:1Y:43:LYS:HZ3	45:1Y:202:3PE:P	2.41	0.43
24:1Y:106:SER:HB3	24:1Y:109:ILE:HD12	2.01	0.43
26:1a:43:TYR:HA	26:1a:46:ASN:HD21	1.83	0.43
27:1b:31:LEU:O	27:1b:35:SER:N	2.50	0.43
30:1e:28:ILE:HD12	30:1e:28:ILE:C	2.43	0.43
32:1g:112:CYS:HB3	41:1p:141:ARG:HD3	2.00	0.43
32:1g:119:GLN:OE1	32:1g:119:GLN:N	2.52	0.43
33:1h:129:ASP:N	33:1h:129:ASP:OD1	2.49	0.43
36:1k:47:ASN:HB3	36:1k:48:GLU:OE2	2.19	0.43
2:1B:81:ARG:HA	2:1B:108:PRO:HD3	1.99	0.43
2:1B:152:THR:HG22	4:1D:188:ARG:HG3	2.01	0.43
3:1C:192:GLN:NE2	17:1Q:72:TRP:CE3	2.86	0.43
4:1D:255:PHE:CE2	4:1D:405:MET:HE1	2.53	0.43
5:1E:87:TYR:CD2	5:1E:87:TYR:N	2.85	0.43
6:1F:53:PRO:HD3	6:1F:127:ARG:NH1	2.33	0.43
6:1F:171:TYR:CD2	6:1F:173:PHE:HB2	2.54	0.43
7:1G:16:GLN:H	7:1G:16:GLN:CD	2.26	0.43
7:1G:237:ASN:CG	7:1G:253:ARG:HE	2.26	0.43
7:1G:360:SER:O	7:1G:490:MET:HE1	2.18	0.43
8:1H:298:LEU:HD23	8:1H:298:LEU:HA	1.83	0.43
12:1L:100:ILE:O	12:1L:104:SER:OG	2.26	0.43
12:1L:341:MET:O	12:1L:345:SER:N	2.50	0.43
12:1L:363:TYR:CD2	12:1L:370:THR:HG21	2.54	0.43
15:1O:25:ILE:HD12	15:1O:168:VAL:HB	2.01	0.43
15:1O:186:LYS:HA	15:1O:186:LYS:HD3	1.80	0.43
15:1O:219:GLU:OE1	15:1O:243:CYS:HA	2.19	0.43
19:1S:41:VAL:O	19:1S:45:LYS:HG2	2.19	0.43
19:1S:49:ASP:N	19:1S:49:ASP:OD1	2.41	0.43
21:1V:37:ILE:HD11	21:1V:99:TRP:HH2	1.83	0.43
21:1V:45:LYS:CB	43:1r:91:LYS:HE2	2.48	0.43
23:1X:43:MET:HE3	27:1b:52:TYR:CE2	2.41	0.43
23:1X:43:MET:HE2	23:1X:43:MET:HB2	1.79	0.43
29:1d:95:LYS:HD3	29:1d:95:LYS:H	1.84	0.43
40:1o:62:LEU:HD22	40:1o:86:TRP:CZ2	2.54	0.43
41:1p:79:LYS:HB3	41:1p:79:LYS:HE2	1.74	0.43
41:1p:81:ILE:HA	41:1p:84:MET:HB2	1.99	0.43
44:1s:73:PRO:HD2	44:1s:74:ARG:HD2	2.01	0.43
1:1A:1:FME:HE1	10:1J:2:THR:HG21	2.00	0.43
1:1A:93:PHE:HE2	1:1A:97:LEU:HD22	1.83	0.43
3:1C:78:LEU:HA	3:1C:93:VAL:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:107:ASP:HA	4:1D:427:GLU:HB2	2.01	0.43
4:1D:247:ALA:HB1	4:1D:265:ILE:HD11	1.99	0.43
4:1D:289:SER:N	4:1D:295:ASP:OD2	2.43	0.43
5:1E:16:ASN:OD1	5:1E:19:THR:OG1	2.25	0.43
6:1F:48:ILE:HG13	6:1F:49:LEU:HD23	2.00	0.43
8:1H:108:MET:HE2	8:1H:108:MET:HA	1.99	0.43
9:1I:27:TRP:CD1	50:1I:203:PC1:H222	2.54	0.43
11:1K:95:LEU:H	14:1N:54:GLU:CD	2.26	0.43
12:1L:98:TRP:NE1	12:1L:102:GLU:OE2	2.51	0.43
12:1L:273:VAL:O	12:1L:277:THR:HG23	2.18	0.43
14:1N:87:THR:HG23	33:1h:126:PRO:HG2	2.00	0.43
14:1N:272:LYS:HE2	33:1h:108:LEU:HD11	2.01	0.43
15:1O:307:GLY:O	15:1O:320:LYS:NZ	2.31	0.43
19:1S:65:TRP:CZ3	19:1S:75:ASN:HB3	2.54	0.43
20:1U:49:GLU:OE1	36:1k:44:TRP:NE1	2.51	0.43
21:1V:45:LYS:HB3	43:1r:91:LYS:HE2	1.99	0.43
23:1X:71:ARG:HH11	23:1X:75:ARG:HH12	1.66	0.43
25:1Z:93:GLU:HG3	30:1e:97:HIS:NE2	2.34	0.43
26:1a:37:ARG:NH2	26:1a:51:ASP:OD2	2.52	0.43
29:1d:31:LEU:HD21	29:1d:69:VAL:HG13	1.99	0.43
34:1i:87:TYR:CE1	41:1p:48:ARG:HG2	2.54	0.43
41:1p:23:THR:HB	41:1p:25:LEU:HD23	2.01	0.43
1:1A:82:ASN:OD1	27:1b:46:ARG:NE	2.52	0.43
3:1C:119:SER:HB3	3:1C:145:HIS:HB2	2.01	0.43
6:1F:104:THR:HA	6:1F:106:LYS:HZ2	1.83	0.43
7:1G:255:HIS:CE1	7:1G:258:ILE:HG12	2.54	0.43
7:1G:346:GLU:H	7:1G:346:GLU:HG2	1.64	0.43
7:1G:367:THR:OG1	7:1G:636:VAL:HG11	2.19	0.43
8:1H:296:LEU:HD13	8:1H:300:LEU:HD23	2.00	0.43
12:1L:26:ILE:HD12	33:1h:26:ARG:NH2	2.34	0.43
12:1L:237:MET:HG3	12:1L:299:LYS:HB3	2.00	0.43
12:1L:435:PRO:HG2	36:1k:56:PHE:CG	2.54	0.43
14:1N:159:MET:O	14:1N:163:LEU:HB2	2.18	0.43
15:1O:269:VAL:HG13	15:1O:270:LEU:HD13	2.00	0.43
20:1T:25:ILE:HD11	20:1T:42:LEU:HD11	2.01	0.43
21:1V:88:SER:O	21:1V:92:LYS:NZ	2.51	0.43
29:1d:95:LYS:HD3	29:1d:95:LYS:N	2.34	0.43
31:1f:28:ARG:HB2	31:1f:57:LYS:HZ2	1.83	0.43
34:1i:18:ARG:NE	39:1n:172:ARG:HH21	2.16	0.43
34:1i:67:SER:O	34:1i:71:VAL:HG23	2.19	0.43
35:1j:12:ARG:HD3	36:1k:50:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:1n:153:LEU:HD23	39:1n:154:PRO:O	2.18	0.43
43:1r:32:LYS:NZ	43:1r:35:GLN:HA	2.33	0.43
4:1D:371:LYS:HD3	4:1D:422:ASP:HB2	2.01	0.43
5:1E:6:LEU:O	5:1E:92:ARG:NH1	2.51	0.43
5:1E:40:GLU:HG2	44:1s:67:SER:HA	2.00	0.43
5:1E:187:ARG:HA	5:1E:187:ARG:HD2	1.67	0.43
6:1F:111:ILE:HG21	6:1F:138:ILE:HD13	2.01	0.43
8:1H:111:LEU:HD12	8:1H:111:LEU:HA	1.87	0.43
10:1J:117:PHE:HB2	10:1J:119:PHE:CE2	2.53	0.43
10:1J:136:PHE:CD2	27:1b:50:TYR:HB3	2.54	0.43
10:1J:162:LEU:O	10:1J:165:VAL:HG12	2.19	0.43
12:1L:64:SER:HB2	34:1i:95:THR:HA	2.01	0.43
12:1L:124:PHE:O	12:1L:127:THR:OG1	2.33	0.43
12:1L:271:LYS:HA	12:1L:274:GLN:NE2	2.33	0.43
12:1L:310:LEU:HA	12:1L:313:MET:HG2	2.00	0.43
13:1M:27:ALA:O	13:1M:31:SER:OG	2.19	0.43
13:1M:313:THR:OG1	13:1M:455:LEU:O	2.25	0.43
15:1O:90:ASP:HA	32:1g:24:ILE:HD12	2.01	0.43
15:1O:240:TYR:O	15:1O:241:LEU:HD13	2.19	0.43
20:1T:62:ILE:HG21	20:1T:79:TYR:HE2	1.83	0.43
22:1W:46:THR:O	22:1W:50:PHE:HB2	2.19	0.43
30:1e:16:TRP:CD1	30:1e:16:TRP:H	2.37	0.43
37:1l:77:ILE:HD11	38:1m:67:TRP:CG	2.53	0.43
37:1l:145:ASP:OD2	37:1l:147:THR:OG1	2.25	0.43
39:1n:13:GLN:HB3	39:1n:17:ARG:NH1	2.33	0.43
39:1n:99:PRO:HB2	39:1n:101:TRP:CD1	2.53	0.43
41:1p:25:LEU:HD23	41:1p:25:LEU:H	1.84	0.43
3:1C:136:ASP:OD2	3:1C:150:ARG:HA	2.18	0.43
4:1D:366:ALA:HB1	4:1D:373:GLU:CD	2.43	0.43
5:1E:168:ASP:O	5:1E:172:ILE:HG12	2.19	0.43
6:1F:343:ILE:O	6:1F:347:ILE:HG13	2.17	0.43
7:1G:622:ARG:O	7:1G:625:GLU:HG2	2.19	0.43
8:1H:141:SER:OG	8:1H:286:MET:SD	2.74	0.43
8:1H:184:MET:HE1	8:1H:293:PHE:CD1	2.53	0.43
11:1K:93:LEU:HD22	14:1N:54:GLU:CD	2.44	0.43
12:1L:287:PHE:HD1	37:1l:108:PHE:HE2	1.66	0.43
13:1M:95:TYR:OH	13:1M:226:ALA:HB3	2.19	0.43
14:1N:167:TRP:HA	14:1N:288:LEU:HD13	2.00	0.43
14:1N:321:LYS:HG2	14:1N:322:GLN:N	2.34	0.43
14:1N:341:PRO:HB2	29:1d:79:GLN:NE2	2.34	0.43
16:1P:206:TYR:CE2	16:1P:313:LYS:HG3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:1Q:69:LEU:HD12	17:1Q:69:LEU:H	1.84	0.43
17:1Q:70:MET:HE3	17:1Q:70:MET:HB3	1.78	0.43
18:1R:51:GLU:OE1	18:1R:92:ARG:HG3	2.19	0.43
20:1T:83:LYS:HG3	20:1T:84:LYS:N	2.33	0.43
20:1U:50:ILE:HD12	20:1U:51:ILE:N	2.34	0.43
22:1W:52:LEU:HD12	22:1W:104:MET:HE2	2.01	0.43
27:1b:4:ILE:HD13	27:1b:4:ILE:HA	1.86	0.43
31:1f:35:THR:HG23	31:1f:38:ARG:HB2	2.00	0.43
31:1f:43:LEU:HB3	31:1f:44:PHE:HD1	1.84	0.43
37:1l:91:THR:HG22	37:1l:91:THR:O	2.19	0.43
39:1n:10:THR:O	39:1n:14:LYS:HG2	2.18	0.43
43:1r:102:ARG:HE	43:1r:102:ARG:C	2.27	0.43
3:1C:73:LYS:HE3	3:1C:73:LYS:HB3	1.94	0.43
4:1D:141:PHE:CZ	4:1D:184:VAL:HG21	2.54	0.43
6:1F:82:MET:HE2	6:1F:82:MET:O	2.19	0.43
6:1F:120:GLU:O	6:1F:123:LEU:HG	2.19	0.43
6:1F:139:ARG:NH1	6:1F:180:GLY:HA3	2.33	0.43
6:1F:376:MET:HE3	6:1F:376:MET:C	2.44	0.43
6:1F:386:PRO:HA	6:1F:430:MET:HE1	2.00	0.43
7:1G:59:ILE:HD12	7:1G:59:ILE:HA	1.75	0.43
7:1G:380:VAL:HB	7:1G:453:LEU:HA	2.01	0.43
8:1H:232:ILE:HD13	8:1H:267:THR:HG21	2.01	0.43
11:1K:55:LEU:HD23	11:1K:55:LEU:HA	1.93	0.43
12:1L:7:LEU:HD11	12:1L:50:PRO:HD3	2.01	0.43
12:1L:434:LYS:NZ	36:1k:52:TYR:HA	2.32	0.43
13:1M:47:GLU:OE2	41:1p:93:ARG:HG2	2.19	0.43
15:1O:202:ILE:O	15:1O:206:TYR:HB2	2.19	0.43
22:1W:23:ARG:C	22:1W:23:ARG:HE	2.27	0.43
23:1X:37:LYS:HZ2	23:1X:37:LYS:HG2	1.59	0.43
26:1a:49:GLU:OE2	26:1a:52:ARG:NH2	2.51	0.43
28:1c:15:LEU:HD23	28:1c:16:LYS:H	1.84	0.43
31:1f:2:ASN:O	31:1f:4:LEU:HD23	2.19	0.43
32:1g:122:GLU:O	41:1p:166:ARG:NH1	2.51	0.43
35:1j:70:ASP:OD1	35:1j:70:ASP:N	2.52	0.43
41:1p:28:PRO:HA	41:1p:31:TYR:HD2	1.83	0.43
42:1q:68:MET:HG2	42:1q:81:MET:HG2	2.01	0.43
3:1C:32:ILE:HD13	3:1C:63:PHE:HZ	1.83	0.42
3:1C:182:ARG:HD2	22:1W:101:THR:HA	2.01	0.42
5:1E:149:VAL:CG1	5:1E:190:ARG:HH22	2.32	0.42
6:1F:358:SER:OG	6:1F:365:CYS:SG	2.60	0.42
7:1G:249:ARG:HD2	7:1G:251:LEU:CD2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:1G:286:ASN:ND2	7:1G:290:LEU:HB3	2.34	0.42
8:1H:107:ALA:HB1	10:1J:57:PHE:HB3	2.01	0.42
8:1H:146:LEU:CD1	8:1H:188:SER:HB2	2.49	0.42
12:1L:37:LYS:NZ	12:1L:105:MET:HE1	2.34	0.42
16:1P:149:LYS:HZ3	54:1P:501:NDP:H1D	1.84	0.42
21:1V:69:GLU:H	21:1V:69:GLU:HG3	1.68	0.42
23:1X:20:SER:HG	26:1a:64:LYS:H	1.63	0.42
24:1Y:130:GLU:HG2	24:1Y:132:TRP:HE1	1.84	0.42
33:1h:36:VAL:HG13	33:1h:40:ILE:HD13	2.01	0.42
35:1j:60:THR:HG23	35:1j:63:GLU:OE1	2.20	0.42
36:1k:26:THR:HB	36:1k:52:TYR:HB2	2.01	0.42
39:1n:158:LYS:NZ	39:1n:159:GLU:O	2.47	0.42
41:1p:96:LYS:HA	41:1p:96:LYS:HD3	1.78	0.42
1:1A:69:ILE:HD12	1:1A:70:ALA:N	2.35	0.42
3:1C:110:TYR:HD1	21:1V:110:GLN:HE22	1.67	0.42
4:1D:130:PRO:HG2	4:1D:138:ARG:HH22	1.84	0.42
5:1E:105:THR:HG23	5:1E:107:PRO:HD2	2.00	0.42
7:1G:239:VAL:HG13	7:1G:251:LEU:HB2	2.00	0.42
7:1G:667:THR:OG1	7:1G:669:LYS:NZ	2.49	0.42
9:1I:99:ARG:NH2	9:1I:101:ASP:OD2	2.45	0.42
10:1J:8:ILE:HG22	10:1J:12:ILE:HD11	2.01	0.42
10:1J:103:MET:SD	10:1J:104:VAL:N	2.92	0.42
13:1M:12:LEU:HB3	13:1M:13:PRO:HD3	2.00	0.42
13:1M:176:PHE:HA	13:1M:179:ILE:HD12	2.01	0.42
16:1P:27:THR:OG1	16:1P:27:THR:O	2.27	0.42
20:1U:37:MET:HE1	20:1U:71:MET:SD	2.58	0.42
21:1V:24:LYS:HE3	21:1V:59:LYS:HA	2.01	0.42
28:1c:19:LEU:O	28:1c:23:THR:HG22	2.19	0.42
37:1l:72:ASN:N	37:1l:75:GLU:OE2	2.51	0.42
37:1l:158:ILE:HG12	40:1o:99:LYS:HE3	2.01	0.42
38:1m:34:GLU:CD	38:1m:34:GLU:H	2.26	0.42
39:1n:42:LEU:O	39:1n:46:ARG:HG2	2.19	0.42
40:1o:30:PHE:CD2	40:1o:33:ARG:HD2	2.54	0.42
4:1D:163:ALA:HB2	8:1H:277:TYR:C	2.43	0.42
4:1D:387:TYR:C	4:1D:387:TYR:CD1	2.97	0.42
6:1F:334:VAL:C	6:1F:335:ILE:HD12	2.45	0.42
8:1H:207:LEU:O	8:1H:209:SER:N	2.51	0.42
12:1L:245:ALA:O	12:1L:249:SER:OG	2.27	0.42
12:1L:279:CYS:O	12:1L:283:ILE:HG22	2.19	0.42
13:1M:115:LEU:HD23	13:1M:115:LEU:HA	1.88	0.42
13:1M:207:MET:HE1	13:1M:240:GLY:HA2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:275:ILE:HD12	15:1O:276:PRO:HD2	2.01	0.42
22:1W:27:GLU:OE1	22:1W:27:GLU:N	2.48	0.42
45:1Y:202:3PE:H221	45:1Y:202:3PE:H2	1.60	0.42
26:1a:58:ASN:C	26:1a:59:ARG:HD2	2.44	0.42
34:1i:101:PRO:HG2	41:1p:16:THR:HG22	2.00	0.42
40:1o:34:LYS:N	40:1o:34:LYS:HD2	2.35	0.42
41:1p:7:ASP:OD1	41:1p:7:ASP:N	2.52	0.42
3:1C:87:GLN:HE22	21:1V:108:ALA:HB3	1.84	0.42
4:1D:266:GLN:HA	4:1D:266:GLN:NE2	2.34	0.42
5:1E:160:TYR:OH	6:1F:145:GLU:OE1	2.24	0.42
6:1F:226:GLU:HG3	6:1F:254:LYS:NZ	2.35	0.42
7:1G:36:GLN:OE1	17:1Q:49:VAL:N	2.52	0.42
7:1G:278:ARG:NH1	7:1G:548:HIS:HB2	2.35	0.42
7:1G:367:THR:HG22	7:1G:369:ALA:H	1.84	0.42
7:1G:474:ALA:HB3	7:1G:490:MET:HB2	2.01	0.42
9:1I:25:LEU:HD12	50:1I:203:PC1:H382	2.01	0.42
10:1J:6:ALA:HB3	10:1J:124:ASP:CG	2.43	0.42
10:1J:139:GLU:O	10:1J:143:ILE:HG12	2.19	0.42
12:1L:81:LYS:C	12:1L:81:LYS:HD2	2.44	0.42
12:1L:270:ASN:O	12:1L:274:GLN:NE2	2.42	0.42
12:1L:310:LEU:HD12	12:1L:310:LEU:H	1.83	0.42
12:1L:548:SER:HB2	38:1m:92:PHE:CD2	2.54	0.42
17:1Q:19:ILE:HB	17:1Q:22:LEU:HD11	2.02	0.42
24:1Y:82:LYS:O	24:1Y:88:ASN:ND2	2.47	0.42
25:1Z:43:LEU:HB3	25:1Z:47:TYR:HE2	1.83	0.42
25:1Z:65:PHE:O	25:1Z:69:ILE:HG12	2.19	0.42
32:1g:43:ASP:C	32:1g:43:ASP:OD2	2.62	0.42
35:1j:59:TRP:CD1	35:1j:59:TRP:N	2.87	0.42
36:1k:18:TYR:OH	36:1k:46:ARG:O	2.37	0.42
42:1q:55:PHE:CZ	42:1q:58:ARG:HD3	2.54	0.42
42:1q:76:ASP:C	42:1q:76:ASP:OD2	2.62	0.42
1:1A:38:GLU:CD	8:1H:126:LYS:HZ2	2.20	0.42
2:1B:62:MET:O	2:1B:62:MET:HG2	2.20	0.42
3:1C:66:ASP:N	3:1C:66:ASP:OD1	2.53	0.42
4:1D:19:MET:HE3	4:1D:19:MET:N	2.28	0.42
4:1D:246:THR:OG1	4:1D:249:ASP:OD2	2.28	0.42
7:1G:64:LYS:HD2	7:1G:64:LYS:C	2.44	0.42
7:1G:405:LYS:HD3	7:1G:405:LYS:HA	1.74	0.42
7:1G:448:LYS:NZ	7:1G:448:LYS:HB3	2.35	0.42
7:1G:537:LEU:HD13	7:1G:541:CYS:CB	2.49	0.42
8:1H:199:ASP:CG	8:1H:279:ARG:HE	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:165:ILE:HD12	9:1I:166:ALA:N	2.35	0.42
11:1K:55:LEU:HG	30:1e:25:PRO:HD3	2.01	0.42
13:1M:2:LEU:HD12	13:1M:6:ILE:HD11	2.01	0.42
13:1M:76:MET:HB3	13:1M:226:ALA:HB1	2.01	0.42
14:1N:197:ASN:ND2	14:1N:200:MET:SD	2.92	0.42
16:1P:235:ARG:HB2	16:1P:340:VAL:HG23	2.00	0.42
17:1Q:57:MET:HB3	17:1Q:84:LEU:H	1.84	0.42
30:1e:11:LEU:HD12	30:1e:13:LEU:HD21	2.01	0.42
31:1f:15:LEU:HD12	31:1f:15:LEU:HA	1.84	0.42
34:1i:127:HIS:HB3	40:1o:84:HIS:HE1	1.84	0.42
35:1j:12:ARG:HD2	36:1k:21:TRP:CZ3	2.54	0.42
37:1l:126:GLN:HE22	58:1l:201:MYR:H31	1.83	0.42
40:1o:52:LEU:HA	40:1o:55:ARG:HD3	2.00	0.42
1:1A:67:LEU:HD12	11:1K:65:VAL:HA	2.02	0.42
1:1A:67:LEU:HD12	11:1K:65:VAL:HG12	1.99	0.42
3:1C:175:ARG:NH1	16:1P:13:ARG:HE	2.17	0.42
3:1C:209:TYR:CD2	3:1C:209:TYR:N	2.87	0.42
5:1E:190:ARG:HA	5:1E:194:GLU:OE2	2.18	0.42
6:1F:185:ILE:O	6:1F:191:ALA:HB3	2.19	0.42
7:1G:544:ILE:HG13	7:1G:559:VAL:O	2.19	0.42
8:1H:142:TYR:O	8:1H:145:THR:OG1	2.24	0.42
10:1J:173:ARG:HG3	10:1J:175:ASN:H	1.84	0.42
13:1M:105:PHE:O	13:1M:109:THR:HG22	2.19	0.42
13:1M:281:ASP:HB3	13:1M:284:SER:HB3	2.00	0.42
14:1N:37:LEU:HD21	14:1N:60:PHE:HD1	1.84	0.42
17:1Q:43:ASN:OD1	17:1Q:45:MET:HG2	2.18	0.42
29:1d:11:LEU:HD21	30:1e:3:PHE:HB3	2.01	0.42
29:1d:94:VAL:HG12	29:1d:101:PHE:CZ	2.55	0.42
35:1j:34:PHE:C	35:1j:34:PHE:CD2	2.98	0.42
39:1n:85:PRO:HA	39:1n:90:TYR:CD2	2.53	0.42
51:1q:201:CDL:H542	51:1q:201:CDL:H512	1.76	0.42
44:1s:46:TYR:CD1	44:1s:50:THR:HG21	2.55	0.42
1:1A:4:MET:SD	1:1A:5:LEU:N	2.93	0.42
6:1F:392:LEU:HG	6:1F:419:ILE:HD11	2.02	0.42
7:1G:321:GLY:O	7:1G:496:ILE:HG23	2.19	0.42
8:1H:105:MET:HE3	8:1H:162:LEU:HD11	2.02	0.42
9:1I:109:TYR:H	9:1I:151:LYS:HB2	1.84	0.42
10:1J:168:ILE:HD13	10:1J:168:ILE:HA	1.84	0.42
12:1L:37:LYS:HE2	12:1L:37:LYS:HB3	1.79	0.42
12:1L:69:MET:HE2	12:1L:70:THR:N	2.35	0.42
12:1L:313:MET:HE3	12:1L:313:MET:HB3	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1M:182:TRP:CE2	41:1p:79:LYS:HE2	2.54	0.42
13:1M:189:SER:OG	24:1Y:130:GLU:OE2	2.37	0.42
13:1M:193:ILE:HD12	13:1M:193:ILE:N	2.35	0.42
16:1P:237:LEU:O	16:1P:241:LEU:HD22	2.20	0.42
20:1T:26:ASP:HB3	20:1T:29:LYS:HE2	2.01	0.42
22:1W:90:LEU:HD12	22:1W:91:GLU:N	2.35	0.42
22:1W:98:LYS:HB3	22:1W:98:LYS:HE3	1.80	0.42
23:1X:79:GLU:HB2	23:1X:80:PRO:HD3	2.01	0.42
24:1Y:36:SER:HB2	24:1Y:55:THR:HA	2.02	0.42
41:1p:89:MET:HA	41:1p:89:MET:HE2	2.02	0.42
1:1A:1:FME:H	1:1A:4:MET:HE1	1.82	0.42
2:1B:46:TRP:CD1	2:1B:75:VAL:HG22	2.55	0.42
4:1D:62:LEU:HD13	4:1D:425:PHE:CE2	2.55	0.42
4:1D:354:GLU:HG2	4:1D:355:GLY:O	2.20	0.42
6:1F:138:ILE:HG23	6:1F:179:ARG:HA	2.01	0.42
6:1F:149:LEU:HA	6:1F:152:ALA:HB3	2.02	0.42
6:1F:188:GLU:HB2	48:1F:501:FMN:C8	2.50	0.42
6:1F:200:GLN:O	6:1F:202:LYS:HG2	2.20	0.42
6:1F:292:ASP:OD1	6:1F:292:ASP:C	2.63	0.42
7:1G:161:ARG:O	7:1G:165:GLU:HG2	2.19	0.42
7:1G:274:LEU:O	7:1G:278:ARG:NH2	2.52	0.42
8:1H:93:TYR:N	8:1H:93:TYR:CD1	2.88	0.42
8:1H:253:GLU:HG3	26:1a:21:MET:CE	2.50	0.42
10:1J:115:ILE:HG22	10:1J:116:ILE:HG12	2.02	0.42
10:1J:163:ILE:O	10:1J:166:VAL:HG22	2.19	0.42
12:1L:61:MET:O	12:1L:82:MET:N	2.52	0.42
12:1L:124:PHE:HA	12:1L:150:MET:HG2	2.02	0.42
12:1L:599:MET:HE2	12:1L:599:MET:HB2	1.91	0.42
14:1N:255:PRO:HG3	14:1N:260:PHE:CD1	2.54	0.42
14:1N:321:LYS:HG2	14:1N:323:MET:H	1.84	0.42
16:1P:40:ARG:HD3	16:1P:40:ARG:HA	1.83	0.42
16:1P:87:HIS:NE2	18:1R:25:ARG:HD2	2.35	0.42
18:1R:16:GLN:HE21	18:1R:18:TYR:HD2	1.66	0.42
21:1V:57:MET:H	21:1V:57:MET:CE	2.32	0.42
33:1h:103:LEU:HD23	33:1h:103:LEU:HA	1.83	0.42
42:1q:11:LEU:HD22	42:1q:11:LEU:H	1.85	0.42
43:1r:26:ARG:HB3	43:1r:30:ILE:HD13	2.00	0.42
1:1A:16:LEU:O	1:1A:20:ILE:HG13	2.19	0.42
2:1B:48:MET:HA	2:1B:48:MET:HE2	2.01	0.42
2:1B:107:MET:HE3	2:1B:107:MET:HB2	1.94	0.42
2:1B:111:ARG:H	16:1P:54:TYR:HH	1.64	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:1D:126:LEU:HG	4:1D:358:VAL:HG22	2.02	0.42
5:1E:96:GLY:H	5:1E:138:THR:HG21	1.85	0.42
6:1F:22:PHE:CD2	6:1F:255:LEU:HD21	2.55	0.42
7:1G:238:ILE:C	7:1G:238:ILE:HD12	2.45	0.42
9:1I:88:PRO:HD2	46:1I:201:SF4:S4	2.59	0.42
10:1J:64:MET:O	10:1J:67:VAL:HG22	2.20	0.42
12:1L:19:ILE:HD11	12:1L:122:VAL:HB	2.01	0.42
14:1N:278:MET:O	14:1N:278:MET:HE3	2.20	0.42
15:1O:139:TYR:HB2	15:1O:144:ILE:HD11	2.01	0.42
29:1d:82:MET:O	29:1d:86:ARG:N	2.37	0.42
33:1h:45:VAL:HG12	41:1p:51:ILE:HD13	2.01	0.42
33:1h:69:HIS:CG	33:1h:70:PRO:HD2	2.55	0.42
35:1j:37:LEU:CB	36:1k:77:PHE:HE1	2.33	0.42
35:1j:66:ILE:HG23	40:1o:107:LEU:HD23	2.01	0.42
39:1n:135:GLU:OE2	39:1n:165:LEU:N	2.52	0.42
2:1B:71:ARG:HA	8:1H:36:GLY:O	2.19	0.42
6:1F:66:ARG:HG2	6:1F:73:PHE:C	2.45	0.42
7:1G:126:ASP:N	7:1G:126:ASP:OD1	2.52	0.42
7:1G:166:ILE:HG23	7:1G:262:TRP:CH2	2.55	0.42
7:1G:283:MET:HG3	7:1G:291:LEU:HB3	2.02	0.42
9:1I:35:GLY:HA3	50:1I:204:PC1:H331	2.01	0.42
10:1J:74:MET:HE3	10:1J:75:ALA:N	2.35	0.42
12:1L:122:VAL:HG12	12:1L:126:ILE:HD11	2.02	0.42
12:1L:252:MET:HG3	12:1L:253:VAL:N	2.35	0.42
12:1L:287:PHE:CZ	12:1L:527:GLY:HA3	2.55	0.42
12:1L:366:MET:HB3	12:1L:369:THR:HB	2.01	0.42
13:1M:163:ALA:O	13:1M:167:ILE:HG12	2.20	0.42
13:1M:253:LEU:HD12	13:1M:253:LEU:HA	1.81	0.42
13:1M:361:MET:HE2	13:1M:361:MET:HB2	1.85	0.42
15:1O:3:TYR:HB3	15:1O:261:MET:CE	2.50	0.42
15:1O:70:ASP:HB3	15:1O:73:LEU:HD23	2.01	0.42
15:1O:174:VAL:HG13	15:1O:178:GLU:HG2	2.02	0.42
15:1O:226:ARG:NH2	15:1O:229:GLU:HG2	2.35	0.42
15:1O:227:GLU:H	15:1O:227:GLU:CD	2.28	0.42
15:1O:308:TYR:OH	29:1d:51:ARG:NH1	2.52	0.42
17:1Q:58:GLU:H	17:1Q:58:GLU:CD	2.06	0.42
22:1W:102:HIS:HA	22:1W:105:ARG:NH1	2.35	0.42
57:1Y:201:PGT:H202	57:1Y:201:PGT:H231	1.93	0.42
29:1d:-1:MET:SD	33:1h:111:ARG:HD2	2.58	0.42
40:1o:105:ARG:HG2	40:1o:109:GLN:HE21	1.85	0.42
2:1B:94:ASN:HD22	3:1C:174:LEU:HG	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1C:10:THR:HG21	43:1r:56:ARG:HD2	2.01	0.41
4:1D:90:LEU:H	4:1D:90:LEU:HD12	1.85	0.41
4:1D:285:VAL:HA	4:1D:286:PRO:HD3	1.89	0.41
4:1D:328:ALA:H	7:1G:126:ASP:HB2	1.85	0.41
5:1E:116:ILE:HG12	5:1E:164:LEU:HD13	2.02	0.41
5:1E:149:VAL:HG11	5:1E:190:ARG:HH22	1.85	0.41
6:1F:91:LYS:HB2	6:1F:91:LYS:HE2	1.87	0.41
7:1G:139:ASP:OD1	7:1G:139:ASP:N	2.52	0.41
7:1G:453:LEU:HB3	7:1G:492:ILE:HG22	2.01	0.41
7:1G:471:SER:HB2	7:1G:646:ASN:ND2	2.35	0.41
8:1H:41:GLY:HA3	8:1H:46:LEU:HD23	2.01	0.41
8:1H:152:SER:HB3	8:1H:301:CYS:HA	2.02	0.41
9:1I:112:ASP:OD2	9:1I:112:ASP:C	2.62	0.41
12:1L:313:MET:O	12:1L:316:THR:HG23	2.20	0.41
12:1L:339:LEU:HD22	12:1L:373:LEU:HD12	2.01	0.41
13:1M:220:HIS:CE1	13:1M:232:ALA:HB2	2.55	0.41
14:1N:26:TRP:NE1	14:1N:86:ILE:HA	2.35	0.41
14:1N:108:LEU:HB3	14:1N:161:SER:HB2	2.02	0.41
14:1N:116:PRO:O	14:1N:119:THR:OG1	2.34	0.41
15:1O:104:ARG:HE	15:1O:104:ARG:HB3	1.62	0.41
16:1P:99:TRP:CD1	16:1P:277:PRO:HD2	2.55	0.41
19:1S:20:ILE:O	19:1S:20:ILE:HD12	2.20	0.41
21:1V:75:GLN:O	21:1V:79:VAL:HG23	2.19	0.41
23:1X:20:SER:OG	26:1a:64:LYS:N	2.39	0.41
33:1h:23:LYS:HD3	33:1h:23:LYS:HA	1.68	0.41
37:1l:135:TYR:HE2	40:1o:45:MET:HE3	1.85	0.41
40:1o:62:LEU:HB2	40:1o:86:TRP:CE2	2.55	0.41
42:1q:96:ASP:OD2	42:1q:100:THR:OG1	2.37	0.41
2:1B:176:TRP:HD1	2:1B:179:ARG:HH21	1.68	0.41
3:1C:32:ILE:HA	21:1V:42:ALA:HB3	2.01	0.41
4:1D:116:GLN:HA	4:1D:194:ILE:HG21	2.02	0.41
4:1D:362:ALA:HB2	4:1D:379:VAL:HG12	2.02	0.41
5:1E:12:THR:OG1	5:1E:14:GLU:OE1	2.34	0.41
5:1E:28:TYR:HA	5:1E:31:ILE:HG13	2.02	0.41
5:1E:146:GLY:HA3	6:1F:142:PHE:HZ	1.85	0.41
6:1F:134:ALA:HB2	6:1F:173:PHE:CZ	2.55	0.41
6:1F:254:LYS:HD3	6:1F:255:LEU:N	2.36	0.41
7:1G:444:LYS:HA	7:1G:444:LYS:HD3	1.88	0.41
8:1H:264:LEU:HD11	26:1a:12:MET:HG2	2.01	0.41
10:1J:152:TRP:HA	10:1J:155:ILE:HD12	2.02	0.41
11:1K:66:PHE:CD2	14:1N:31:ILE:HD12	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:1L:264:TYR:CD2	12:1L:265:PRO:HD3	2.55	0.41
12:1L:480:THR:N	12:1L:482:MET:HE1	2.34	0.41
14:1N:69:MET:HG2	14:1N:97:MET:SD	2.59	0.41
14:1N:159:MET:O	14:1N:159:MET:HE3	2.20	0.41
14:1N:159:MET:SD	14:1N:278:MET:HE1	2.59	0.41
14:1N:206:LEU:O	14:1N:210:THR:HG23	2.19	0.41
14:1N:238:PRO:HB2	45:1N:401:3PE:O32	2.20	0.41
14:1N:332:LEU:HD23	14:1N:336:VAL:HG11	2.01	0.41
15:1O:59:ALA:O	15:1O:63:THR:HG22	2.20	0.41
19:1S:19:ARG:HD3	19:1S:53:LEU:HD12	2.03	0.41
21:1V:59:LYS:HE2	21:1V:59:LYS:HB2	1.69	0.41
22:1W:57:LYS:HG3	22:1W:58:GLN:N	2.35	0.41
25:1Z:31:SER:O	25:1Z:34:SER:OG	2.32	0.41
25:1Z:120:MET:HB2	30:1e:68:ARG:CZ	2.50	0.41
30:1e:12:ASP:OD1	30:1e:16:TRP:HD1	2.03	0.41
30:1e:21:SER:HB3	33:1h:133:ILE:HD13	2.02	0.41
34:1i:6:ASP:OD1	34:1i:6:ASP:N	2.53	0.41
40:1o:33:ARG:NH2	40:1o:100:GLU:OE2	2.41	0.41
41:1p:48:ARG:HA	41:1p:51:ILE:HG22	2.02	0.41
2:1B:125:TYR:CE2	9:1I:88:PRO:HB2	2.55	0.41
3:1C:211:GLN:NE2	21:1V:114:PRO:O	2.53	0.41
6:1F:188:GLU:OE2	6:1F:405:CYS:HB2	2.20	0.41
7:1G:148:THR:O	7:1G:148:THR:OG1	2.38	0.41
7:1G:403:ASP:HA	17:1Q:127:ARG:NH2	2.34	0.41
7:1G:492:ILE:O	7:1G:493:LEU:HD23	2.20	0.41
11:1K:67:ALA:HA	11:1K:70:GLU:OE2	2.20	0.41
12:1L:10:THR:O	12:1L:13:ILE:HG22	2.20	0.41
12:1L:147:VAL:HG21	12:1L:252:MET:HB2	2.02	0.41
12:1L:187:ALA:HA	13:1M:383:THR:HG22	2.01	0.41
12:1L:396:ILE:HD13	12:1L:396:ILE:HA	1.86	0.41
14:1N:122:ILE:C	14:1N:122:ILE:HD12	2.45	0.41
16:1P:36:ASN:ND2	16:1P:40:ARG:HH22	2.18	0.41
16:1P:107:GLU:O	16:1P:111:VAL:HG12	2.20	0.41
16:1P:208:VAL:O	16:1P:212:LYS:NZ	2.52	0.41
18:1R:40:ALA:O	18:1R:44:ILE:HG22	2.20	0.41
21:1V:18:THR:OG1	21:1V:21:GLU:OE2	2.37	0.41
21:1V:21:GLU:O	21:1V:25:ILE:HG13	2.20	0.41
22:1W:59:GLY:O	22:1W:63:VAL:HG23	2.20	0.41
22:1W:66:MET:HA	22:1W:69:LYS:NZ	2.35	0.41
25:1Z:62:ILE:HG22	27:1b:48:THR:HG23	2.01	0.41
33:1h:91:MET:HE3	33:1h:91:MET:HB3	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:1o:38:MET:HG2	40:1o:57:TYR:CE1	2.55	0.41
42:1q:54:GLN:HB2	42:1q:59:HIS:HA	2.01	0.41
43:1r:45:SER:O	43:1r:51:ASN:ND2	2.53	0.41
44:1s:52:LEU:HD13	44:1s:55:ASN:HD22	1.84	0.41
4:1D:217:ASN:CG	43:1r:22:LYS:HB2	2.45	0.41
5:1E:201:SER:O	5:1E:202:LEU:HD23	2.20	0.41
6:1F:44:LYS:O	6:1F:48:ILE:HG23	2.20	0.41
6:1F:154:ARG:HH12	44:1s:58:LEU:N	2.19	0.41
6:1F:254:LYS:HD3	6:1F:255:LEU:H	1.85	0.41
6:1F:322:LEU:HG	6:1F:329:LEU:HB2	2.01	0.41
6:1F:385:ARG:HB2	6:1F:388:GLU:OE1	2.20	0.41
7:1G:38:PRO:HG3	7:1G:123:PHE:CD2	2.55	0.41
7:1G:171:ASP:O	7:1G:185:THR:HG23	2.21	0.41
7:1G:229:ASP:N	7:1G:236:SER:O	2.48	0.41
7:1G:343:LEU:HD22	7:1G:507:TYR:CZ	2.55	0.41
7:1G:364:LEU:HG	7:1G:492:ILE:O	2.20	0.41
7:1G:584:LYS:HG3	17:1Q:36:ARG:NH1	2.35	0.41
8:1H:32:GLN:HB2	8:1H:34:ARG:HG3	2.00	0.41
8:1H:241:LEU:HD12	8:1H:241:LEU:HA	1.85	0.41
10:1J:52:LEU:HD13	10:1J:52:LEU:HA	1.86	0.41
10:1J:99:MET:O	10:1J:103:MET:HG3	2.20	0.41
13:1M:261:PHE:HB2	13:1M:302:MET:HE2	2.03	0.41
14:1N:175:LEU:HD21	14:1N:227:THR:HA	2.02	0.41
14:1N:190:MET:HE2	14:1N:190:MET:HB3	1.80	0.41
16:1P:196:LEU:HD12	16:1P:196:LEU:HA	1.92	0.41
16:1P:278:TRP:CD1	16:1P:278:TRP:N	2.87	0.41
20:1T:54:MET:HE1	20:1T:62:ILE:HG13	2.02	0.41
20:1T:58:PHE:HB2	20:1T:60:PHE:CE1	2.56	0.41
20:1U:11:ILE:O	20:1U:15:VAL:N	2.45	0.41
23:1X:97:ARG:HH21	25:1Z:53:TRP:HH2	1.68	0.41
23:1X:171:MET:HB2	29:1d:30:ARG:HD2	2.03	0.41
29:1d:86:ARG:O	29:1d:90:MET:HB2	2.21	0.41
32:1g:92:GLU:HG2	41:1p:64:HIS:HE1	1.85	0.41
35:1j:56:PRO:HB3	40:1o:102:GLU:OE2	2.20	0.41
40:1o:18:PRO:HA	40:1o:21:MET:SD	2.60	0.41
40:1o:69:LYS:HE3	40:1o:69:LYS:HB3	1.82	0.41
2:1B:88:VAL:HG21	2:1B:136:CYS:SG	2.60	0.41
3:1C:72:PHE:HB3	3:1C:96:LEU:HB3	2.02	0.41
5:1E:213:VAL:HG12	6:1F:44:LYS:HD2	2.03	0.41
6:1F:29:HIS:CD2	6:1F:29:HIS:H	2.39	0.41
6:1F:231:SER:O	6:1F:234:ILE:HG13	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:337:MET:HG3	6:1F:341:THR:OG1	2.20	0.41
7:1G:326:GLU:OE1	7:1G:326:GLU:N	2.48	0.41
7:1G:378:LEU:HD21	7:1G:439:PHE:CE1	2.56	0.41
8:1H:204:GLU:HA	8:1H:208:VAL:O	2.20	0.41
10:1J:68:PHE:O	10:1J:72:THR:HG23	2.21	0.41
10:1J:129:ASP:OD2	10:1J:129:ASP:C	2.64	0.41
12:1L:183:VAL:HG23	13:1M:382:ILE:HG21	2.02	0.41
12:1L:368:PHE:HE1	35:1j:28:PHE:HD2	1.66	0.41
12:1L:428:PHE:CD2	12:1L:505:ASN:HB3	2.56	0.41
13:1M:16:TRP:HA	13:1M:93:LYS:HD3	2.01	0.41
13:1M:389:SER:O	13:1M:392:THR:HG22	2.20	0.41
13:1M:407:SER:O	13:1M:410:MET:HG2	2.20	0.41
15:1O:85:ASP:OD1	15:1O:85:ASP:N	2.52	0.41
15:1O:281:GLU:H	15:1O:281:GLU:CD	2.28	0.41
20:1T:45:LEU:HG	22:1W:64:ARG:HH22	1.85	0.41
23:1X:58:GLU:OE1	23:1X:58:GLU:N	2.38	0.41
25:1Z:87:LEU:HD23	25:1Z:87:LEU:HA	1.85	0.41
25:1Z:105:LYS:O	25:1Z:105:LYS:HG3	2.19	0.41
32:1g:50:ASP:OD2	32:1g:50:ASP:C	2.63	0.41
34:1i:48:LYS:HA	34:1i:51:GLN:HG2	2.01	0.41
34:1i:102:ARG:HB3	40:1o:49:GLN:HG2	2.03	0.41
37:1l:4:VAL:HG23	37:1l:8:MET:HE2	2.03	0.41
41:1p:30:THR:O	41:1p:34:LYS:HG2	2.20	0.41
42:1q:6:VAL:CG1	51:1q:201:CDL:HA61	2.48	0.41
42:1q:83:PRO:HG2	42:1q:86:TRP:HB2	2.03	0.41
42:1q:86:TRP:CE3	42:1q:98:PRO:HD2	2.56	0.41
43:1r:32:LYS:O	43:1r:32:LYS:HD2	2.21	0.41
44:1s:58:LEU:HD12	44:1s:62:ARG:HH12	1.84	0.41
6:1F:94:VAL:HG11	6:1F:192:LEU:HD21	2.02	0.41
9:1I:9:GLU:CD	9:1I:9:GLU:N	2.79	0.41
9:1I:12:MET:HE1	9:1I:20:ARG:HH12	1.86	0.41
9:1I:72:SER:HB2	18:1R:47:GLN:HE21	1.85	0.41
11:1K:40:LEU:O	11:1K:44:SER:OG	2.25	0.41
12:1L:316:THR:OG1	12:1L:325:ALA:HB2	2.21	0.41
13:1M:150:LEU:O	13:1M:154:LEU:HD23	2.20	0.41
13:1M:309:PHE:O	13:1M:313:THR:HG23	2.20	0.41
13:1M:312:ALA:O	13:1M:316:MET:N	2.49	0.41
14:1N:82:GLY:O	14:1N:83:GLN:NE2	2.54	0.41
14:1N:316:GLN:NE2	15:1O:60:ASP:OD1	2.54	0.41
45:1N:401:3PE:O14	15:1O:303:LYS:NZ	2.48	0.41
15:1O:23:LYS:HG3	15:1O:167:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:56:ILE:O	15:1O:99:TRP:NE1	2.45	0.41
15:1O:64:GLY:O	28:1c:4:ILE:HG23	2.20	0.41
16:1P:23:VAL:O	16:1P:48:PRO:HD2	2.21	0.41
16:1P:91:VAL:HG23	16:1P:126:VAL:HG21	2.03	0.41
16:1P:271:GLU:HG2	16:1P:280:THR:HG22	2.03	0.41
18:1R:71:VAL:HG12	18:1R:72:TYR:H	1.85	0.41
19:1S:12:LYS:HG2	19:1S:13:LEU:N	2.35	0.41
20:1T:7:THR:O	20:1T:11:ILE:HG13	2.20	0.41
24:1Y:87:LEU:O	24:1Y:91:ILE:HG12	2.21	0.41
25:1Z:21:TYR:CD2	25:1Z:21:TYR:C	2.98	0.41
37:1l:18:GLU:OE2	37:1l:18:GLU:N	2.31	0.41
37:1l:65:ASP:OD2	37:1l:73:TRP:N	2.53	0.41
37:1l:82:ASP:O	37:1l:88:ARG:HD2	2.20	0.41
41:1p:139:GLN:O	41:1p:143:SER:OG	2.36	0.41
43:1r:107:LYS:H	43:1r:107:LYS:CE	2.27	0.41
1:1A:1:FME:CN	25:1Z:142:TRP:HB3	2.51	0.41
1:1A:54:LYS:HD2	4:1D:71:GLU:OE1	2.21	0.41
2:1B:145:TYR:N	9:1I:141:THR:O	2.50	0.41
3:1C:40:VAL:HG23	3:1C:50:ILE:CD1	2.50	0.41
3:1C:105:ILE:HD13	3:1C:105:ILE:HA	1.89	0.41
3:1C:141:PHE:HD2	22:1W:20:ILE:HD11	1.86	0.41
4:1D:69:SER:N	4:1D:72:MET:O	2.49	0.41
4:1D:357:GLN:OE1	43:1r:59:ARG:NH2	2.42	0.41
5:1E:93:LYS:HG3	5:1E:94:PRO:CD	2.50	0.41
5:1E:149:VAL:HB	6:1F:257:ASN:ND2	2.28	0.41
6:1F:115:PRO:HD2	6:1F:116:HIS:CD2	2.56	0.41
7:1G:67:ALA:O	7:1G:71:MET:HG2	2.21	0.41
7:1G:286:ASN:N	7:1G:290:LEU:O	2.48	0.41
9:1I:69:ARG:HG3	9:1I:73:GLY:HA2	2.02	0.41
12:1L:253:VAL:HG13	12:1L:310:LEU:HD21	2.03	0.41
12:1L:511:LEU:HD11	39:1n:38:TYR:CE2	2.56	0.41
13:1M:100:ILE:HD12	13:1M:101:LEU:N	2.35	0.41
13:1M:168:GLN:HE21	33:1h:104:ARG:HD2	1.84	0.41
13:1M:197:LEU:HD23	13:1M:197:LEU:HA	1.86	0.41
13:1M:405:LEU:HA	13:1M:405:LEU:HD13	1.83	0.41
14:1N:270:MET:CG	14:1N:279:PRO:HG3	2.51	0.41
15:1O:311:ASP:OD1	15:1O:311:ASP:N	2.53	0.41
16:1P:80:SER:HA	16:1P:83:LYS:HE3	2.02	0.41
16:1P:248:VAL:HG23	16:1P:334:VAL:HG11	2.02	0.41
20:1T:36:PHE:CD1	20:1T:40:LEU:HD12	2.56	0.41
20:1T:63:PRO:HB2	20:1T:65:ILE:HG13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:1V:22:ARG:HD2	21:1V:22:ARG:HA	1.77	0.41
23:1X:109:CYS:HB3	23:1X:113:LYS:HG3	2.01	0.41
50:1f:101:PC1:H12	50:1f:101:PC1:H152	2.03	0.41
32:1g:48:ASP:OD2	32:1g:48:ASP:N	2.53	0.41
33:1h:26:ARG:O	33:1h:30:LEU:HB2	2.19	0.41
37:1l:34:TYR:HD1	37:1l:48:PRO:HB3	1.86	0.41
42:1q:29:ARG:HH22	42:1q:65:THR:C	2.28	0.41
1:1A:29:ALA:C	1:1A:30:TYR:HD2	2.29	0.41
1:1A:93:PHE:C	1:1A:93:PHE:CD2	2.96	0.41
3:1C:41:GLN:OE1	43:1r:67:ILE:HD12	2.20	0.41
3:1C:184:VAL:HG13	3:1C:186:GLU:OE2	2.21	0.41
3:1C:204:GLU:HA	17:1Q:50:ASN:ND2	2.21	0.41
4:1D:72:MET:HE1	4:1D:409:HIS:N	2.36	0.41
4:1D:357:GLN:HA	4:1D:384:SER:HA	2.02	0.41
5:1E:124:LEU:HG	5:1E:126:ILE:HG12	2.02	0.41
6:1F:34:LYS:HE2	6:1F:34:LYS:HB2	1.77	0.41
6:1F:65:LEU:HD23	6:1F:242:PHE:CZ	2.56	0.41
7:1G:70:ALA:O	7:1G:72:PRO:HD3	2.20	0.41
12:1L:67:HIS:HA	12:1L:77:SER:OG	2.20	0.41
12:1L:313:MET:HG2	12:1L:313:MET:H	1.59	0.41
13:1M:134:THR:HG21	14:1N:302:LEU:HD13	2.02	0.41
13:1M:436:LEU:HD23	13:1M:436:LEU:C	2.46	0.41
14:1N:217:MET:SD	14:1N:326:LEU:HB2	2.61	0.41
18:1R:37:GLU:OE1	18:1R:37:GLU:N	2.32	0.41
29:1d:58:LEU:HA	29:1d:58:LEU:HD22	1.89	0.41
30:1e:80:ARG:NH1	30:1e:80:ARG:HA	2.34	0.41
33:1h:85:LYS:O	33:1h:89:LYS:HB2	2.21	0.41
33:1h:94:LEU:HD23	33:1h:94:LEU:HA	1.83	0.41
35:1j:62:GLU:OE1	35:1j:63:GLU:N	2.53	0.41
37:1l:156:TYR:CD2	40:1o:33:ARG:HB3	2.54	0.41
39:1n:138:GLN:O	39:1n:142:GLU:HG2	2.21	0.41
40:1o:13:SER:C	40:1o:14:LYS:HD2	2.45	0.41
40:1o:30:PHE:CG	40:1o:33:ARG:HD2	2.56	0.41
42:1q:56:PHE:HZ	43:1r:33:ARG:HH11	1.67	0.41
2:1B:176:TRP:HA	2:1B:179:ARG:HE	1.86	0.41
3:1C:41:GLN:NE2	43:1r:65:PRO:O	2.54	0.41
3:1C:126:ALA:HB2	4:1D:253:TYR:C	2.46	0.41
4:1D:137:ILE:HG12	4:1D:203:LEU:HD21	2.02	0.41
4:1D:242:ILE:HD12	4:1D:409:HIS:HD2	1.86	0.41
5:1E:122:LYS:HD3	5:1E:122:LYS:HA	1.94	0.41
5:1E:207:LYS:HA	5:1E:207:LYS:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:413:TRP:N	6:1F:413:TRP:CD1	2.86	0.41
6:1F:417:GLY:HA2	6:1F:420:ARG:HE	1.86	0.41
7:1G:28:GLN:NE2	17:1Q:114:LYS:O	2.54	0.41
7:1G:80:LEU:HD23	7:1G:80:LEU:HA	1.94	0.41
7:1G:335:LEU:HD23	7:1G:335:LEU:HA	1.76	0.41
8:1H:100:LEU:HD22	8:1H:160:TYR:HB2	2.03	0.41
8:1H:206:GLU:HG2	8:1H:207:LEU:CD2	2.47	0.41
8:1H:267:THR:O	8:1H:270:PHE:HB2	2.21	0.41
10:1J:68:PHE:CD1	11:1K:27:MET:HE1	2.56	0.41
10:1J:122:LEU:HD23	10:1J:122:LEU:HA	1.84	0.41
10:1J:167:VAL:HG23	14:1N:42:PRO:HB3	2.02	0.41
11:1K:55:LEU:H	30:1e:24:GLN:HE22	1.67	0.41
11:1K:57:ASN:O	11:1K:60:PRO:HD2	2.21	0.41
12:1L:88:MET:C	12:1L:91:PRO:HD2	2.45	0.41
12:1L:108:MET:HE1	12:1L:242:PRO:HD2	2.03	0.41
12:1L:131:LEU:HD12	12:1L:143:GLY:C	2.46	0.41
12:1L:283:ILE:HB	37:1l:112:MET:HE2	2.02	0.41
12:1L:319:ILE:O	12:1L:321:GLN:HG2	2.20	0.41
13:1M:40:SER:HA	32:1g:76:PHE:CE2	2.56	0.41
13:1M:51:ASN:N	13:1M:51:ASN:HD22	2.19	0.41
13:1M:69:THR:HG23	13:1M:234:VAL:HG21	2.02	0.41
13:1M:76:MET:SD	13:1M:76:MET:N	2.86	0.41
13:1M:135:ARG:HE	45:1N:401:3PE:H362	1.86	0.41
13:1M:201:MET:HE1	13:1M:261:PHE:CZ	2.55	0.41
13:1M:388:TRP:CE2	38:1m:108:ARG:HD2	2.55	0.41
14:1N:104:MET:HE2	14:1N:104:MET:HB2	1.87	0.41
14:1N:270:MET:H	14:1N:270:MET:HG2	1.60	0.41
15:1O:94:TYR:CD1	15:1O:148:CYS:HB3	2.56	0.41
15:1O:204:ASN:O	15:1O:208:LYS:HG2	2.21	0.41
15:1O:309:ASN:HB3	15:1O:311:ASP:OD1	2.21	0.41
16:1P:141:SER:O	16:1P:147:ARG:NH2	2.54	0.41
16:1P:183:ALA:O	16:1P:186:ARG:HG2	2.21	0.41
19:1S:44:LYS:NZ	19:1S:48:PRO:HB3	2.36	0.41
20:1T:83:LYS:HE2	20:1T:83:LYS:HB2	1.93	0.41
20:1U:46:ASP:OD1	39:1n:44:ARG:NH2	2.54	0.41
22:1W:47:VAL:HG11	22:1W:56:VAL:HG22	2.03	0.41
23:1X:30:HIS:HA	23:1X:34:GLN:NE2	2.36	0.41
25:1Z:6:VAL:HA	43:1r:39:LYS:HG3	2.02	0.41
30:1e:83:ASP:N	30:1e:83:ASP:OD2	2.52	0.41
33:1h:32:THR:O	33:1h:35:PRO:HD2	2.21	0.41
34:1i:57:LYS:HB2	34:1i:57:LYS:HE2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:1i:109:ILE:HD13	34:1i:112:THR:H	1.86	0.41
34:1i:116:ILE:HD12	34:1i:116:ILE:O	2.21	0.41
37:1l:6:LYS:HE3	37:1l:9:PHE:HD2	1.84	0.41
37:1l:69:LEU:HD22	37:1l:85:ILE:HD11	2.03	0.41
39:1n:91:GLU:HB2	39:1n:94:GLU:HB2	2.03	0.41
42:1q:9:ARG:HD3	51:1q:201:CDL:CA3	2.46	0.41
1:1A:22:PHE:HB3	1:1A:23:TRP:HE3	1.86	0.41
3:1C:197:PHE:HA	7:1G:220:TRP:O	2.21	0.41
4:1D:80:ILE:C	4:1D:80:ILE:HD12	2.46	0.41
4:1D:328:ALA:HA	4:1D:331:SER:O	2.21	0.41
5:1E:30:ARG:HG2	44:1s:56:VAL:HG11	2.02	0.41
5:1E:111:ARG:NH2	6:1F:260:GLY:O	2.45	0.41
5:1E:191:PHE:CG	44:1s:38:TYR:HB2	2.56	0.41
6:1F:48:ILE:HG13	6:1F:49:LEU:N	2.35	0.41
7:1G:237:ASN:O	7:1G:259:ASN:ND2	2.52	0.41
7:1G:331:LEU:HA	7:1G:334:LEU:HB3	2.03	0.41
8:1H:20:LEU:HD23	8:1H:228:TYR:CD1	2.55	0.41
8:1H:42:PRO:HB3	42:1q:27:LEU:HD21	2.03	0.41
8:1H:85:MET:HE1	8:1H:105:MET:HA	2.02	0.41
12:1L:124:PHE:CA	12:1L:150:MET:HG2	2.51	0.41
13:1M:269:MET:HG2	13:1M:270:ILE:N	2.36	0.41
13:1M:367:LEU:HD23	13:1M:367:LEU:HA	1.80	0.41
14:1N:15:SER:O	14:1N:19:LEU:N	2.45	0.41
15:1O:153:ASN:HB3	15:1O:157:LYS:HZ1	1.84	0.41
15:1O:270:LEU:O	15:1O:273:THR:OG1	2.24	0.41
16:1P:35:VAL:HA	16:1P:38:LEU:HB2	2.03	0.41
18:1R:73:ILE:HD12	18:1R:73:ILE:C	2.45	0.41
20:1T:54:MET:HA	20:1T:57:GLU:OE2	2.21	0.41
20:1T:84:LYS:HZ3	20:1T:86:VAL:HB	1.86	0.41
20:1U:70:LEU:HA	20:1U:75:GLU:OE2	2.21	0.41
22:1W:47:VAL:HA	22:1W:52:LEU:CD2	2.50	0.41
22:1W:54:ILE:HD12	22:1W:54:ILE:C	2.46	0.41
22:1W:87:LYS:O	22:1W:87:LYS:NZ	2.29	0.41
24:1Y:35:VAL:HG23	45:1Y:202:3PE:H252	2.03	0.41
32:1g:37:LEU:HB3	32:1g:44:SER:OG	2.21	0.41
43:1r:49:SER:OG	43:1r:50:ASN:N	2.51	0.41
1:1A:105:GLU:OE1	1:1A:111:LEU:HD22	2.21	0.40
4:1D:77:ASP:OD2	4:1D:77:ASP:C	2.64	0.40
4:1D:322:GLU:CD	4:1D:322:GLU:H	2.29	0.40
4:1D:345:LEU:HD12	4:1D:345:LEU:HA	1.75	0.40
6:1F:205:LEU:HD11	6:1F:404:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1F:294:LEU:O	6:1F:294:LEU:HD12	2.22	0.40
7:1G:378:LEU:HD23	7:1G:443:LEU:HD11	2.03	0.40
7:1G:391:PHE:CD1	7:1G:391:PHE:C	3.00	0.40
8:1H:2:PHE:CZ	8:1H:6:ILE:HD11	2.56	0.40
9:1I:18:THR:HA	27:1b:12:TRP:CH2	2.56	0.40
9:1I:113:MET:HB2	9:1I:147:LEU:HB3	2.03	0.40
11:1K:93:LEU:O	11:1K:93:LEU:HD13	2.21	0.40
12:1L:272:LEU:O	12:1L:275:THR:OG1	2.32	0.40
12:1L:346:ILE:HD11	12:1L:359:MET:HE2	2.03	0.40
13:1M:169:ASN:ND2	14:1N:272:LYS:HG3	2.36	0.40
13:1M:201:MET:HE1	13:1M:261:PHE:CE1	2.56	0.40
13:1M:243:MET:HB2	13:1M:301:ILE:HG12	2.03	0.40
13:1M:418:LYS:HA	39:1n:94:GLU:OE2	2.21	0.40
15:1O:30:ASN:OD1	15:1O:31:ILE:HD12	2.21	0.40
18:1R:55:ARG:HE	18:1R:55:ARG:HB3	1.76	0.40
19:1S:19:ARG:HA	19:1S:53:LEU:O	2.21	0.40
21:1V:80:ILE:H	21:1V:80:ILE:HG13	1.69	0.40
23:1X:109:CYS:O	23:1X:112:ASP:N	2.41	0.40
26:1a:1:MET:HE2	51:1q:201:CDL:O1	2.21	0.40
26:1a:2:TRP:HE3	26:1a:2:TRP:O	2.04	0.40
37:1l:8:MET:HB3	38:1m:66:ARG:NH1	2.35	0.40
44:1s:40:ASN:ND2	44:1s:43:HIS:HB3	2.36	0.40
3:1C:15:ASN:OD1	3:1C:15:ASN:C	2.64	0.40
3:1C:39:GLN:HA	3:1C:39:GLN:OE1	2.21	0.40
3:1C:128:ASN:C	3:1C:128:ASN:OD1	2.64	0.40
3:1C:211:GLN:OE1	3:1C:211:GLN:HA	2.21	0.40
4:1D:98:GLN:O	4:1D:101:PRO:HD2	2.20	0.40
7:1G:365:ASN:HB2	7:1G:488:LYS:CB	2.51	0.40
7:1G:629:ASN:HB3	19:1S:57:CYS:HB2	2.02	0.40
8:1H:76:ILE:N	8:1H:76:ILE:HD13	2.36	0.40
8:1H:232:ILE:H	8:1H:232:ILE:HG12	1.67	0.40
9:1I:69:ARG:NE	9:1I:73:GLY:O	2.50	0.40
9:1I:153:LYS:HB2	42:1q:124:TYR:CE1	2.57	0.40
10:1J:127:ILE:H	10:1J:127:ILE:HG13	1.67	0.40
11:1K:12:PHE:CE2	11:1K:36:MET:HG2	2.57	0.40
12:1L:371:THR:O	12:1L:374:ILE:HG13	2.21	0.40
12:1L:593:ILE:O	12:1L:597:ILE:HG12	2.21	0.40
18:1R:26:VAL:O	18:1R:29:SER:OG	2.30	0.40
19:1S:32:VAL:O	19:1S:36:ILE:HG13	2.21	0.40
20:1T:62:ILE:HD12	20:1T:62:ILE:C	2.46	0.40
20:1U:29:LYS:H	20:1U:29:LYS:HD3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1U:52:MET:HE2	20:1U:52:MET:HB3	1.82	0.40
38:1m:22:TYR:CD2	39:1n:64:ARG:NH1	2.90	0.40
38:1m:65:ILE:H	38:1m:65:ILE:HG13	1.74	0.40
38:1m:91:LEU:O	38:1m:96:PRO:HD3	2.20	0.40
39:1n:21:ARG:CZ	39:1n:21:ARG:HB3	2.51	0.40
40:1o:74:PRO:HD3	41:1p:27:ASN:HA	2.03	0.40
40:1o:107:LEU:HD23	40:1o:107:LEU:HA	1.82	0.40
1:1A:104:TYR:CD2	1:1A:104:TYR:C	2.98	0.40
2:1B:42:ARG:HB2	2:1B:164:GLN:HB3	2.02	0.40
4:1D:107:ASP:HB3	4:1D:114:ASN:ND2	2.31	0.40
4:1D:204:PRO:HA	9:1I:175:TYR:CZ	2.55	0.40
4:1D:350:LYS:HD3	4:1D:350:LYS:HA	1.91	0.40
5:1E:87:TYR:N	5:1E:87:TYR:HD2	2.20	0.40
6:1F:305:PRO:HB3	6:1F:417:GLY:HA3	2.03	0.40
7:1G:231:MET:HB2	7:1G:267:THR:HG22	2.04	0.40
7:1G:286:ASN:OD1	7:1G:290:LEU:N	2.45	0.40
9:1I:165:ILE:HG13	9:1I:165:ILE:H	1.67	0.40
10:1J:23:LYS:HA	10:1J:23:LYS:HD2	1.97	0.40
10:1J:52:LEU:HD21	10:1J:143:ILE:HD11	2.03	0.40
11:1K:53:PHE:HB3	11:1K:56:ALA:HB3	2.02	0.40
12:1L:207:GLU:C	12:1L:209:PRO:HD3	2.47	0.40
12:1L:314:MET:HE2	12:1L:314:MET:HB2	1.74	0.40
12:1L:481:THR:C	12:1L:482:MET:HE3	2.46	0.40
13:1M:216:LEU:HB3	13:1M:217:PRO:HD3	2.03	0.40
14:1N:137:ALA:HB3	14:1N:138:PRO:HD3	2.03	0.40
14:1N:147:GLN:H	14:1N:147:GLN:CD	2.29	0.40
15:1O:57:HIS:ND1	15:1O:68:PRO:HB3	2.37	0.40
20:1U:36:PHE:HB2	20:1U:37:MET:HE3	2.03	0.40
23:1X:81:PHE:CG	23:1X:106:PHE:HE2	2.39	0.40
26:1a:22:ALA:C	26:1a:26:ILE:HD12	2.46	0.40
34:1i:60:ILE:HA	34:1i:63:THR:HG22	2.04	0.40
35:1j:18:THR:O	35:1j:21:GLN:HG2	2.21	0.40
37:1l:128:VAL:HG23	40:1o:97:ARG:HB3	2.04	0.40
38:1m:105:LYS:HA	38:1m:105:LYS:HD3	1.93	0.40
41:1p:122:GLN:C	41:1p:122:GLN:OE1	2.64	0.40
4:1D:176:LYS:NZ	43:1r:26:ARG:HH11	2.18	0.40
4:1D:180:PHE:CD2	4:1D:211:ILE:HG22	2.57	0.40
4:1D:209:ASP:O	4:1D:213:GLU:HG2	2.20	0.40
8:1H:130:ILE:O	8:1H:134:ARG:NH1	2.54	0.40
8:1H:179:TRP:CD1	8:1H:180:PRO:HD3	2.56	0.40
9:1I:81:LYS:HD2	9:1I:84:GLU:OE2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:1I:146:GLU:HG2	42:1q:124:TYR:O	2.21	0.40
12:1L:118:PHE:O	12:1L:122:VAL:HG23	2.20	0.40
12:1L:550:SER:HB3	13:1M:275:ILE:HD12	2.02	0.40
13:1M:230:VAL:O	13:1M:234:VAL:HG12	2.22	0.40
13:1M:278:ARG:HH21	37:1l:83:MET:N	2.20	0.40
14:1N:116:PRO:CG	14:1N:181:TYR:HE1	2.35	0.40
14:1N:236:LYS:HB2	14:1N:311:MET:SD	2.61	0.40
16:1P:193:LEU:O	16:1P:257:PRO:HA	2.21	0.40
16:1P:292:MET:SD	16:1P:292:MET:N	2.94	0.40
17:1Q:33:ARG:HE	17:1Q:33:ARG:HB3	1.69	0.40
17:1Q:35:VAL:HG22	17:1Q:59:PHE:CE2	2.56	0.40
17:1Q:126:LYS:HD2	17:1Q:126:LYS:HA	1.78	0.40
18:1R:20:ASP:OD1	18:1R:21:GLY:N	2.48	0.40
20:1T:22:TYR:OH	20:1T:24:LYS:HD3	2.22	0.40
20:1T:78:ASP:OD1	20:1T:79:TYR:N	2.55	0.40
20:1U:70:LEU:HD12	20:1U:76:ILE:HA	2.03	0.40
22:1W:42:GLU:HA	22:1W:45:ASN:HD21	1.87	0.40
22:1W:127:ASP:OD1	22:1W:127:ASP:N	2.54	0.40
25:1Z:93:GLU:OE1	30:1e:94:PRO:HG2	2.22	0.40
39:1n:140:GLN:H	39:1n:140:GLN:CD	2.29	0.40
40:1o:92:LEU:HA	40:1o:95:VAL:HG12	2.04	0.40
41:1p:159:LYS:HE3	41:1p:159:LYS:HB3	1.83	0.40
43:1r:32:LYS:HD2	43:1r:32:LYS:C	2.46	0.40
2:1B:49:THR:HG21	2:1B:59:MET:HE2	2.04	0.40
3:1C:43:SER:HA	43:1r:65:PRO:HA	2.01	0.40
4:1D:169:TRP:HH2	9:1I:37:THR:HG22	1.87	0.40
5:1E:86:PHE:C	5:1E:86:PHE:CD2	2.99	0.40
5:1E:88:THR:HG23	6:1F:182:GLY:O	2.21	0.40
5:1E:153:MET:CE	47:1E:301:FES:S2	2.95	0.40
6:1F:139:ARG:HB3	6:1F:142:PHE:CD2	2.57	0.40
6:1F:307:ILE:HD11	6:1F:311:VAL:HB	2.03	0.40
7:1G:210:SER:OG	7:1G:213:TYR:HB3	2.22	0.40
7:1G:302:ARG:O	7:1G:306:MET:HG2	2.22	0.40
8:1H:281:ARG:O	8:1H:285:LEU:HB2	2.21	0.40
10:1J:120:ASN:N	11:1K:1:FME:O	2.52	0.40
12:1L:125:LEU:HD23	12:1L:125:LEU:HA	1.78	0.40
12:1L:152:PHE:CD1	12:1L:168:ALA:HB1	2.57	0.40
12:1L:247:LEU:HB3	12:1L:252:MET:HG2	2.03	0.40
12:1L:418:LEU:HD13	12:1L:418:LEU:HA	1.97	0.40
12:1L:559:GLU:HA	12:1L:563:PRO:HG2	2.03	0.40
13:1M:147:LEU:HD23	13:1M:147:LEU:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:1O:251:GLN:HB3	15:1O:255:THR:OG1	2.21	0.40
17:1Q:112:LYS:HG2	17:1Q:113:PRO:HD2	2.04	0.40
21:1V:94:LEU:O	21:1V:97:LYS:HD3	2.22	0.40
25:1Z:137:THR:OG1	25:1Z:138:TYR:N	2.55	0.40
29:1d:61:GLN:HA	29:1d:64:TYR:HD2	1.86	0.40
30:1e:9:LEU:HB2	30:1e:11:LEU:CD2	2.51	0.40
31:1f:25:TYR:HA	31:1f:28:ARG:HG2	2.03	0.40
38:1m:21:GLU:O	38:1m:24:ILE:HG23	2.21	0.40
40:1o:94:TYR:O	40:1o:98:MET:HE1	2.21	0.40
42:1q:3:LEU:HG	51:1q:201:CDL:HB61	2.03	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%)	104 (92%)	9 (8%)	0	100	100
2	1B	153/258 (59%)	142 (93%)	11 (7%)	0	100	100
3	1C	207/264 (78%)	196 (95%)	11 (5%)	0	100	100
4	1D	427/476 (90%)	395 (92%)	31 (7%)	1 (0%)	43	72
5	1E	212/249 (85%)	192 (91%)	19 (9%)	1 (0%)	24	57
6	1F	430/464 (93%)	395 (92%)	35 (8%)	0	100	100
7	1G	697/727 (96%)	650 (93%)	44 (6%)	3 (0%)	30	61
8	1H	316/318 (99%)	291 (92%)	23 (7%)	2 (1%)	21	54
9	1I	174/239 (73%)	166 (95%)	8 (5%)	0	100	100
10	1J	173/175 (99%)	161 (93%)	11 (6%)	1 (1%)	21	54
11	1K	96/98 (98%)	88 (92%)	8 (8%)	0	100	100
12	1L	604/606 (100%)	554 (92%)	47 (8%)	3 (0%)	24	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	1M	457/459 (100%)	437 (96%)	20 (4%)	0	100	100
14	1N	345/347 (99%)	323 (94%)	22 (6%)	0	100	100
15	1O	318/357 (89%)	293 (92%)	25 (8%)	0	100	100
16	1P	340/377 (90%)	320 (94%)	20 (6%)	0	100	100
17	1Q	127/175 (73%)	117 (92%)	10 (8%)	0	100	100
18	1R	94/123 (76%)	80 (85%)	14 (15%)	0	100	100
19	1S	85/99 (86%)	78 (92%)	7 (8%)	0	100	100
20	1T	83/156 (53%)	75 (90%)	8 (10%)	0	100	100
20	1U	84/156 (54%)	76 (90%)	8 (10%)	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%)	161 (95%)	8 (5%)	0	100	100
24	1Y	137/141 (97%)	132 (96%)	5 (4%)	0	100	100
25	1Z	139/144 (96%)	126 (91%)	13 (9%)	0	100	100
26	1a	68/70 (97%)	66 (97%)	2 (3%)	0	100	100
27	1b	81/84 (96%)	72 (89%)	9 (11%)	0	100	100
28	1c	47/76 (62%)	43 (92%)	4 (8%)	0	100	100
29	1d	117/123 (95%)	111 (95%)	5 (4%)	1 (1%)	14	46
30	1e	97/106 (92%)	93 (96%)	4 (4%)	0	100	100
31	1f	55/135 (41%)	50 (91%)	4 (7%)	1 (2%)	6	34
32	1g	98/154 (64%)	89 (91%)	8 (8%)	1 (1%)	12	45
33	1h	136/189 (72%)	134 (98%)	2 (2%)	0	100	100
34	1i	124/128 (97%)	120 (97%)	4 (3%)	0	100	100
35	1j	69/105 (66%)	66 (96%)	3 (4%)	0	100	100
36	1k	79/98 (81%)	73 (92%)	6 (8%)	0	100	100
37	1l	154/186 (83%)	140 (91%)	14 (9%)	0	100	100
38	1m	126/129 (98%)	117 (93%)	9 (7%)	0	100	100
39	1n	170/179 (95%)	161 (95%)	9 (5%)	0	100	100
40	1o	120/137 (88%)	116 (97%)	4 (3%)	0	100	100
41	1p	171/176 (97%)	168 (98%)	3 (2%)	0	100	100
42	1q	143/145 (99%)	134 (94%)	8 (6%)	1 (1%)	18	51

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	1r	90/114 (79%)	79 (88%)	11 (12%)	0	100	100
44	1s	43/471 (9%)	42 (98%)	1 (2%)	0	100	100
All	All	8194/9744 (84%)	7630 (93%)	549 (7%)	15 (0%)	44	72

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	1E	97	LYS
8	1H	92	PRO
29	1d	53	VAL
42	1q	142	THR
7	1G	47	SER
8	1H	208	VAL
32	1g	25	ARG
7	1G	186	TYR
31	1f	36	ALA
12	1L	464	ALA
4	1D	87	THR
7	1G	367	THR
12	1L	387	THR
12	1L	549	ALA
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%)	95 (96%)	4 (4%)	28	54
2	1B	131/212 (62%)	127 (97%)	4 (3%)	35	59
3	1C	190/227 (84%)	177 (93%)	13 (7%)	14	42
4	1D	371/405 (92%)	357 (96%)	14 (4%)	29	55
5	1E	183/207 (88%)	171 (93%)	12 (7%)	15	43
6	1F	346/368 (94%)	331 (96%)	15 (4%)	26	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	1G	588/610 (96%)	546 (93%)	42 (7%)	13	40
8	1H	274/274 (100%)	255 (93%)	19 (7%)	14	41
9	1I	151/201 (75%)	142 (94%)	9 (6%)	17	45
10	1J	140/140 (100%)	133 (95%)	7 (5%)	22	49
11	1K	84/84 (100%)	78 (93%)	6 (7%)	13	40
12	1L	539/539 (100%)	507 (94%)	32 (6%)	18	45
13	1M	408/408 (100%)	382 (94%)	26 (6%)	16	43
14	1N	310/310 (100%)	296 (96%)	14 (4%)	24	51
15	1O	283/307 (92%)	270 (95%)	13 (5%)	24	51
16	1P	296/323 (92%)	279 (94%)	17 (6%)	18	46
17	1Q	117/152 (77%)	111 (95%)	6 (5%)	21	49
18	1R	79/97 (81%)	71 (90%)	8 (10%)	7	30
19	1S	77/82 (94%)	74 (96%)	3 (4%)	28	54
20	1T	79/133 (59%)	75 (95%)	4 (5%)	21	49
20	1U	79/133 (59%)	77 (98%)	2 (2%)	42	63
21	1V	100/101 (99%)	96 (96%)	4 (4%)	28	54
22	1W	107/112 (96%)	100 (94%)	7 (6%)	15	43
23	1X	153/154 (99%)	143 (94%)	10 (6%)	15	43
24	1Y	101/102 (99%)	95 (94%)	6 (6%)	18	45
25	1Z	123/124 (99%)	116 (94%)	7 (6%)	18	46
26	1a	58/58 (100%)	56 (97%)	2 (3%)	32	57
27	1b	69/70 (99%)	64 (93%)	5 (7%)	13	40
28	1c	45/66 (68%)	42 (93%)	3 (7%)	15	42
29	1d	107/109 (98%)	100 (94%)	7 (6%)	15	43
30	1e	87/94 (93%)	84 (97%)	3 (3%)	32	57
31	1f	54/113 (48%)	51 (94%)	3 (6%)	19	47
32	1g	92/129 (71%)	91 (99%)	1 (1%)	65	74
33	1h	121/158 (77%)	118 (98%)	3 (2%)	42	63
34	1i	119/120 (99%)	112 (94%)	7 (6%)	18	45
35	1j	62/84 (74%)	58 (94%)	4 (6%)	15	43
36	1k	63/76 (83%)	58 (92%)	5 (8%)	11	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
37	1l	141/161 (88%)	132 (94%)	9 (6%)	16	43
38	1m	113/114 (99%)	109 (96%)	4 (4%)	32	57
39	1n	156/160 (98%)	153 (98%)	3 (2%)	50	67
40	1o	110/120 (92%)	104 (94%)	6 (6%)	19	47
41	1p	154/156 (99%)	150 (97%)	4 (3%)	40	62
42	1q	131/131 (100%)	122 (93%)	9 (7%)	14	41
43	1r	85/98 (87%)	81 (95%)	4 (5%)	23	50
44	1s	44/351 (12%)	41 (93%)	3 (7%)	14	42
All	All	7219/8272 (87%)	6830 (95%)	389 (5%)	21	47

All (389) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1A	15	SER
1	1A	46	SER
1	1A	75	LEU
1	1A	101	SER
2	1B	74	VAL
2	1B	129	SER
2	1B	132	VAL
2	1B	133	VAL
3	1C	52	ILE
3	1C	62	THR
3	1C	109	THR
3	1C	130	TYR
3	1C	134	ILE
3	1C	140	VAL
3	1C	151	ILE
3	1C	152	LEU
3	1C	199	LEU
3	1C	201	SER
3	1C	206	PHE
3	1C	209	TYR
3	1C	214	GLU
4	1D	18	VAL
4	1D	42	THR
4	1D	45	SER
4	1D	79	HIS
4	1D	87	THR

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Mol	Chain	Res	Type
4	1D	97	LEU
4	1D	199	VAL
4	1D	203	LEU
4	1D	224	GLU
4	1D	269	LEU
4	1D	277	VAL
4	1D	284	ASP
4	1D	376	VAL
4	1D	399	LEU
5	1E	18	ASP
5	1E	73	LEU
5	1E	78	MET
5	1E	99	HIS
5	1E	154	VAL
5	1E	164	LEU
5	1E	165	THR
5	1E	169	ILE
5	1E	172	ILE
5	1E	183	LYS
5	1E	187	ARG
5	1E	207	LYS
6	1F	25	LEU
6	1F	32	ARG
6	1F	44	LYS
6	1F	48	ILE
6	1F	62	THR
6	1F	80	SER
6	1F	120	GLU
6	1F	129	MET
6	1F	175	VAL
6	1F	228	VAL
6	1F	253	THR
6	1F	267	THR
6	1F	334	VAL
6	1F	343	ILE
6	1F	363	THR
7	1G	13	VAL
7	1G	18	VAL
7	1G	37	ILE
7	1G	40	PHE
7	1G	59	ILE
7	1G	93	VAL

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Mol	Chain	Res	Type
7	1G	116	LEU
7	1G	119	GLN
7	1G	142	ILE
7	1G	148	THR
7	1G	154	ILE
7	1G	185	THR
7	1G	187	ILE
7	1G	193	SER
7	1G	227	SER
7	1G	239	VAL
7	1G	242	THR
7	1G	244	THR
7	1G	269	PHE
7	1G	293	TYR
7	1G	329	VAL
7	1G	345	THR
7	1G	356	THR
7	1G	360	SER
7	1G	404	LEU
7	1G	415	LEU
7	1G	453	LEU
7	1G	455	SER
7	1G	464	THR
7	1G	481	SER
7	1G	514	ILE
7	1G	533	THR
7	1G	536	ASP
7	1G	537	LEU
7	1G	548	HIS
7	1G	567	THR
7	1G	631	VAL
7	1G	650	LYS
7	1G	651	LEU
7	1G	667	THR
7	1G	677	ILE
7	1G	703	ILE
8	1H	28	LEU
8	1H	45	LEU
8	1H	56	VAL
8	1H	72	ILE
8	1H	80	SER
8	1H	87	VAL

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Mol	Chain	Res	Type
8	1H	110	SER
8	1H	113	VAL
8	1H	119	SER
8	1H	157	ASN
8	1H	163	SER
8	1H	188	SER
8	1H	201	THR
8	1H	266	LEU
8	1H	268	ILE
8	1H	280	PHE
8	1H	285	LEU
8	1H	294	LEU
8	1H	297	THR
9	1I	31	VAL
9	1I	67	LEU
9	1I	68	ARG
9	1I	94	ILE
9	1I	104	ARG
9	1I	110	ASP
9	1I	123	GLN
9	1I	140	SER
9	1I	155	LEU
10	1J	56	VAL
10	1J	61	LEU
10	1J	102	CYS
10	1J	127	ILE
10	1J	130	THR
10	1J	171	ILE
10	1J	173	ARG
11	1K	10	MET
11	1K	44	SER
11	1K	54	THR
11	1K	78	LEU
11	1K	90	VAL
11	1K	98	CYS
12	1L	6	SER
12	1L	36	VAL
12	1L	66	TRP
12	1L	70	THR
12	1L	71	LEU
12	1L	92	VAL
12	1L	132	VAL

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Mol	Chain	Res	Type
12	1L	137	LEU
12	1L	159	HIS
12	1L	183	VAL
12	1L	193	SER
12	1L	206	ASN
12	1L	217	LEU
12	1L	247	LEU
12	1L	285	THR
12	1L	316	THR
12	1L	323	HIS
12	1L	345	SER
12	1L	346	ILE
12	1L	366	MET
12	1L	377	SER
12	1L	394	LEU
12	1L	404	THR
12	1L	419	THR
12	1L	471	ASN
12	1L	494	THR
12	1L	502	LEU
12	1L	517	SER
12	1L	561	ILE
12	1L	562	LEU
12	1L	569	ILE
12	1L	589	LEU
13	1M	9	THR
13	1M	23	ILE
13	1M	26	ASN
13	1M	33	LEU
13	1M	34	ILE
13	1M	65	LEU
13	1M	69	THR
13	1M	86	LYS
13	1M	88	THR
13	1M	97	THR
13	1M	123	GLU
13	1M	134	THR
13	1M	189	SER
13	1M	209	LEU
13	1M	228	SER
13	1M	265	SER
13	1M	284	SER

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Mol	Chain	Res	Type
13	1M	344	LEU
13	1M	350	THR
13	1M	359	TRP
13	1M	363	SER
13	1M	365	THR
13	1M	405	LEU
13	1M	410	MET
13	1M	420	THR
13	1M	431	THR
14	1N	85	THR
14	1N	87	THR
14	1N	108	LEU
14	1N	123	SER
14	1N	140	SER
14	1N	154	MET
14	1N	163	LEU
14	1N	191	THR
14	1N	226	THR
14	1N	270	MET
14	1N	276	ILE
14	1N	296	LEU
14	1N	325	LEU
14	1N	340	THR
15	1O	35	LYS
15	1O	78	SER
15	1O	98	SER
15	1O	103	SER
15	1O	104	ARG
15	1O	116	LEU
15	1O	164	LEU
15	1O	221	LEU
15	1O	240	TYR
15	1O	242	LYS
15	1O	250	ASP
15	1O	269	VAL
15	1O	270	LEU
16	1P	19	ILE
16	1P	27	THR
16	1P	30	LEU
16	1P	43	SER
16	1P	45	VAL
16	1P	56	THR

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Mol	Chain	Res	Type
16	1P	65	LEU
16	1P	71	MET
16	1P	101	THR
16	1P	143	SER
16	1P	171	ILE
16	1P	224	LYS
16	1P	258	LEU
16	1P	273	SER
16	1P	290	SER
16	1P	303	LEU
16	1P	317	VAL
17	1Q	21	THR
17	1Q	39	VAL
17	1Q	44	ASN
17	1Q	104	ASP
17	1Q	123	SER
17	1Q	128	THR
18	1R	5	SER
18	1R	9	GLU
18	1R	11	VAL
18	1R	12	THR
18	1R	58	SER
18	1R	71	VAL
18	1R	83	THR
18	1R	84	CYS
19	1S	58	SER
19	1S	76	VAL
19	1S	89	THR
20	1T	7	THR
20	1T	26	ASP
20	1T	48	VAL
20	1T	70	LEU
20	1U	44	SER
20	1U	72	CYS
21	1V	3	LEU
21	1V	37	ILE
21	1V	71	LEU
21	1V	99	TRP
22	1W	30	ARG
22	1W	52	LEU
22	1W	69	LYS
22	1W	70	ASN

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Mol	Chain	Res	Type
22	1W	74	THR
22	1W	79	VAL
22	1W	124	VAL
23	1X	14	VAL
23	1X	62	VAL
23	1X	73	ILE
23	1X	88	ILE
23	1X	94	GLN
23	1X	99	CYS
23	1X	111	LEU
23	1X	124	LEU
23	1X	128	THR
23	1X	150	ASN
24	1Y	52	VAL
24	1Y	68	ILE
24	1Y	85	ASP
24	1Y	94	CYS
24	1Y	126	MET
24	1Y	134	VAL
25	1Z	71	LEU
25	1Z	100	ASP
25	1Z	110	VAL
25	1Z	124	LEU
25	1Z	127	LEU
25	1Z	129	THR
25	1Z	133	ILE
26	1a	21	MET
26	1a	53	CYS
27	1b	33	SER
27	1b	44	ILE
27	1b	48	THR
27	1b	51	ASN
27	1b	65	VAL
28	1c	9	HIS
28	1c	24	SER
28	1c	31	LEU
29	1d	3	SER
29	1d	31	LEU
29	1d	32	VAL
29	1d	40	CYS
29	1d	54	VAL
29	1d	58	LEU

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Mol	Chain	Res	Type
29	1d	90	MET
30	1e	5	VAL
30	1e	67	LEU
30	1e	98	LEU
31	1f	21	VAL
31	1f	43	LEU
31	1f	52	GLU
32	1g	101	GLU
33	1h	25	MET
33	1h	29	ILE
33	1h	89	LYS
34	1i	13	GLN
34	1i	14	LEU
34	1i	28	SER
34	1i	63	THR
34	1i	98	GLU
34	1i	110	LEU
34	1i	126	HIS
35	1j	7	ILE
35	1j	26	GLU
35	1j	44	SER
35	1j	60	THR
36	1k	29	GLU
36	1k	31	VAL
36	1k	61	SER
36	1k	78	VAL
36	1k	88	GLU
37	1l	16	THR
37	1l	26	LYS
37	1l	33	ASP
37	1l	63	ASP
37	1l	69	LEU
37	1l	85	ILE
37	1l	96	VAL
37	1l	118	VAL
37	1l	128	VAL
38	1m	16	THR
38	1m	58	VAL
38	1m	82	THR
38	1m	122	GLN
39	1n	18	LEU
39	1n	52	ASN

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Mol	Chain	Res	Type
39	1n	158	LYS
40	1o	19	LEU
40	1o	39	VAL
40	1o	45	MET
40	1o	63	ILE
40	1o	77	LEU
40	1o	109	GLN
41	1p	63	TYR
41	1p	81	ILE
41	1p	82	LEU
41	1p	150	SER
42	1q	7	LEU
42	1q	63	ILE
42	1q	77	VAL
42	1q	78	ASP
42	1q	95	ASP
42	1q	100	THR
42	1q	104	THR
42	1q	125	VAL
42	1q	138	VAL
43	1r	7	ILE
43	1r	34	THR
43	1r	49	SER
43	1r	70	SER
44	1s	41	LEU
44	1s	42	GLN
44	1s	43	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (79) such sidechains are listed below:

Mol	Chain	Res	Type
2	1B	61	HIS
2	1B	106	GLN
3	1C	88	ASN
4	1D	54	GLN
4	1D	84	HIS
4	1D	98	GLN
4	1D	149	ASN
4	1D	273	GLN
4	1D	280	GLN
4	1D	398	HIS
5	1E	9	HIS

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Mol	Chain	Res	Type
5	1E	37	ASN
5	1E	121	GLN
6	1F	150	GLN
6	1F	224	ASN
6	1F	416	GLN
6	1F	436	GLN
7	1G	51	ASN
7	1G	476	ASN
7	1G	582	GLN
7	1G	655	GLN
8	1H	230	ASN
11	1K	50	ASN
11	1K	57	ASN
12	1L	2	ASN
12	1L	25	ASN
12	1L	59	GLN
12	1L	135	ASN
12	1L	332	HIS
13	1M	26	ASN
13	1M	103	GLN
13	1M	168	GLN
13	1M	415	GLN
14	1N	36	ASN
14	1N	63	GLN
14	1N	120	GLN
14	1N	134	GLN
14	1N	174	GLN
14	1N	197	ASN
14	1N	289	ASN
14	1N	309	ASN
15	1O	76	ASN
15	1O	92	ASN
15	1O	147	GLN
16	1P	44	GLN
16	1P	67	GLN
16	1P	131	HIS
16	1P	180	ASN
16	1P	203	GLN
16	1P	288	HIS
17	1Q	50	ASN
19	1S	61	GLN
20	1T	47	GLN

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Mol	Chain	Res	Type
20	1U	33	ASN
20	1U	35	HIS
21	1V	70	GLN
21	1V	110	GLN
23	1X	15	GLN
23	1X	63	ASN
26	1a	46	ASN
28	1c	35	HIS
29	1d	61	GLN
30	1e	69	GLN
30	1e	97	HIS
31	1f	5	GLN
35	1j	13	GLN
37	1l	55	GLN
37	1l	56	GLN
37	1l	66	HIS
37	1l	126	GLN
38	1m	54	ASN
39	1n	61	GLN
40	1o	84	HIS
41	1p	55	HIS
41	1p	103	ASN
41	1p	160	GLN
42	1q	13	GLN
44	1s	55	ASN
44	1s	71	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	FME	1K	1	11	8,9,10	0.56	0	8,9,11	0.99	1 (12%)
8	FME	1H	1	8	8,9,10	0.55	0	8,9,11	1.08	1 (12%)
1	FME	1A	1	1	8,9,10	0.52	0	8,9,11	1.09	1 (12%)
14	FME	1N	1	14	8,9,10	0.56	0	8,9,11	0.98	1 (12%)
12	FME	1L	1	12	8,9,10	0.54	0	8,9,11	0.94	1 (12%)
34	SAC	1i	1	-	7,8,9	0.58	0	7,9,11	1.15	1 (14%)
13	FME	1M	1	13	8,9,10	0.54	0	8,9,11	0.96	1 (12%)
10	FME	1J	1	10	8,9,10	0.56	0	8,9,11	0.91	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
11	FME	1K	1	11	-	1/7/9/11	-
8	FME	1H	1	8	-	0/7/9/11	-
1	FME	1A	1	1	-	1/7/9/11	-
14	FME	1N	1	14	-	0/7/9/11	-
12	FME	1L	1	12	-	0/7/9/11	-
34	SAC	1i	1	-	-	0/7/8/10	-
13	FME	1M	1	13	-	3/7/9/11	-
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	-2.97	117.13	124.77
8	1H	1	FME	O-C-CA	-2.76	117.68	124.77
11	1K	1	FME	O-C-CA	-2.72	117.77	124.77
1	1A	1	FME	O-C-CA	-2.67	117.89	124.77
14	1N	1	FME	O-C-CA	-2.58	118.13	124.77
13	1M	1	FME	O-C-CA	-2.52	118.28	124.77
12	1L	1	FME	O-C-CA	-2.49	118.36	124.77
10	1J	1	FME	O-C-CA	-2.29	118.89	124.77

There are no chirality outliers.

All (5) 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
1	1A	1	FME	CB-CG-SD-CE
13	1M	1	FME	CB-CA-N-CN

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	1K	1	FME	4	0
1	1A	1	FME	7	0
14	1N	1	FME	1	0
13	1M	1	FME	2	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	$\# Z > 2$
51	CDL	1q	201	-	60,60,99	0.31	0	66,72,111	0.85	5 (7%)
46	SF4	1B	201	2	0,12,12	-	-	-		
51	CDL	1N	402	-	76,76,99	0.29	0	82,88,111	0.39	0
45	3PE	1Y	203	-	50,50,50	0.27	0	53,55,55	0.43	0
58	MYR	1l	201	-	13,14,15	0.31	0	12,13,15	0.30	0
50	PC1	1I	204	-	43,43,53	0.29	0	49,51,61	0.36	0
54	NDP	1P	501	-	51,52,52	0.52	0	71,80,80	0.76	2 (2%)
45	3PE	1N	401	-	50,50,50	0.27	0	53,55,55	0.38	0
45	3PE	1A	201	-	46,46,50	0.29	0	49,51,55	0.39	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	SF4	1G	802	7	0,12,12	-	-	-		
47	FES	1E	301	5	0,4,4	-	-	-		
50	PC1	1J	201	-	34,34,53	0.32	0	40,42,61	0.33	0
52	GTP	1O	401	53	33,34,34	0.61	0	50,54,54	0.58	0
45	3PE	1L	703	-	41,41,50	0.31	0	44,46,55	1.26	5 (11%)
48	FMN	1F	501	-	33,33,33	0.60	0	48,50,50	0.64	1 (2%)
46	SF4	1F	502	6	0,12,12	-	-	-		
50	PC1	1I	203	-	53,53,53	0.27	0	59,61,61	0.34	0
50	PC1	1f	101	-	45,45,53	0.28	0	51,53,61	0.36	0
47	FES	1G	803	7	0,4,4	-	-	-		
45	3PE	1Y	202	-	30,30,50	0.35	0	33,35,55	0.65	1 (3%)
56	EHZ	1n	201	-	31,36,37	0.21	0	36,44,47	1.10	1 (2%)
46	SF4	1G	801	7	0,12,12	-	-	-		
46	SF4	1I	201	9	0,12,12	-	-	-		
50	PC1	1L	702	-	43,43,53	0.30	0	49,51,61	0.35	0
57	PGT	1Y	201	-	50,50,50	0.49	0	53,56,56	0.49	0
46	SF4	1I	202	9	0,12,12	-	-	-		
56	EHZ	1W	201	-	31,36,37	0.18	0	36,44,47	1.41	1 (2%)
45	3PE	1L	701	-	45,45,50	0.29	0	48,50,55	0.31	0

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
51	CDL	1q	201	-	-	16/71/71/110	-
46	SF4	1B	201	2	-	-	0/6/5/5
51	CDL	1N	402	-	-	6/87/87/110	-
45	3PE	1Y	203	-	-	8/54/54/54	-
58	MYR	1l	201	-	-	2/12/12/13	-
50	PC1	1I	204	-	-	3/47/47/57	-
54	NDP	1P	501	-	-	7/34/77/77	0/5/5/5
45	3PE	1N	401	-	-	10/54/54/54	-
45	3PE	1A	201	-	-	3/50/50/54	-
46	SF4	1G	802	7	-	-	0/6/5/5
47	FES	1E	301	5	-	-	0/1/1/1
50	PC1	1J	201	-	-	2/38/38/57	-
52	GTP	1O	401	53	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	3PE	1L	703	-	-	6/45/45/54	-
48	FMN	1F	501	-	-	1/18/18/18	0/3/3/3
46	SF4	1F	502	6	-	-	0/6/5/5
50	PC1	1I	203	-	-	5/57/57/57	-
50	PC1	1f	101	-	-	5/49/49/57	-
47	FES	1G	803	7	-	-	0/1/1/1
45	3PE	1Y	202	-	-	6/34/34/54	-
56	EHZ	1n	201	-	-	9/42/44/45	-
46	SF4	1G	801	7	-	-	0/6/5/5
46	SF4	1I	201	9	-	-	0/6/5/5
50	PC1	1L	702	-	-	5/47/47/57	-
57	PGT	1Y	201	-	-	23/55/55/55	-
46	SF4	1I	202	9	-	-	0/6/5/5
56	EHZ	1W	201	-	-	3/42/44/45	-
45	3PE	1L	701	-	-	4/49/49/54	-

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	1W	201	EHZ	C10-S1-C9	7.74	124.73	101.84
56	1n	201	EHZ	C10-S1-C9	6.09	119.86	101.84
45	1L	703	3PE	O21-C21-C22	6.07	124.61	111.48
54	1P	501	NDP	P2B-O2B-C2B	-3.78	113.33	123.43
51	1q	201	CDL	OB4-PB2-OB2	3.36	122.78	107.57
45	1L	703	3PE	O21-C21-O22	-2.73	117.32	123.70
54	1P	501	NDP	O4D-C1D-C2D	-2.63	100.98	106.62
45	1L	703	3PE	C2-O21-C21	2.61	124.04	117.80
45	1L	703	3PE	O21-C2-C1	2.37	116.86	108.34
51	1q	201	CDL	OB5-PB2-OB3	-2.28	99.89	108.94
45	1Y	202	3PE	O21-C21-C22	2.18	116.20	111.48
48	1F	501	FMN	C4-N3-C2	-2.13	121.87	125.64
51	1q	201	CDL	OA6-CA4-CA3	2.10	115.89	108.34
51	1q	201	CDL	OA4-PA1-OA3	2.08	122.11	112.44
45	1L	703	3PE	O21-C2-C3	2.05	115.68	108.34
51	1q	201	CDL	OB4-PB2-OB3	2.00	121.76	112.44

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	1L	703	3PE	O22-C21-O21-C2
45	1L	703	3PE	C22-C21-O21-C2
45	1N	401	3PE	C1-O11-P-O14
45	1Y	202	3PE	C1-O11-P-O14
45	1Y	202	3PE	O32-C31-O31-C3
45	1Y	202	3PE	C32-C31-O31-C3
45	1Y	202	3PE	O22-C21-O21-C2
45	1Y	202	3PE	C22-C21-O21-C2
45	1Y	203	3PE	C1-O11-P-O14
50	1I	204	PC1	C1-O11-P-O14
50	1J	201	PC1	C1-O11-P-O14
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	1N	402	CDL	OA6-CA4-CA6-OA8
51	1q	201	CDL	CA2-OA2-PA1-OA4
51	1q	201	CDL	CA2-OA2-PA1-OA5
51	1q	201	CDL	CA3-OA5-PA1-OA2
56	1W	201	EHZ	O2-C9-S1-C10
56	1W	201	EHZ	C8-C9-S1-C10
56	1n	201	EHZ	C18-C17-C20-O6
56	1n	201	EHZ	C19-C17-C20-O6
56	1n	201	EHZ	O2-C9-S1-C10
56	1n	201	EHZ	C8-C9-S1-C10
57	1Y	201	PGT	C32-C31-O2-C2
57	1Y	201	PGT	C1-O3P-P-O4P
57	1Y	201	PGT	C4-O4P-P-O3P
57	1Y	201	PGT	C5-C4-O4P-P
57	1Y	201	PGT	C4-C5-C6-O6
57	1Y	201	PGT	O5-C5-C6-O6
57	1Y	201	PGT	O11-C11-O3-C3
57	1Y	201	PGT	C12-C11-O3-C3
58	1l	201	MYR	O1-C1-C2-C3
57	1Y	201	PGT	O31-C31-O2-C2
51	1q	201	CDL	O1-C1-CA2-OA2
52	1O	401	GTP	O4'-C4'-C5'-O5'
45	1Y	203	3PE	C2-C1-O11-P
51	1q	201	CDL	CB2-C1-CA2-OA2
51	1q	201	CDL	CA2-C1-CB2-OB2
54	1P	501	NDP	C2D-C1D-N1N-C2N
52	1O	401	GTP	C3'-C4'-C5'-O5'
51	1q	201	CDL	O1-C1-CB2-OB2
54	1P	501	NDP	C2D-C1D-N1N-C6N

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Mol	Chain	Res	Type	Atoms
57	1Y	201	PGT	C40-C41-C42-C43
57	1Y	201	PGT	C14-C15-C16-C17
57	1Y	201	PGT	C15-C16-C17-C18
57	1Y	201	PGT	C21-C22-C23-C24
56	1n	201	EHZ	C12-C13-C14-N2
57	1Y	201	PGT	C34-C35-C36-C37
51	1q	201	CDL	C51-C52-C53-C54
50	1I	203	PC1	C24-C25-C26-C27
45	1Y	203	3PE	C35-C36-C37-C38
57	1Y	201	PGT	C32-C33-C34-C35
45	1Y	203	3PE	C3C-C3D-C3E-C3F
45	1L	703	3PE	O11-C1-C2-O21
57	1Y	201	PGT	C44-C45-C46-C47
45	1N	401	3PE	O31-C31-C32-C33
50	1I	203	PC1	O31-C31-C32-C33
51	1N	402	CDL	CA3-CA4-CA6-OA8
51	1q	201	CDL	C53-C54-C55-C56
51	1q	201	CDL	OB5-CB3-CB4-OB6
56	1n	201	EHZ	O3-C12-C13-C14
54	1P	501	NDP	C3B-C2B-O2B-P2B
56	1W	201	EHZ	C5-C6-C7-C8
45	1Y	203	3PE	O11-C1-C2-O21
45	1A	201	3PE	C12-C11-O13-P
45	1Y	203	3PE	C12-C11-O13-P
50	1J	201	PC1	O13-C11-C12-N
58	1l	201	MYR	C3-C4-C5-C6
51	1q	201	CDL	OB5-CB3-CB4-CB6
45	1N	401	3PE	C2-C1-O11-P
54	1P	501	NDP	C1B-C2B-O2B-P2B
54	1P	501	NDP	O4D-C1D-N1N-C2N
51	1q	201	CDL	CA3-CA4-CA6-OA8
56	1n	201	EHZ	C16-C17-C20-O6
45	1N	401	3PE	C3A-C3B-C3C-C3D
50	1I	203	PC1	C1-O11-P-O14
50	1L	702	PC1	C1-O11-P-O12
50	1L	702	PC1	C1-O11-P-O13
50	1f	101	PC1	C11-O13-P-O14
51	1q	201	CDL	CA2-OA2-PA1-OA3
51	1q	201	CDL	CA3-OA5-PA1-OA3
57	1Y	201	PGT	C1-O3P-P-O1P
57	1Y	201	PGT	C4-O4P-P-O1P
51	1N	402	CDL	C55-C56-C57-C58

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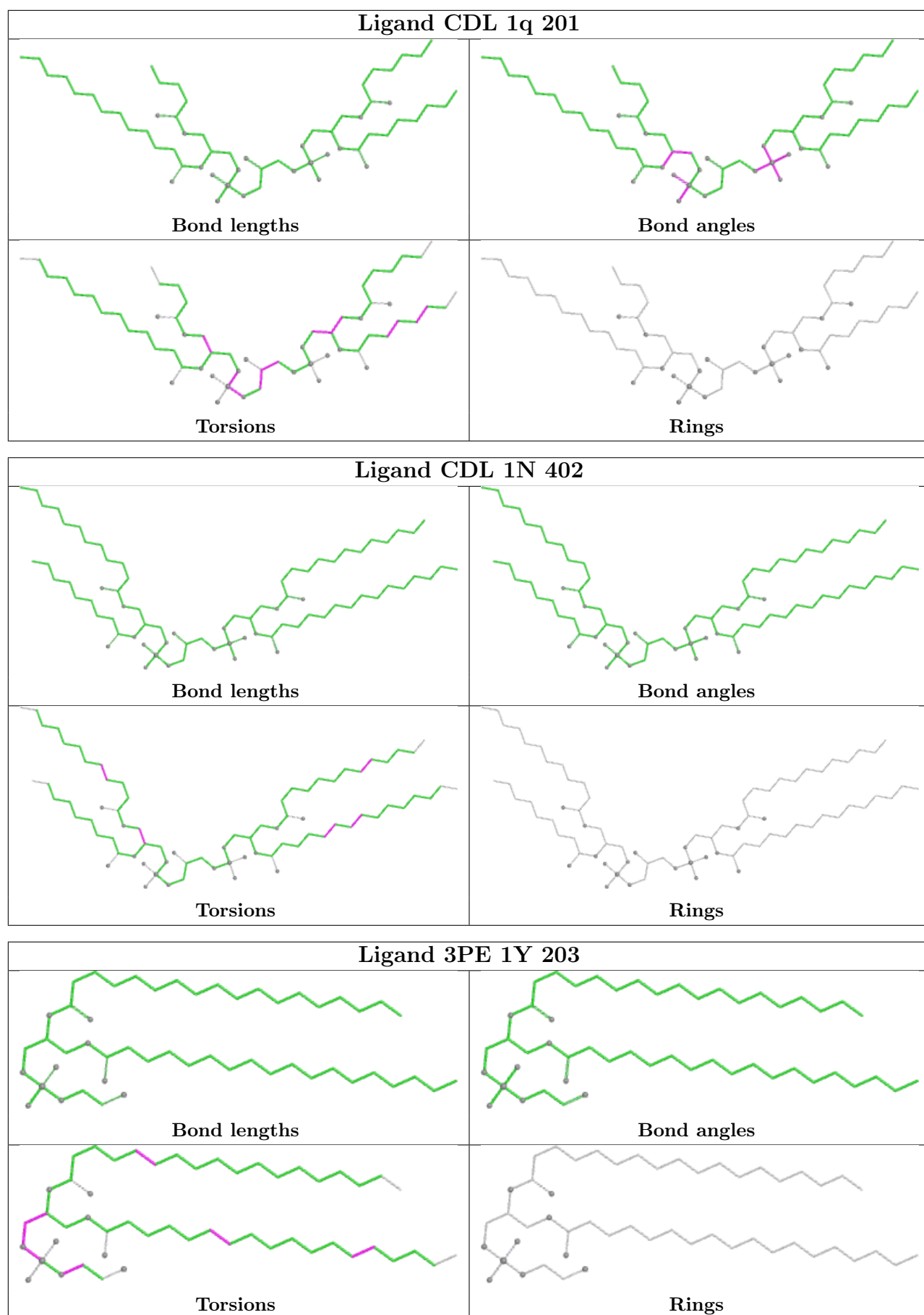
Mol	Chain	Res	Type	Atoms
52	1O	401	GTP	C4'-C5'-O5'-PA
45	1N	401	3PE	C34-C35-C36-C37
45	1Y	203	3PE	C24-C25-C26-C27
45	1N	401	3PE	O11-C1-C2-O21
54	1P	501	NDP	O4D-C1D-N1N-C6N
45	1A	201	3PE	C24-C25-C26-C27
56	1n	201	EHZ	N1-C12-C13-C14
45	1N	401	3PE	C2-C3-O31-C31
45	1L	701	3PE	C22-C23-C24-C25
45	1A	201	3PE	O21-C2-C3-O31
56	1n	201	EHZ	C13-C14-N2-C15
45	1L	703	3PE	C1-C2-C3-O31
45	1L	703	3PE	C1-C2-O21-C21
57	1Y	201	PGT	C2-C1-O3P-P
51	1q	201	CDL	OB6-CB4-CB6-OB8
51	1N	402	CDL	C76-C77-C78-C79
50	1L	702	PC1	C1-C2-C3-O31
54	1P	501	NDP	O4D-C4D-C5D-O5D
57	1Y	201	PGT	C31-C32-C33-C34
45	1L	701	3PE	C33-C34-C35-C36
45	1Y	203	3PE	O11-C1-C2-C3
45	1N	401	3PE	O21-C2-C3-O31
45	1L	701	3PE	C35-C36-C37-C38
51	1q	201	CDL	CB3-CB4-CB6-OB8
51	1N	402	CDL	C53-C54-C55-C56
50	1I	203	PC1	O32-C31-C32-C33
57	1Y	201	PGT	C39-C40-C41-C42
57	1Y	201	PGT	C41-C42-C43-C44
50	1I	204	PC1	C11-C12-N-C13
45	1N	401	3PE	O32-C31-C32-C33
50	1I	203	PC1	C3E-C3F-C3G-C3H
45	1N	401	3PE	C39-C3A-C3B-C3C
45	1Y	202	3PE	O21-C2-C3-O31
50	1f	101	PC1	C36-C37-C38-C39
48	1F	501	FMN	N10-C1'-C2'-O2'
45	1L	701	3PE	C37-C38-C39-C3A
50	1f	101	PC1	C21-C22-C23-C24
57	1Y	201	PGT	C20-C21-C22-C23
50	1I	204	PC1	C11-C12-N-C14
50	1L	702	PC1	O31-C31-C32-C33
45	1L	703	3PE	C32-C33-C34-C35
51	1N	402	CDL	C32-C33-C34-C35

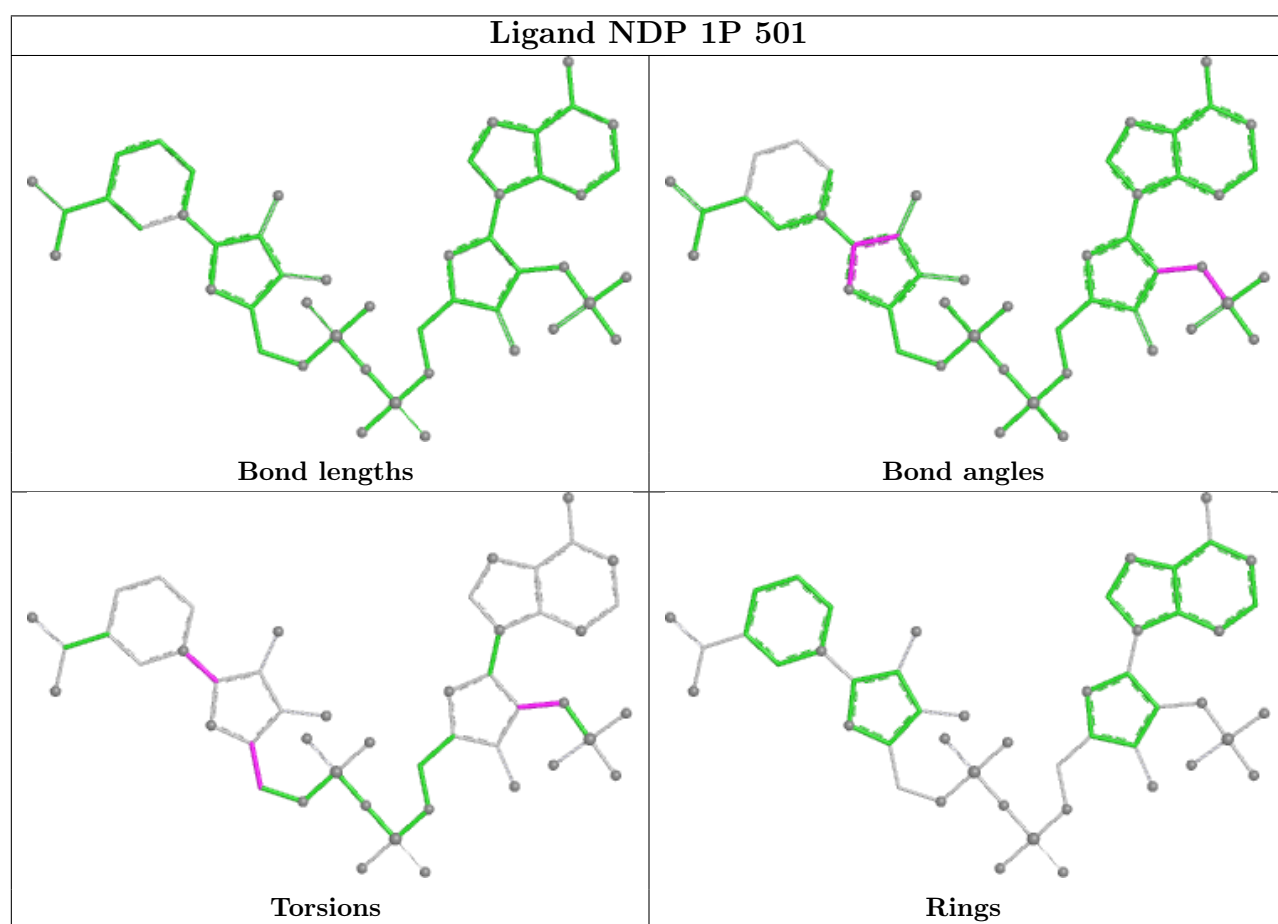
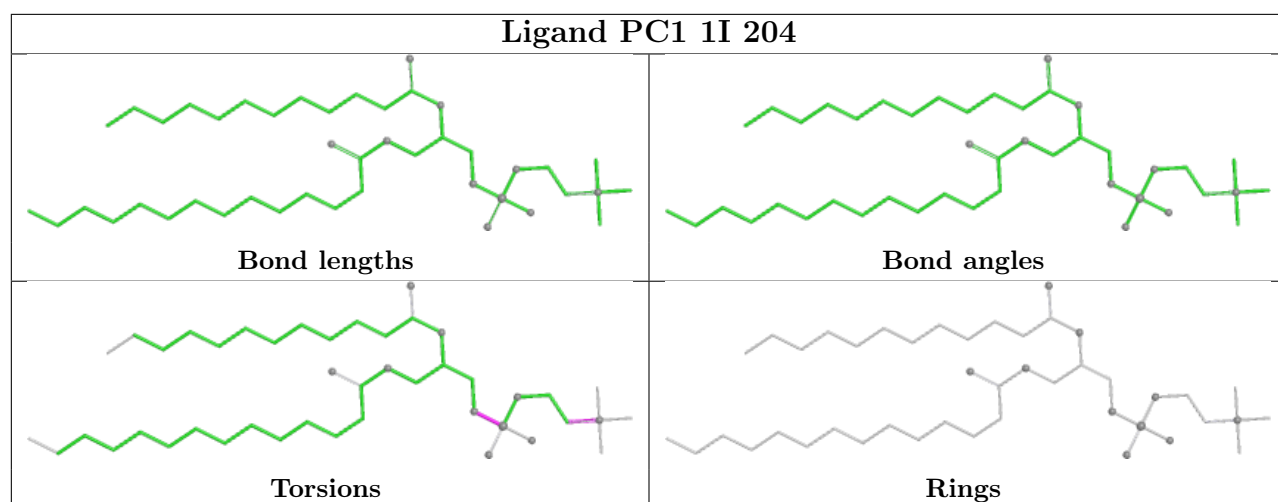
There are no ring outliers.

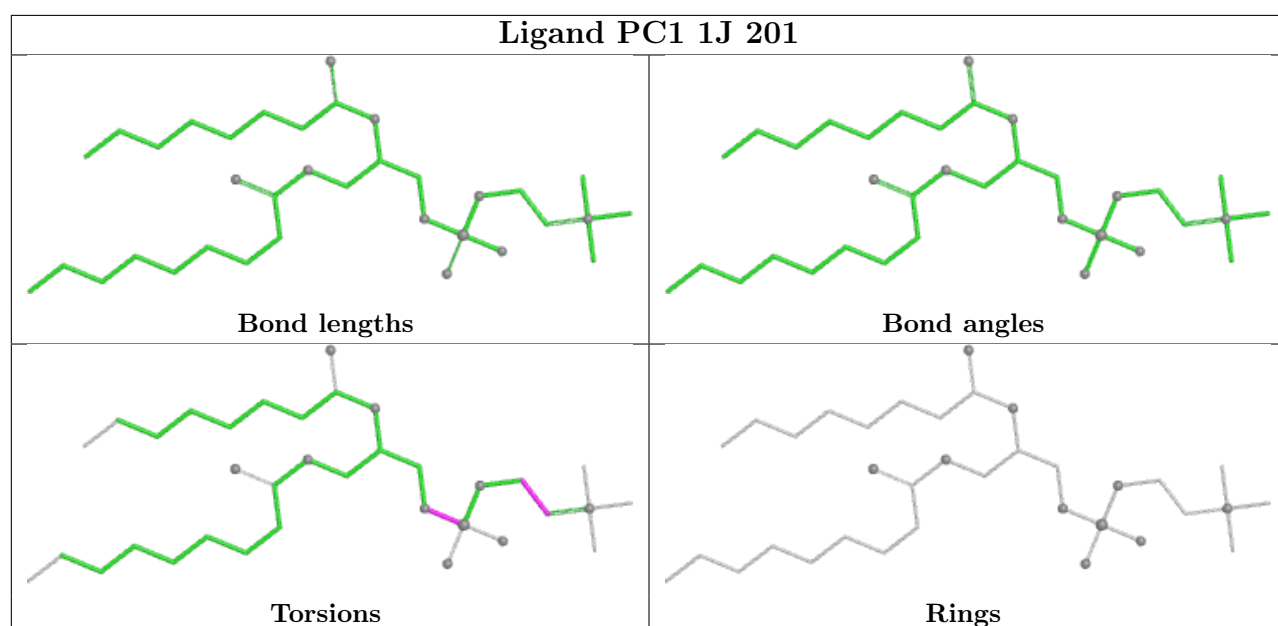
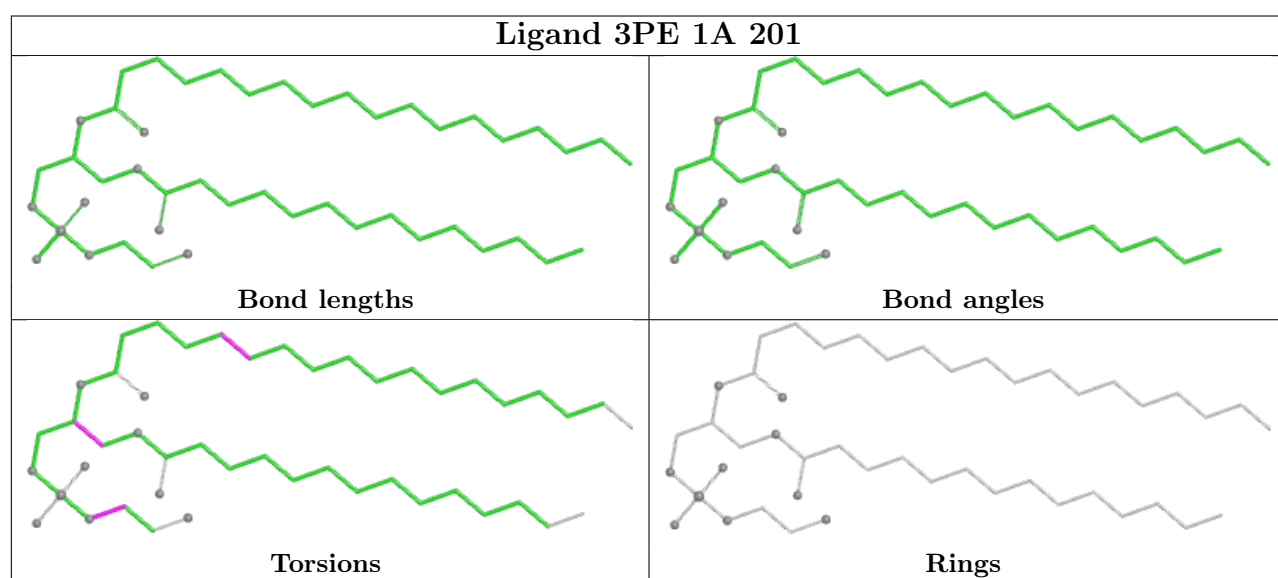
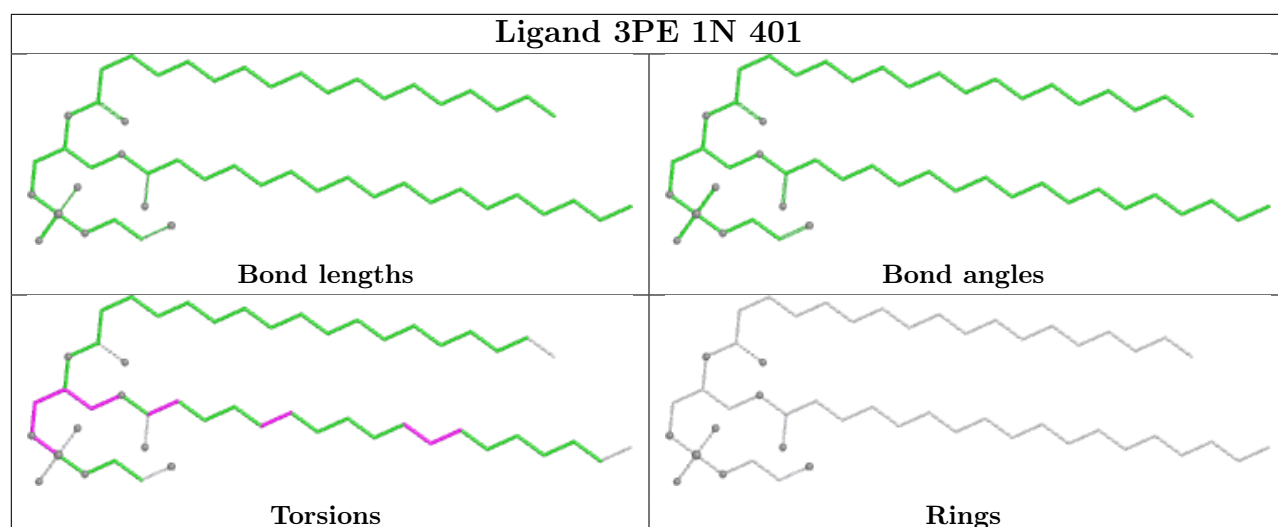
23 monomers are involved in 92 short contacts:

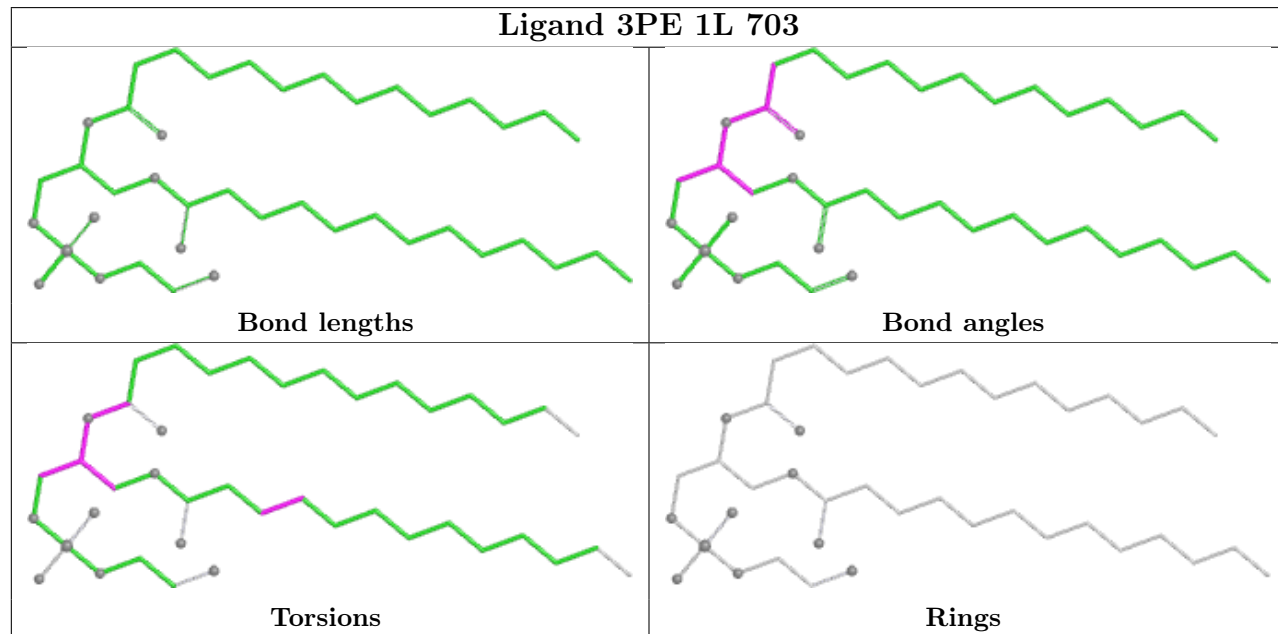
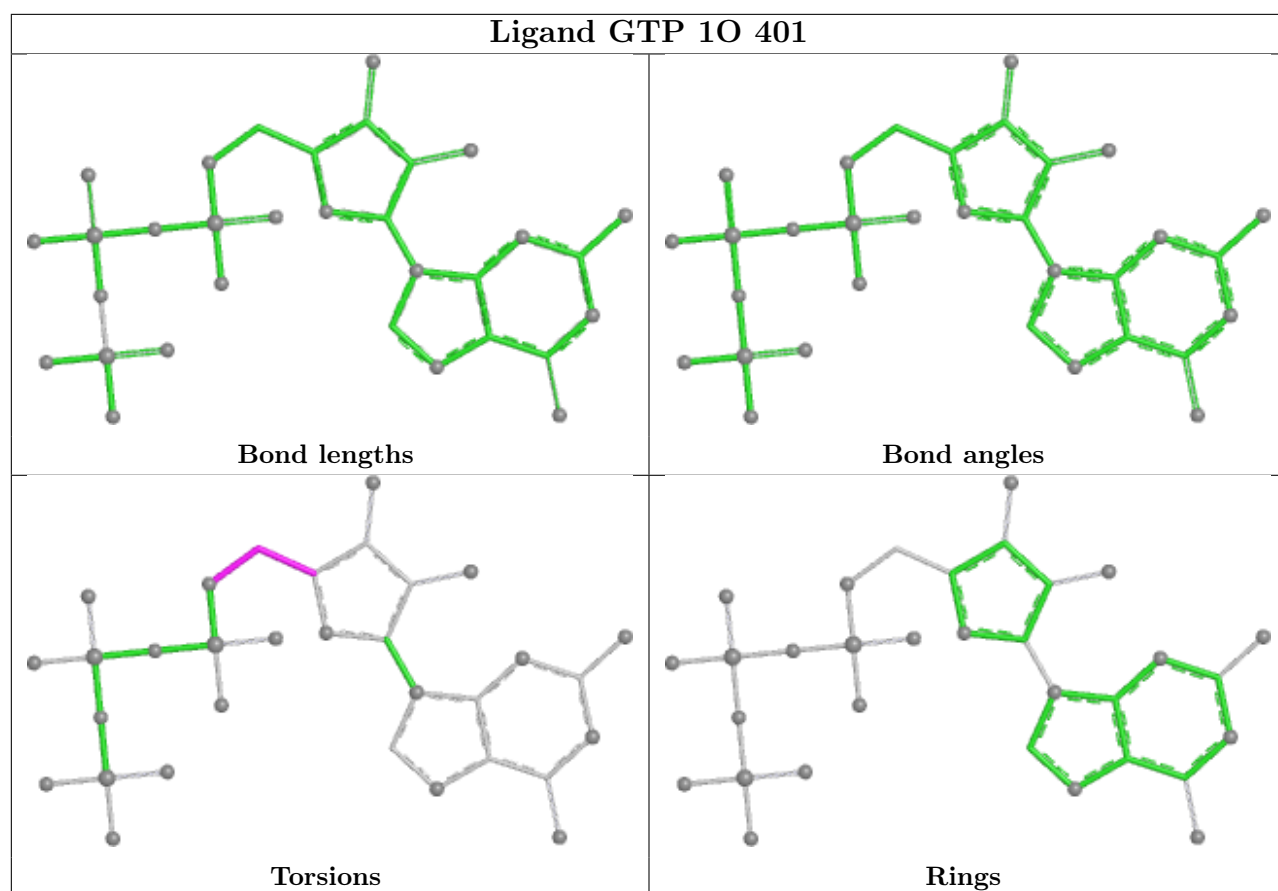
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	1q	201	CDL	14	0
46	1B	201	SF4	1	0
51	1N	402	CDL	4	0
58	1l	201	MYR	1	0
50	1I	204	PC1	8	0
54	1P	501	NDP	6	0
45	1N	401	3PE	6	0
45	1A	201	3PE	7	0
47	1E	301	FES	2	0
52	1O	401	GTP	3	0
45	1L	703	3PE	2	0
48	1F	501	FMN	3	0
46	1F	502	SF4	1	0
50	1I	203	PC1	5	0
50	1f	101	PC1	3	0
47	1G	803	FES	3	0
45	1Y	202	3PE	7	0
46	1G	801	SF4	2	0
46	1I	201	SF4	1	0
50	1L	702	PC1	1	0
57	1Y	201	PGT	8	0
56	1W	201	EHZ	1	0
45	1L	701	3PE	3	0

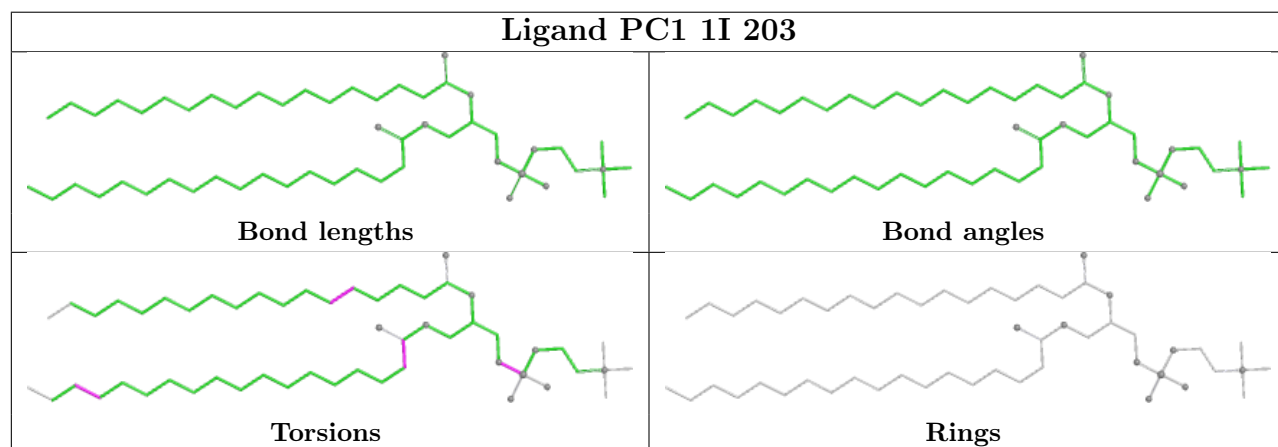
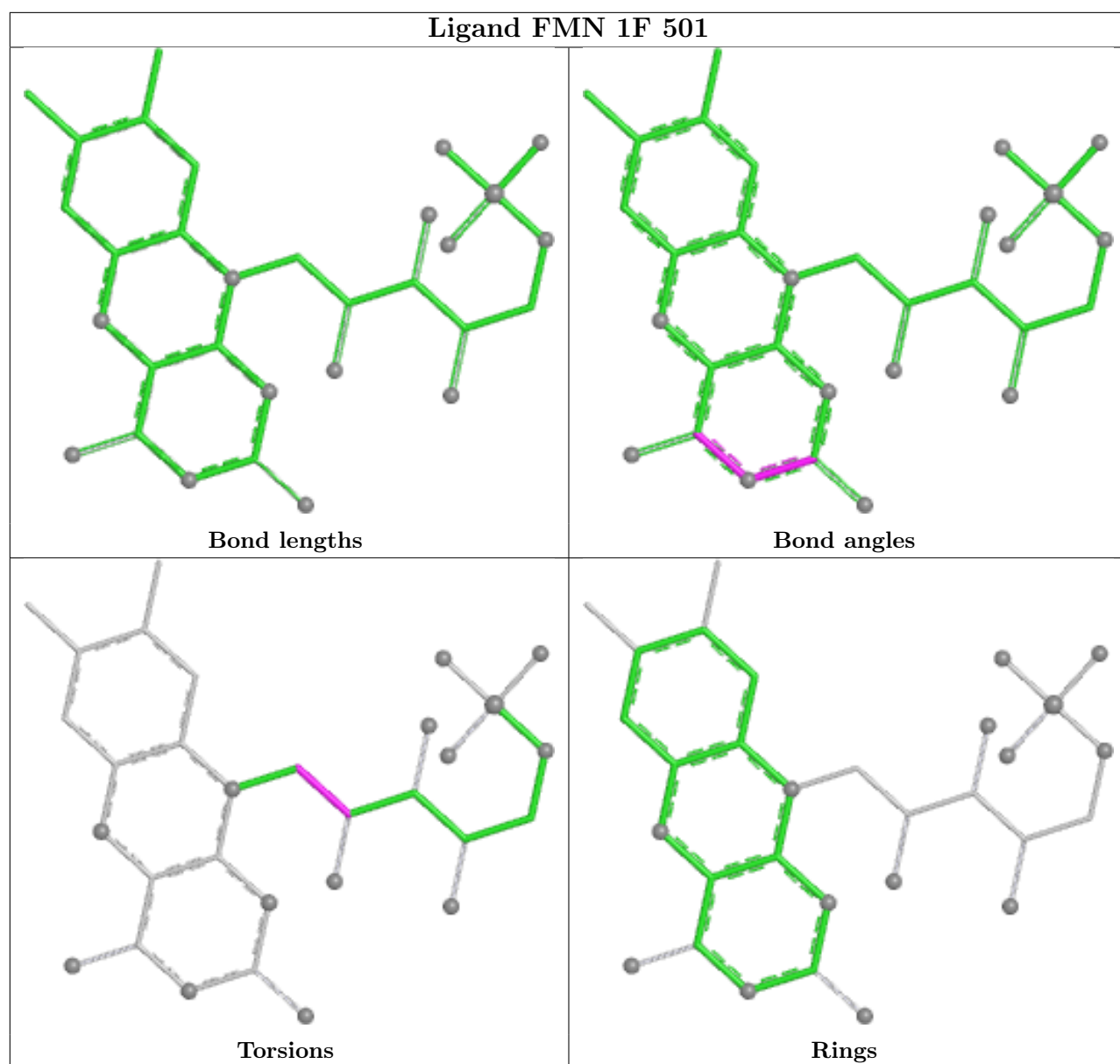
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

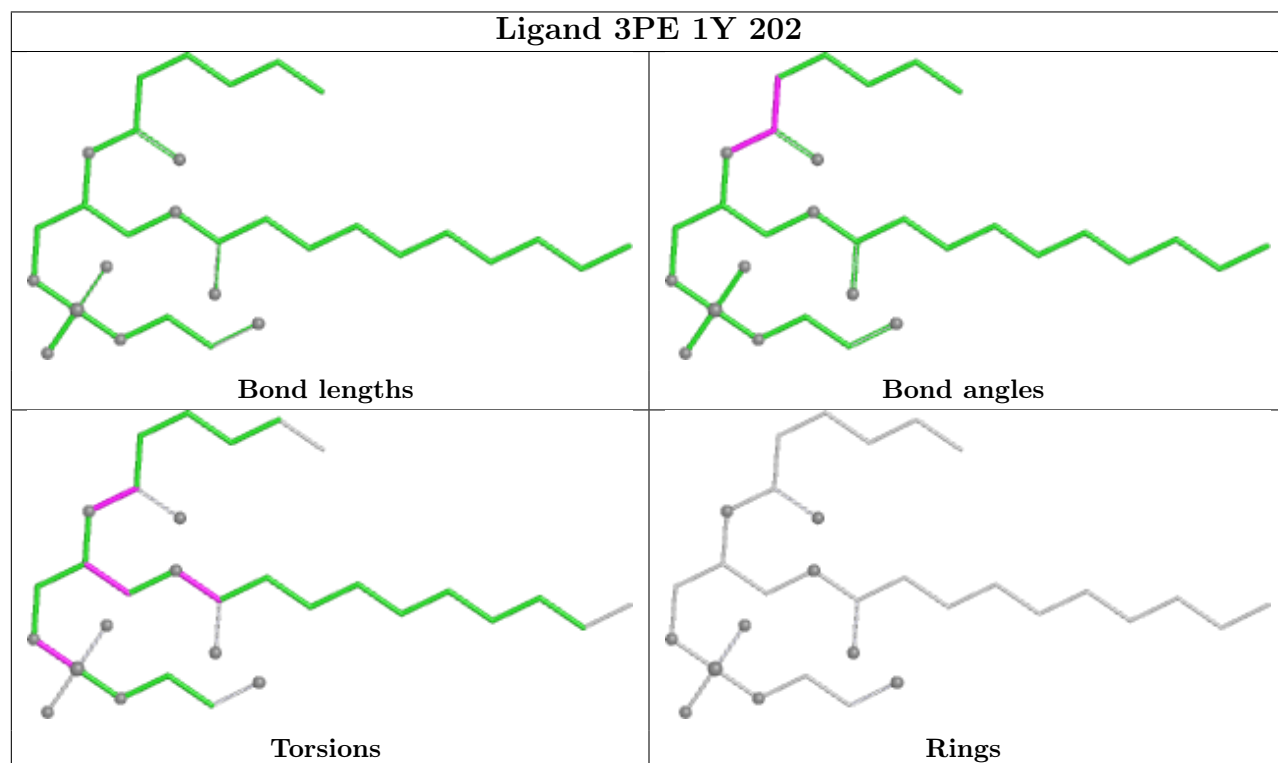
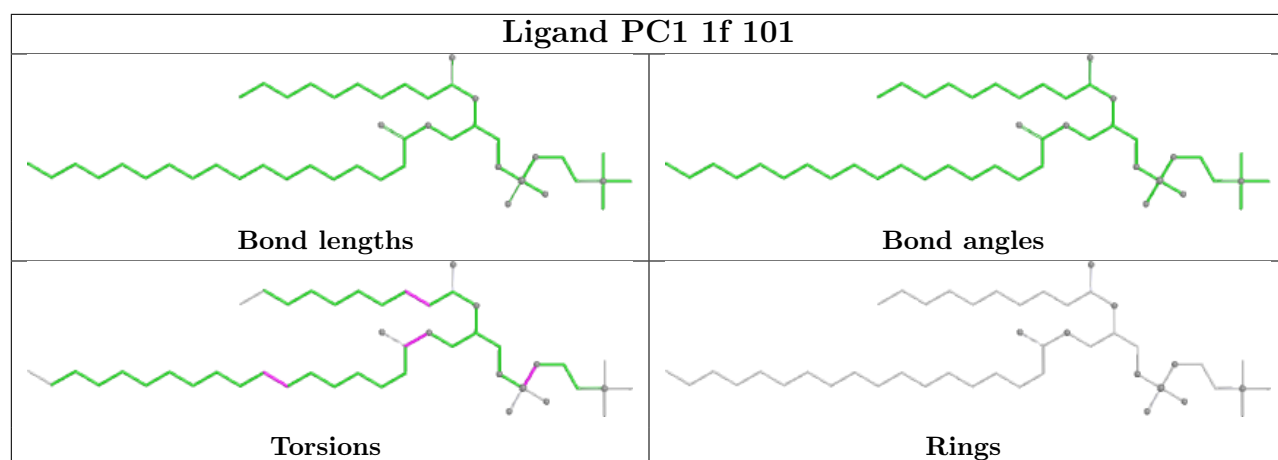


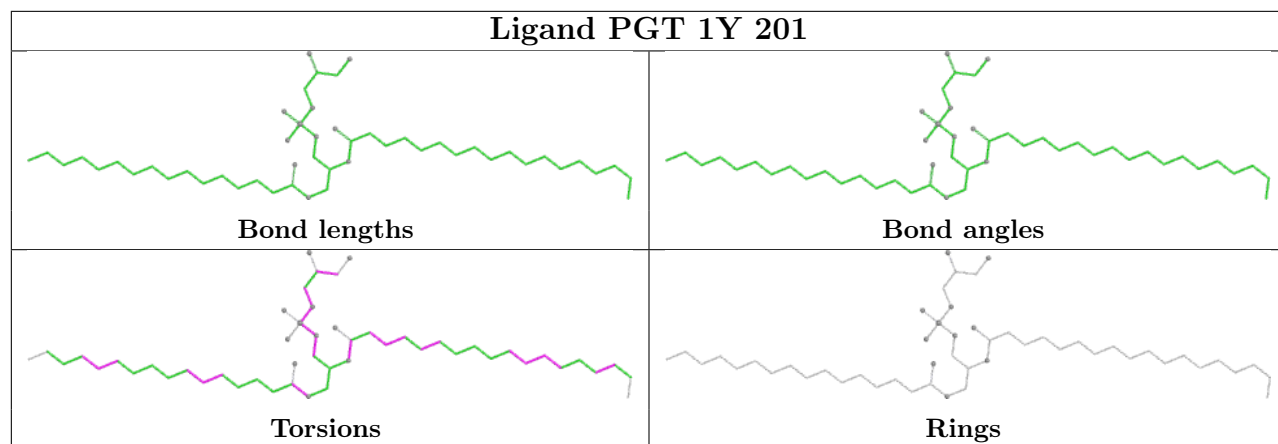
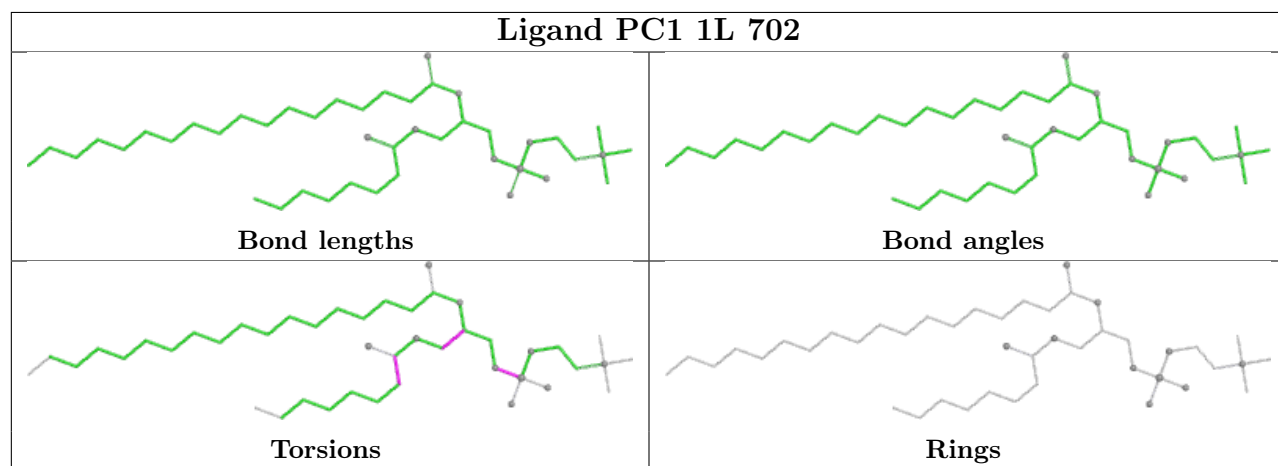
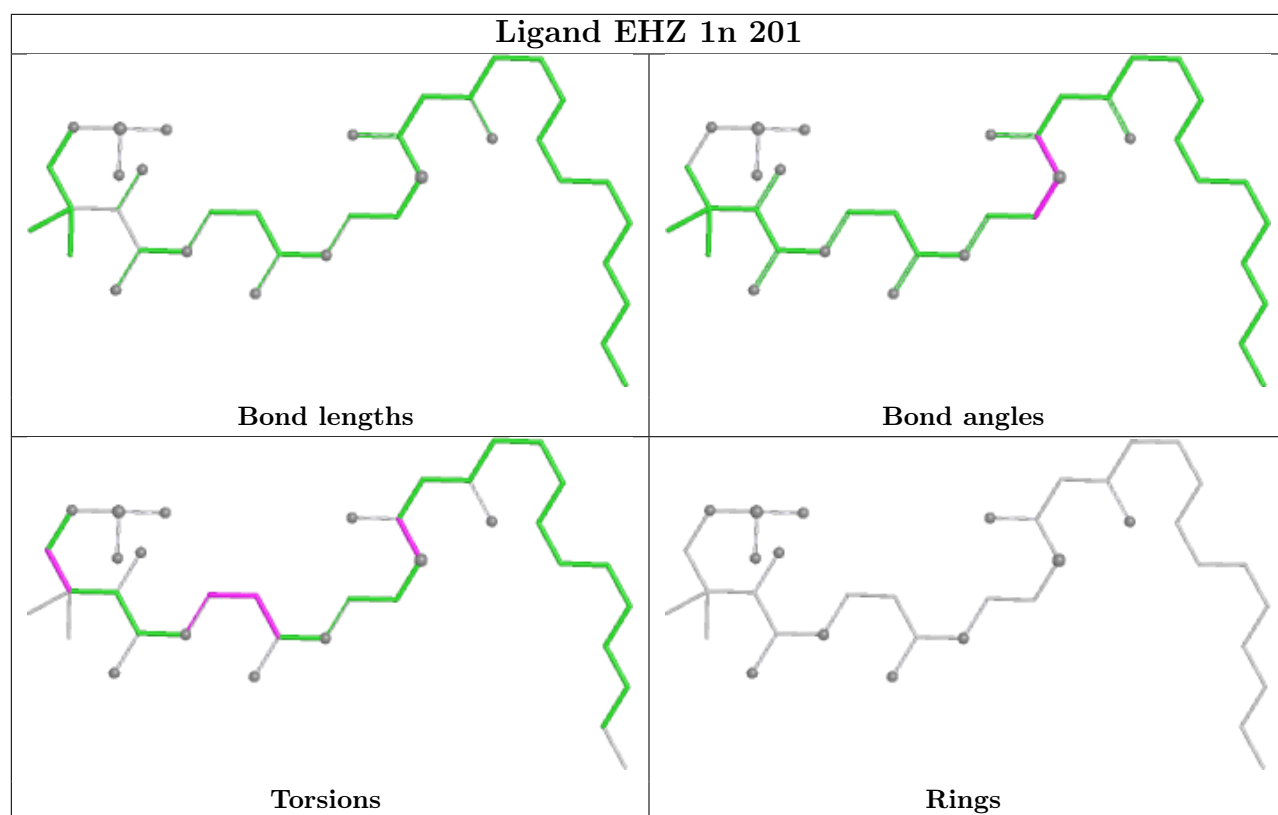


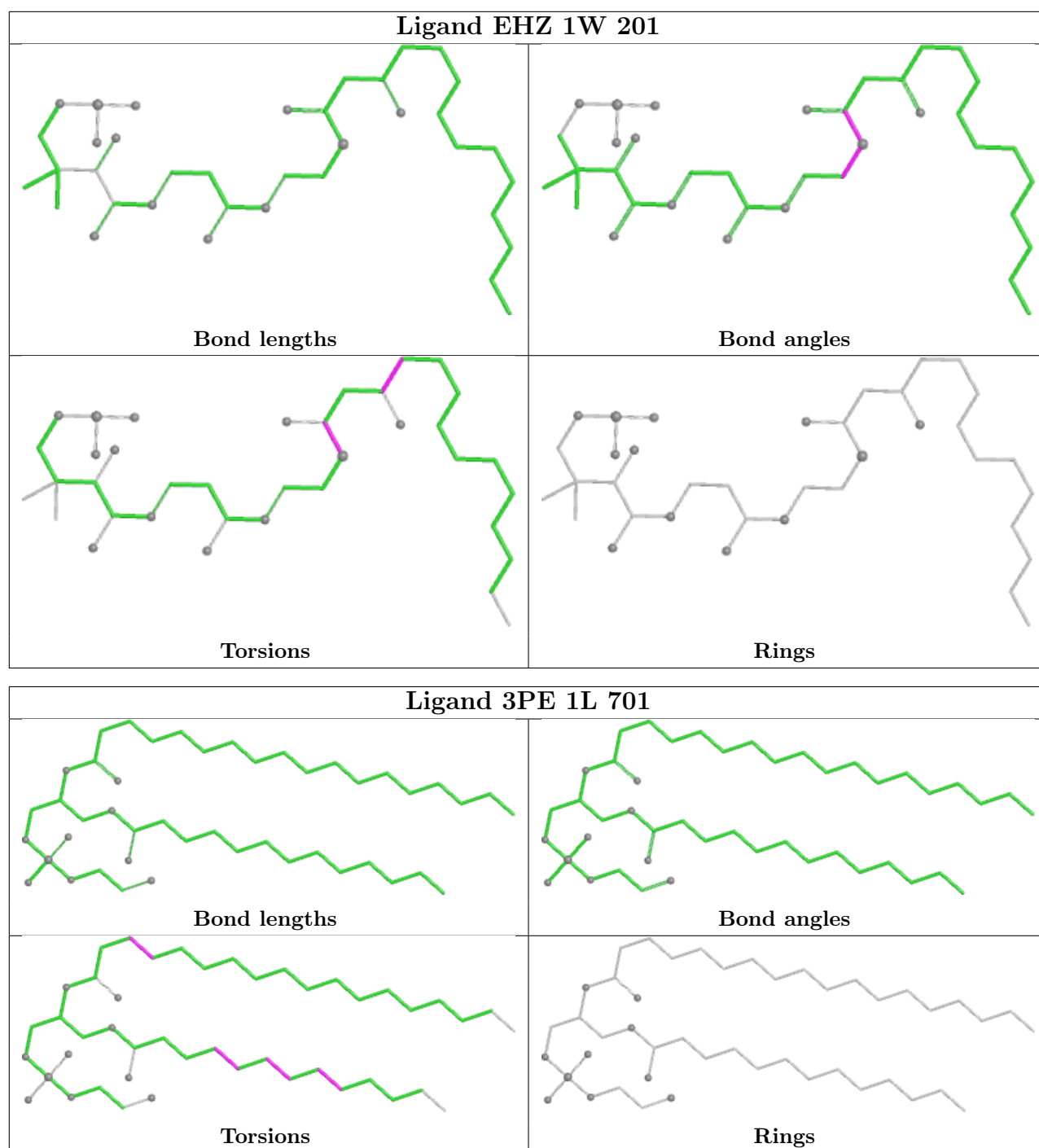












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

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

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1i	1:SAC	C	2:GLY	N	5.00
1	1r	1:ALA	C	2:SER	N	3.05

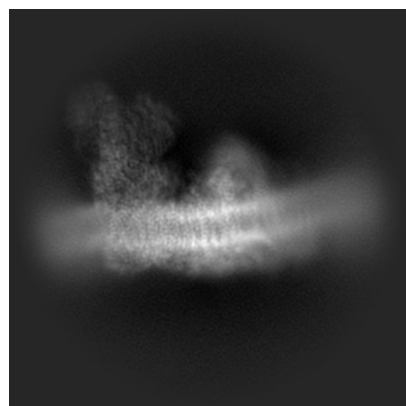
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-42169. These allow visual inspection of the internal detail of the map and identification of artifacts.

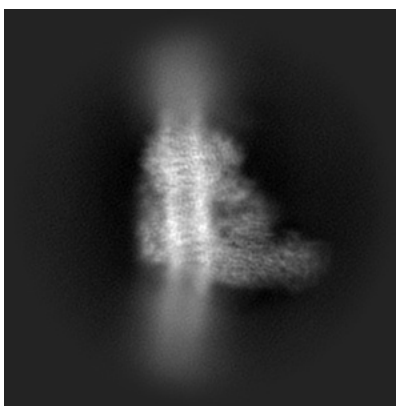
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

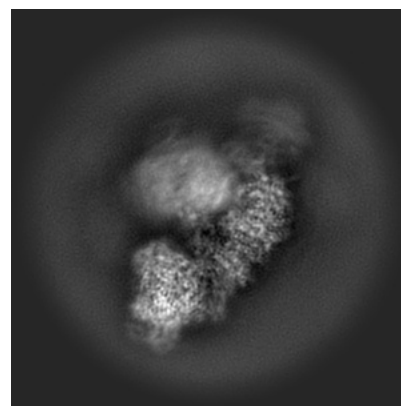
6.1.1 Primary map



X

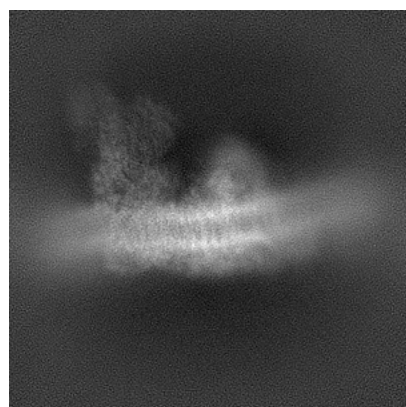


Y

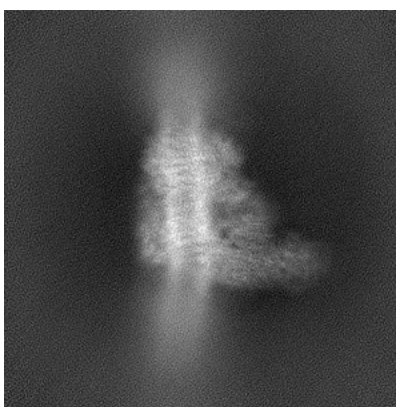


Z

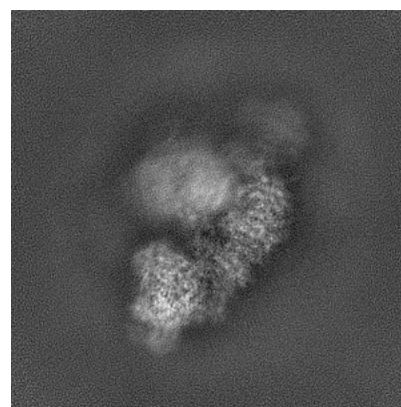
6.1.2 Raw map



X



Y

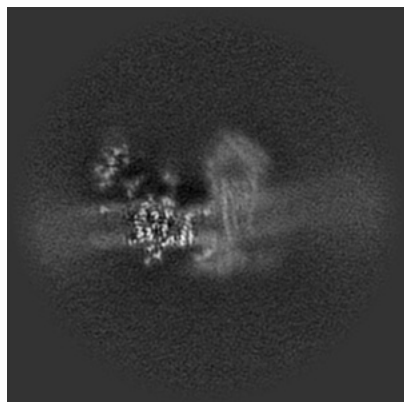


Z

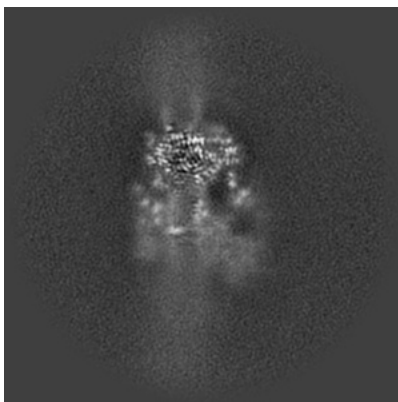
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

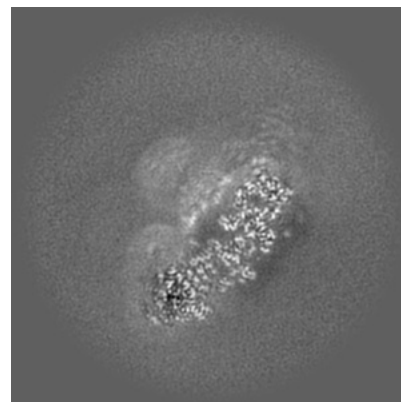
6.2.1 Primary map



X Index: 160



Y Index: 160

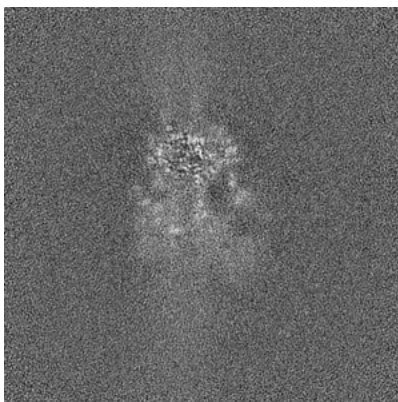


Z Index: 160

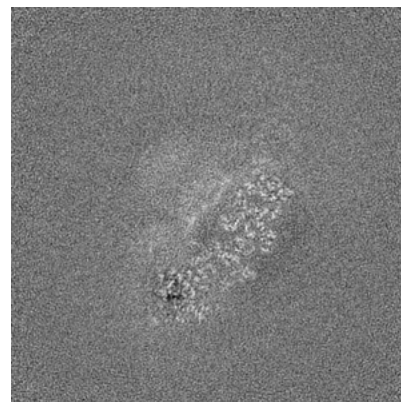
6.2.2 Raw map



X Index: 160



Y Index: 160

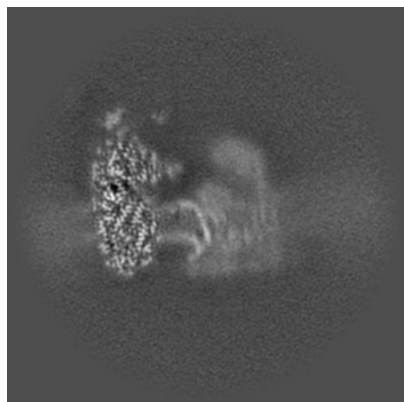


Z Index: 160

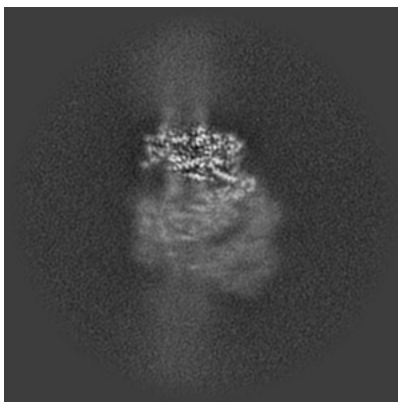
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

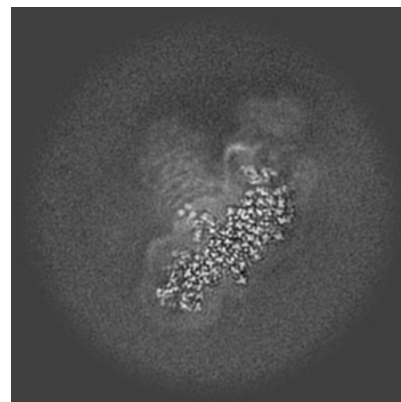
6.3.1 Primary map



X Index: 141

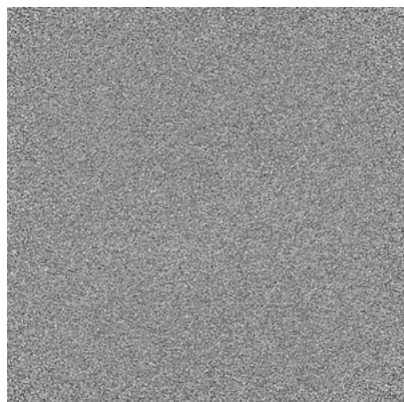


Y Index: 173

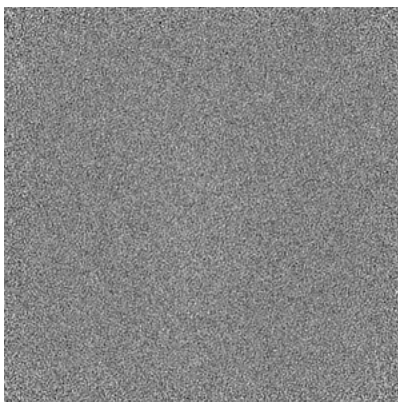


Z Index: 134

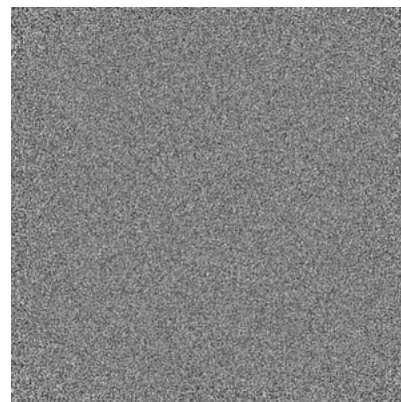
6.3.2 Raw map



X Index: 0



Y Index: 0

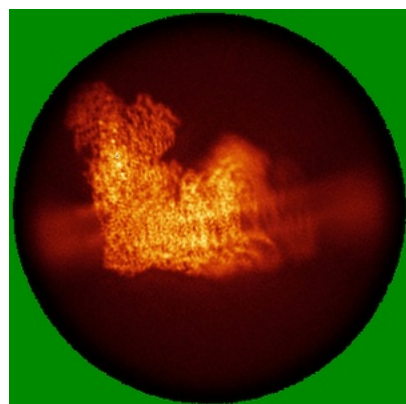


Z Index: 0

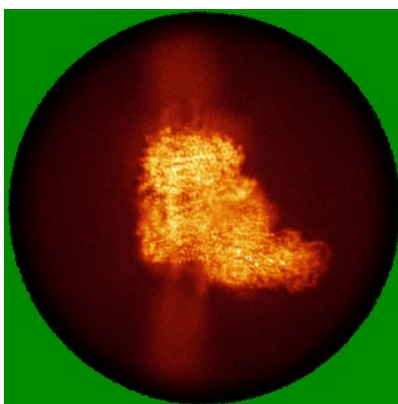
The images above show the largest variance slices of the map in three orthogonal directions.

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

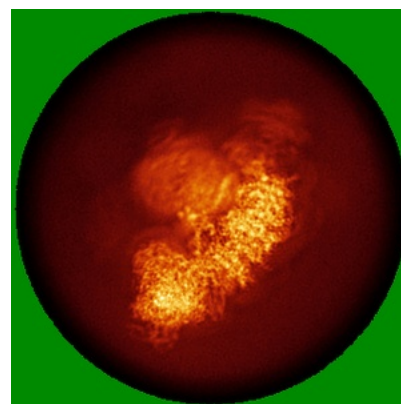
6.4.1 Primary map



X

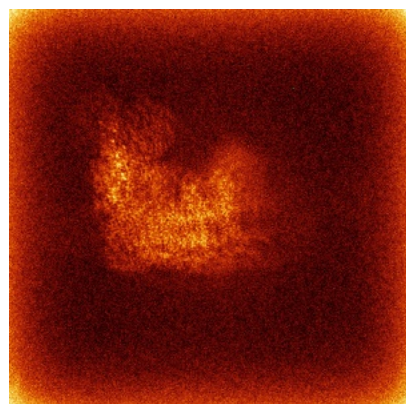


Y

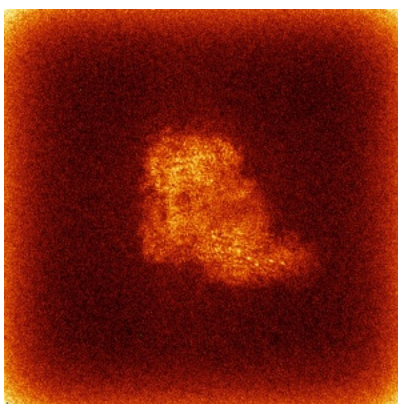


Z

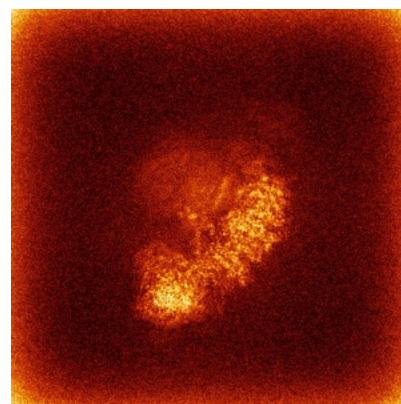
6.4.2 Raw map



X



Y

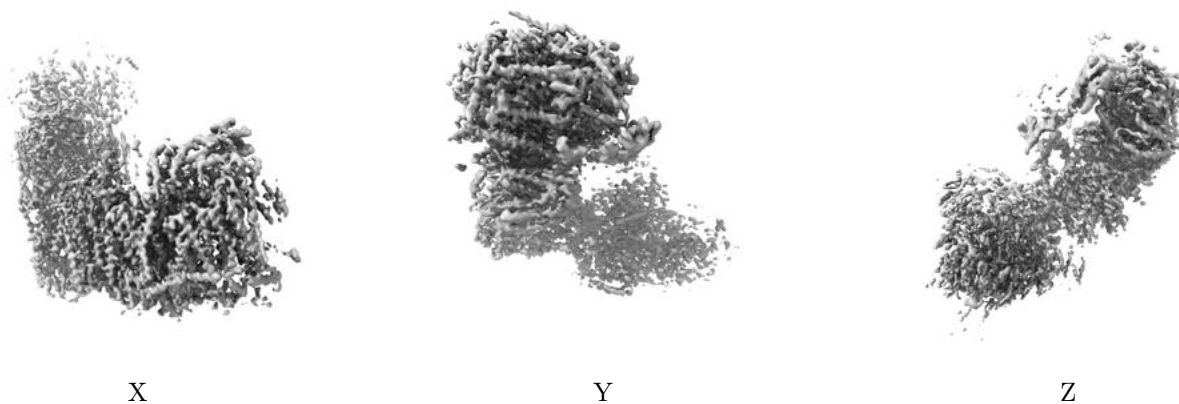


Z

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.

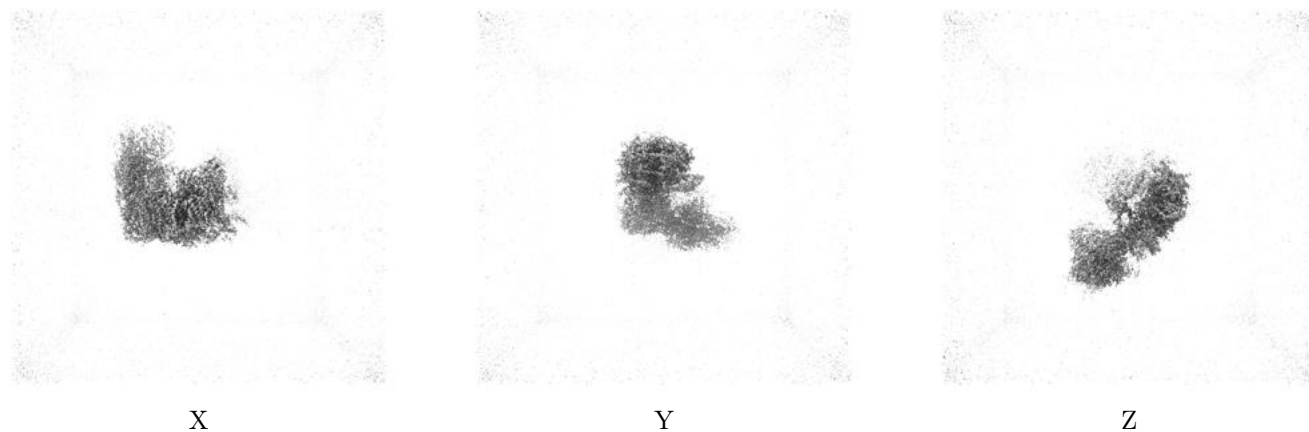
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.12. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

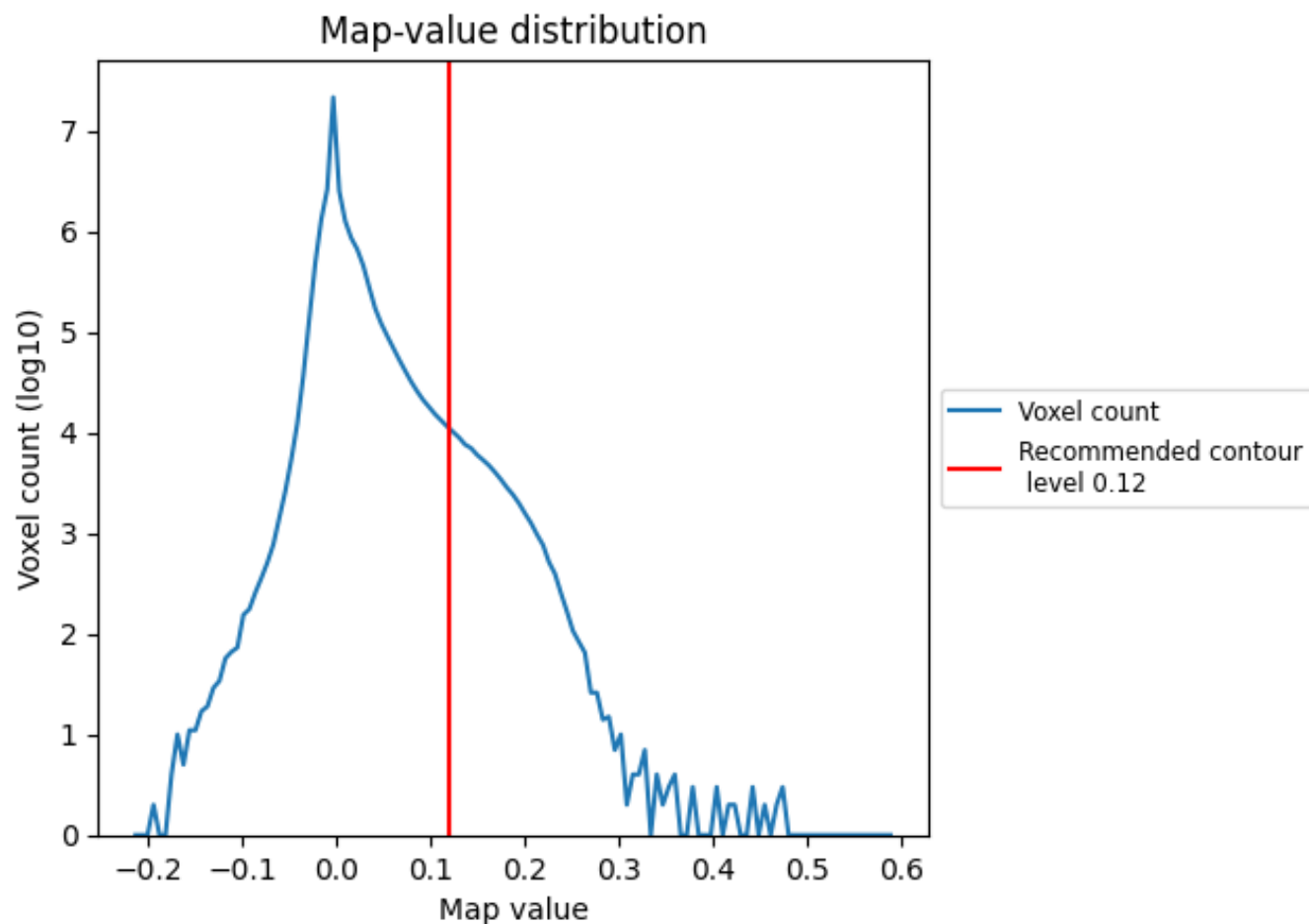
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

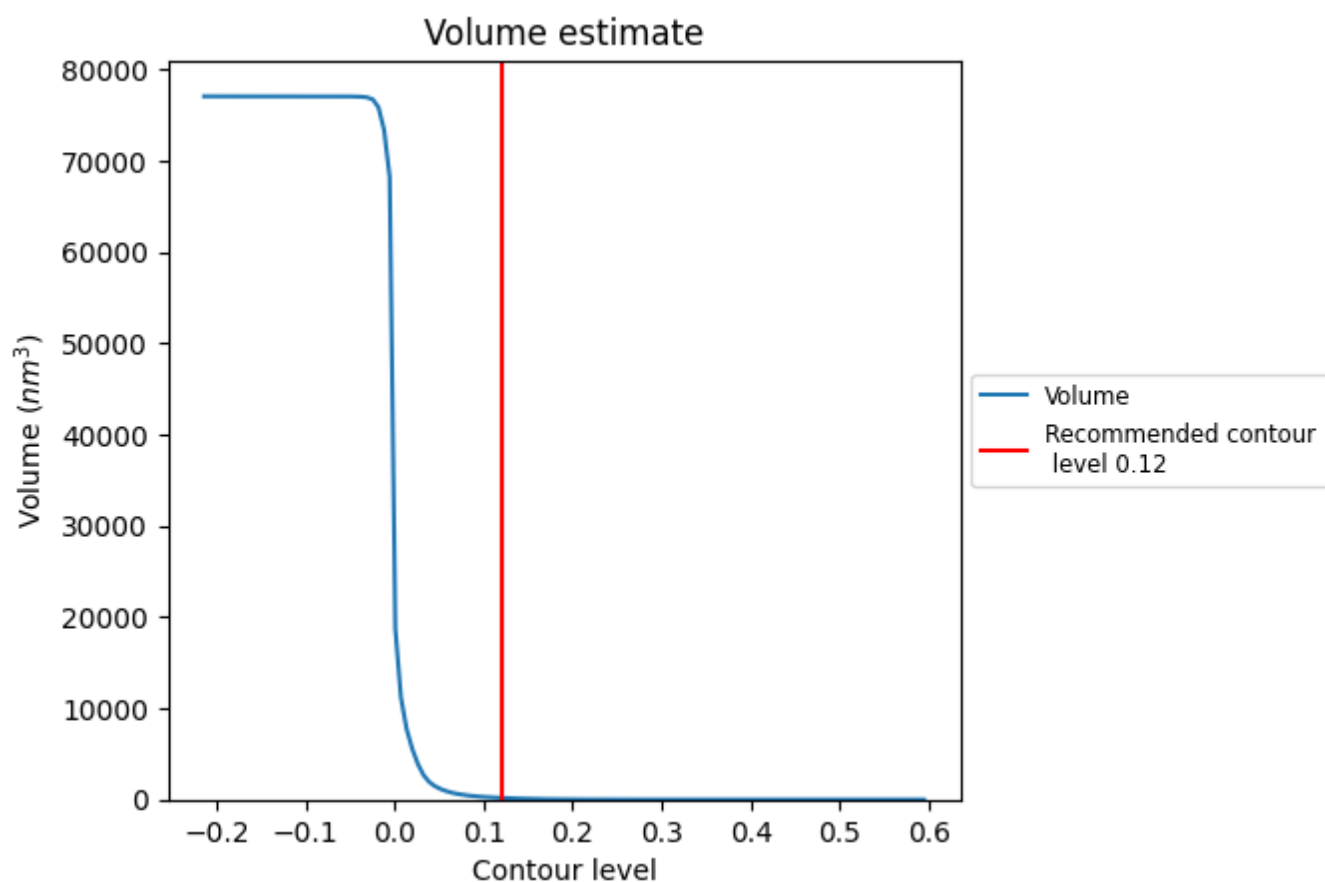
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

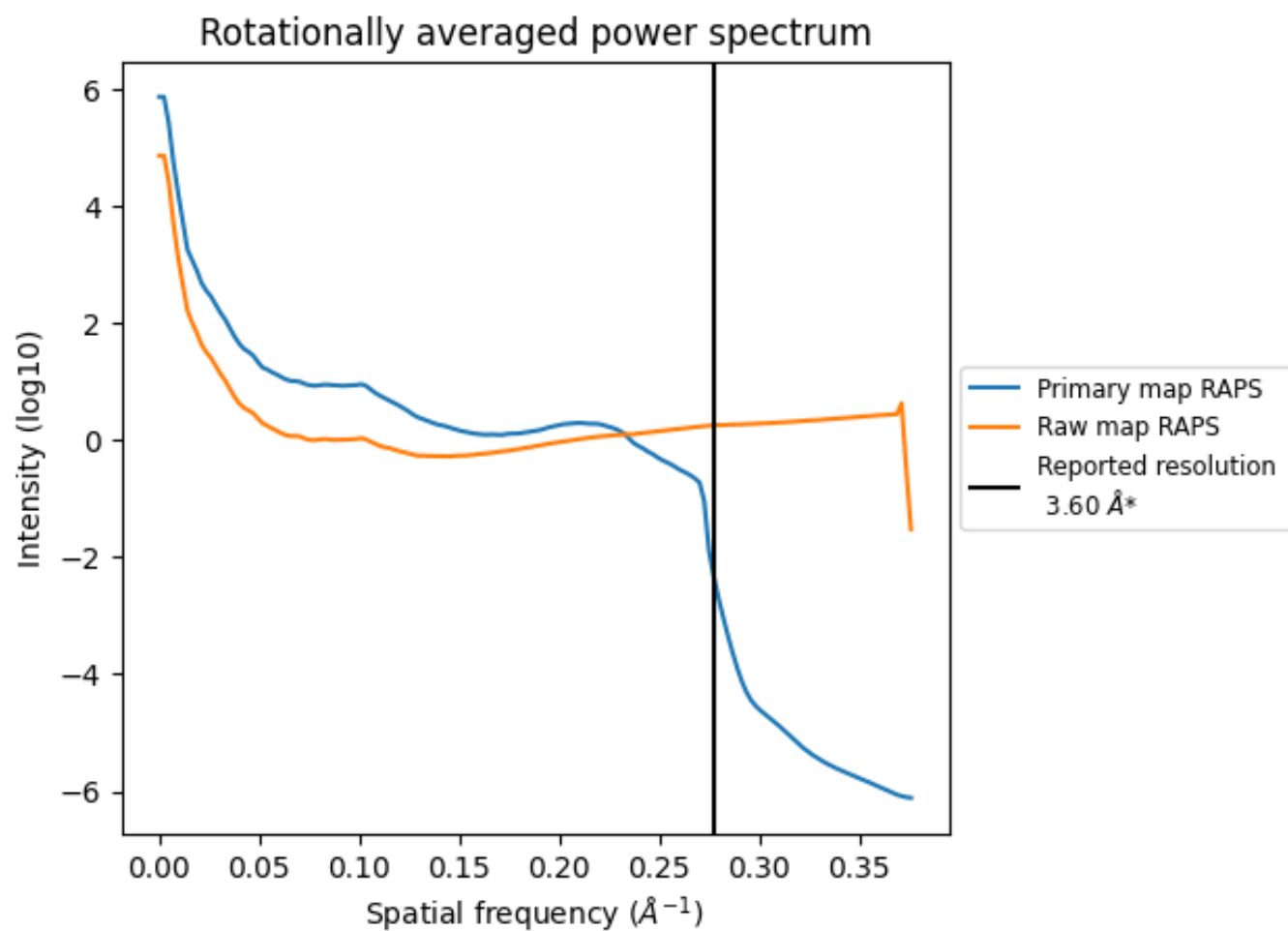
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 181 nm³; this corresponds to an approximate mass of 163 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](#)

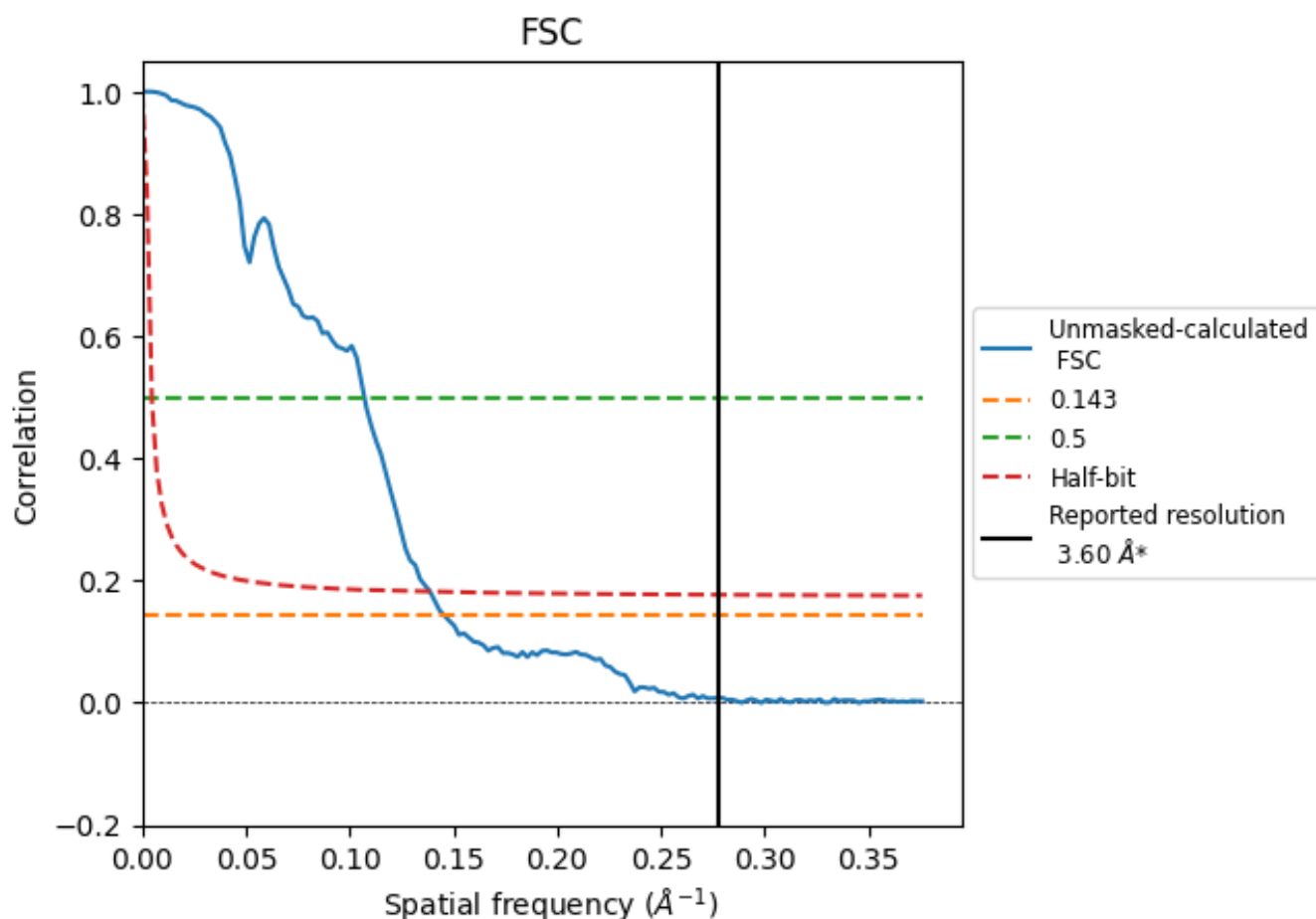


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

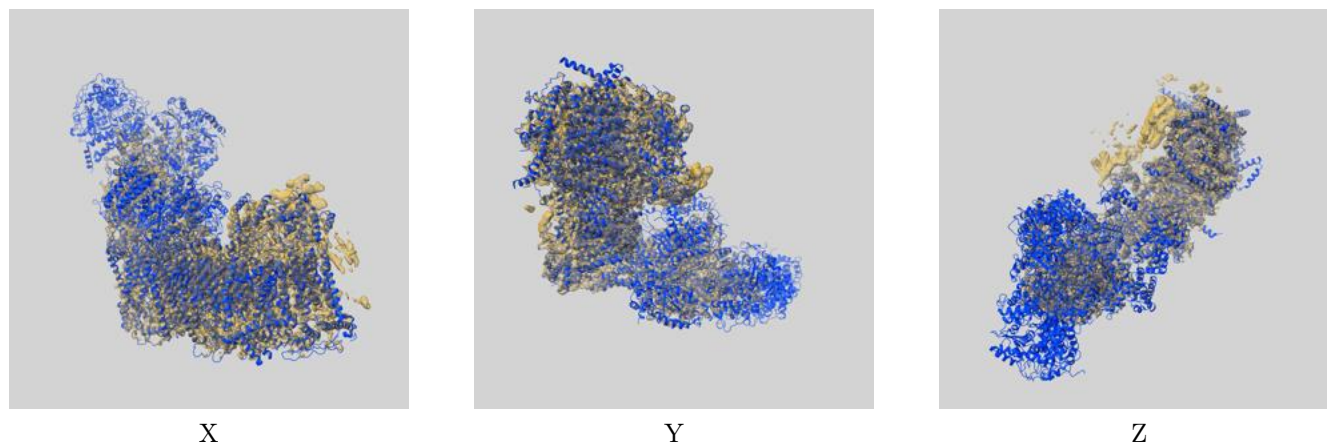
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.87	9.34	7.20

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.87 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

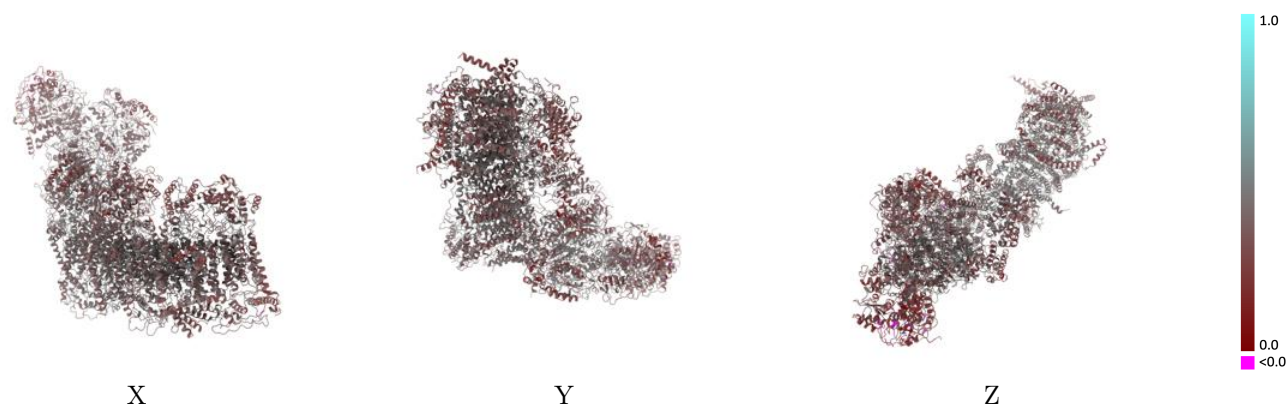
This section contains information regarding the fit between EMDB map EMD-42169 and PDB model 8UES. Per-residue inclusion information can be found in section [3](#) on page [21](#).

9.1 Map-model overlay [i](#)



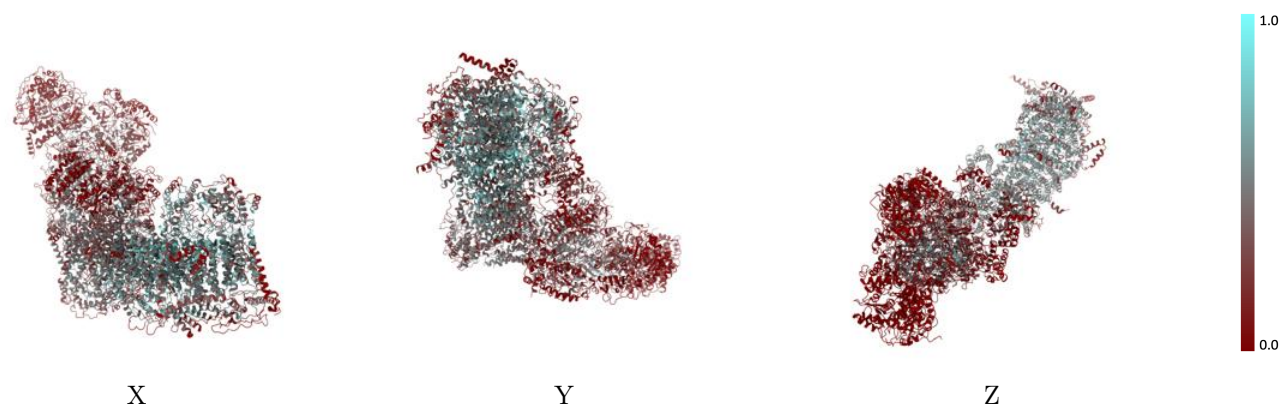
The images above show the 3D surface view of the map at the recommended contour level 0.12 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



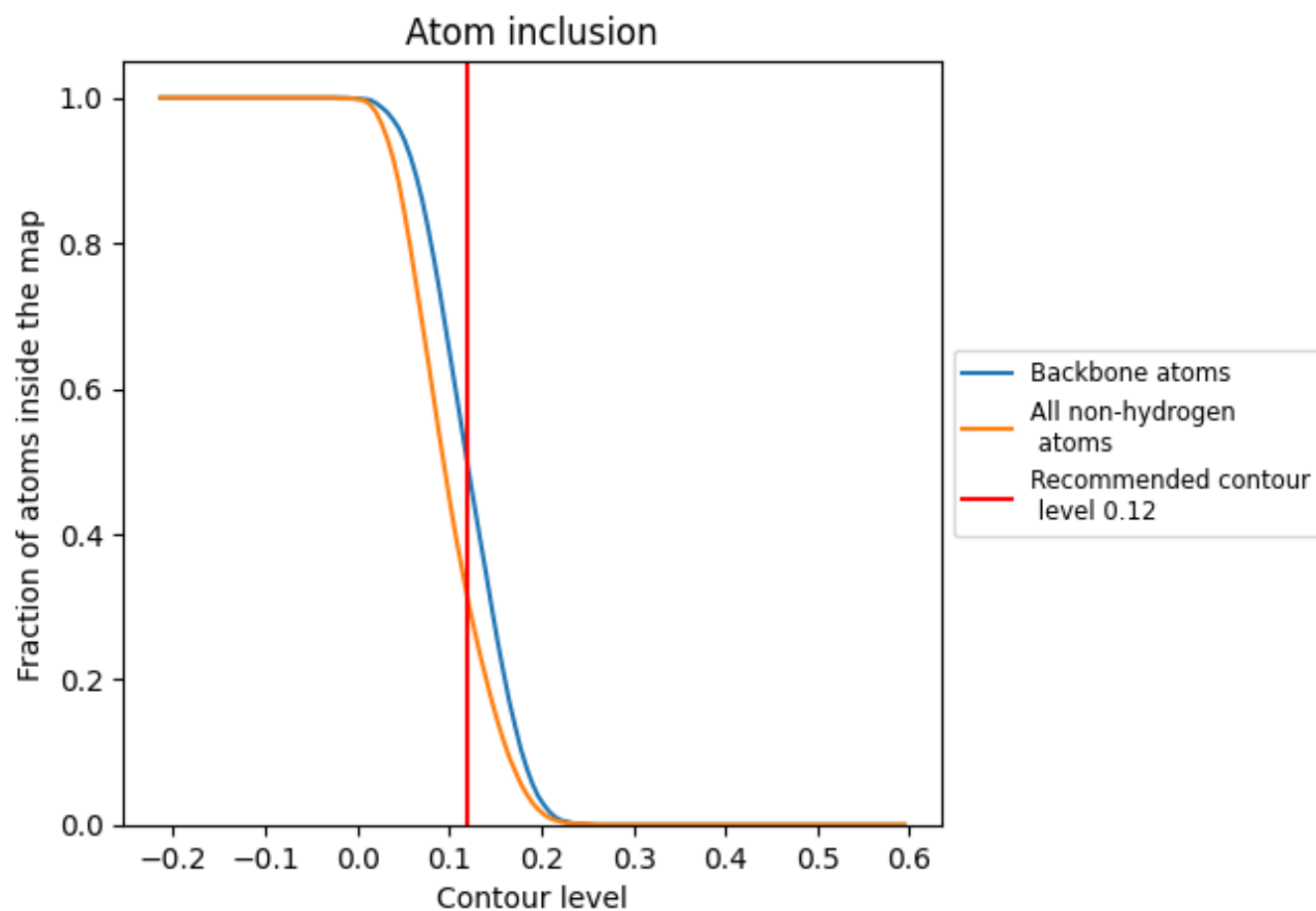
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.12).

9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 31% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.12) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.3100	 0.3800
1A	 0.2840	 0.3840
1B	 0.3950	 0.4320
1C	 0.1910	 0.4110
1D	 0.3410	 0.4120
1E	 0.0040	 0.2970
1F	 0.0090	 0.2810
1G	 0.1260	 0.3660
1H	 0.4090	 0.4160
1I	 0.4090	 0.4200
1J	 0.3100	 0.3730
1K	 0.4190	 0.4080
1L	 0.5480	 0.4000
1M	 0.6040	 0.4360
1N	 0.5030	 0.4250
1O	 0.1880	 0.3600
1P	 0.1110	 0.3450
1Q	 0.1270	 0.3760
1R	 0.1550	 0.4050
1S	 0.0130	 0.2940
1T	 0.0410	 0.2690
1U	 0.4260	 0.3490
1V	 0.0510	 0.3420
1W	 0.1360	 0.3460
1X	 0.3390	 0.4070
1Y	 0.4450	 0.3790
1Z	 0.3580	 0.4130
1a	 0.4380	 0.4050
1b	 0.3230	 0.4120
1c	 0.2860	 0.3610
1d	 0.4730	 0.4160
1e	 0.4220	 0.4270
1f	 0.2900	 0.3850
1g	 0.4080	 0.3800
1h	 0.4720	 0.4170



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Chain	Atom inclusion	Q-score
1i	 0.2480	 0.3510
1j	 0.3160	 0.3660
1k	 0.3130	 0.3460
1l	 0.4300	 0.3910
1m	 0.5090	 0.3760
1n	 0.4620	 0.3560
1o	 0.2920	 0.3240
1p	 0.4050	 0.3870
1q	 0.2220	 0.4100
1r	 0.1870	 0.4020
1s	 0.0000	 0.2530