



Full wwPDB EM Validation Report ⓘ

Mar 21, 2026 – 06:27 PM UTC

PDB ID : 7AR8 / pdb_00007ar8
EMDB ID : EMD-11876
Title : Cryo-EM structure of Arabidopsis thaliana complex-I (closed conformation)
Authors : Klusch, N.; Kuelbrandt, W.; Yildiz, O.
Deposited on : 2020-10-23
Resolution : 3.53 Å(reported)

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

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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

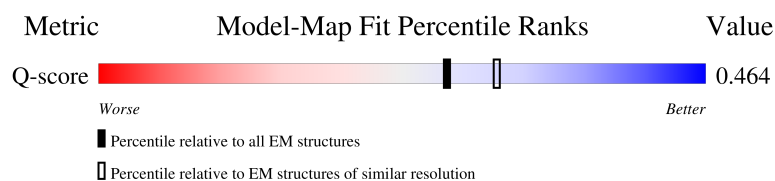
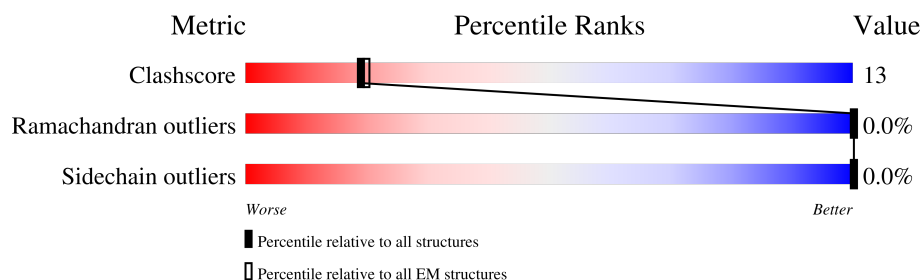
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.53 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	12947 (3.03 - 4.02)

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	A	119	8% 60% 18% 23%
2	B	218	49% 23% 28%
3	C	190	71% 27%
4	D	394	71% 27%

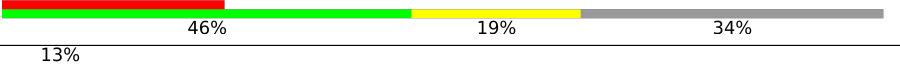
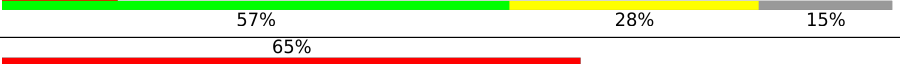
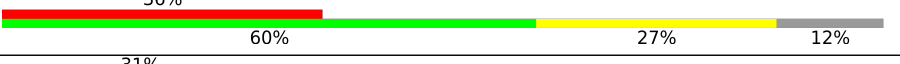
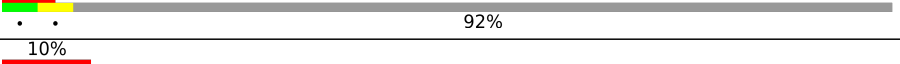
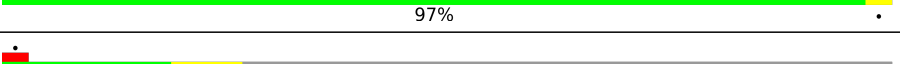
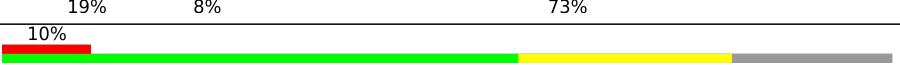
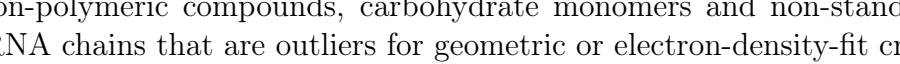
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Mol	Chain	Length	Quality of chain
5	E	255	
6	F	486	
7	G	748	
8	H	325	
9	I	222	
10	J	205	
11	K	100	
12	L	669	
13	M	495	
14	N	499	
15	O	159	
16	P	402	
17	Q	154	
18	R	110	
19	S	97	
20	T	122	
21	U	126	
22	V	169	
23	W	133	
24	X	106	
25	Z	143	
26	a	65	
27	b	65	
28	c	88	
29	d	81	

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Mol	Chain	Length	Quality of chain
30	e	83	
31	f	106	
32	g	114	
33	i	98	
34	j	69	
35	k	72	
36	l	125	
37	m	71	
38	n	117	
39	o	103	
40	p	106	
41	q	159	
42	r	131	
43	u	30	
44	v	113	
45	x	256	
46	y	278	
47	z	275	

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
48	SF4	F	501	-	-	X	-
49	FES	E	500	-	-	X	-

2 Entry composition

There are 61 unique types of molecules in this entry. The entry contains 61461 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	A	92	Total	C	N	O	S	0	0
			785	556	108	117	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	157	Total	C	N	O	S	0	0
			1244	797	218	215	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	185	Total	C	N	O	S	0	0
			1581	1021	271	283	6		

- Molecule 4 is a protein called NADH dehydrogenase subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	385	Total	C	N	O	S	0	0
			3077	1954	542	557	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	363	SER	LEU	variant	UNP A0A2P2CLH2

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	192	Total	C	N	O	S	0	0
			1500	954	248	287	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	434	Total	C	N	O	S	0	0
			3368	2125	600	618	25		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	688	Total	C	N	O	S	0	0
			5252	3291	921	1001	39		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	324	Total	C	N	O	S	0	0
			2536	1719	386	416	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	169	Total	C	N	O	S	0	0
			1381	869	234	268	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	138	Total	C	N	O	S	0	0
			1093	742	168	175	8		

- Molecule 11 is a protein called NADH dehydrogenase subunit 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	90	Total	C	N	O	S	0	0
			707	476	109	115	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	615	Total	C	N	O	S	0	0
			4807	3191	748	832	36		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP B5TM94

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	487	Total	C	N	O	S	0	0
			3887	2627	601	636	23		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	326	LEU	PRO	conflict	UNP B5TM93

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	488	Total	C	N	O	S	0	0
			3820	2573	577	642	28		

- Molecule 15 is a protein called AT3G07480.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	122	Total	C	N	O	S	0	0
			956	598	169	185	4		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	332	Total	C	N	O	S	0	0
			2560	1643	439	463	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	119	Total	C	N	O	S	0	0
			939	600	163	175	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	62	Total	C	N	O	S	0	0
			482	304	84	89	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	93	Total	C	N	O	S	0	0
			727	459	129	133	6		

- Molecule 20 is a protein called Acyl carrier protein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	84	Total	C	N	O	S	0	0
			667	421	105	138	3		

- Molecule 21 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	79	Total	C	N	O	S	0	0
			616	387	98	130	1		

- Molecule 22 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	140	Total	C	N	O	S	0	0
			1123	712	187	219	5		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	110	Total	C	N	O	S	0	0
			893	571	159	160	3		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	97	Total	C	N	O	S	0	0
			767	480	132	143	12		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	124	Total	C	N	O	S	0	0
			990	635	174	176	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	58	Total	C	N	O	S	0	0
			469	302	84	78	5		

- Molecule 27 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	39	Total	C	N	O	S	0	0
			288	190	47	48	3		

- Molecule 28 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	73	Total	C	N	O	S	0	0
			595	384	110	95	6		

- Molecule 29 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	73	Total	C	N	O	S	0	0
			574	368	104	97	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	64	Total	C	N	O	S	0	0
			546	338	102	99	7		

- Molecule 31 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	98	Total	C	N	O	S	0	0
			734	473	118	138	5		

- Molecule 32 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	75	Total	C	N	O	S	0	0
			615	396	107	109	3		

- Molecule 33 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	i	83	Total	C	N	O	S	0	0
			721	458	132	126	5		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	j	51	Total	C	N	O	S	0	0
			415	275	73	64	3		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	k	47	Total	C	N	O	S	0	0
			374	238	71	62	3		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	l	50	Total	C	N	O	0	0
			384	255	61	68		

- Molecule 37 is a protein called B15 – 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	69	Total	C	N	O	S	0	0
			569	364	106	97	2		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	n	109	Total	C	N	O	S	0	0
			911	580	170	160	1		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	o	77	Total	C	N	O	S	0	0
			631	398	109	114	10		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	p	93	Total	C	N	O	S	0	0
			778	493	144	137	4		

- Molecule 41 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	q	65	Total	C	N	O	0	0
			536	342	95	99		

- Molecule 42 is a protein called Furry.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	r	10	Total	C	N	O	0	0
			88	57	17	14		

- Molecule 43 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	u	30	Total	C	N	O	0	0
			150	90	30	30		

- Molecule 44 is a protein called Uncharacterized protein At2g27730, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	v	30	Total	C	N	O	0	0
			226	147	39	40		

- Molecule 45 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	x	211	Total	C	N	O	S	0	0
			1637	1049	281	302	5		

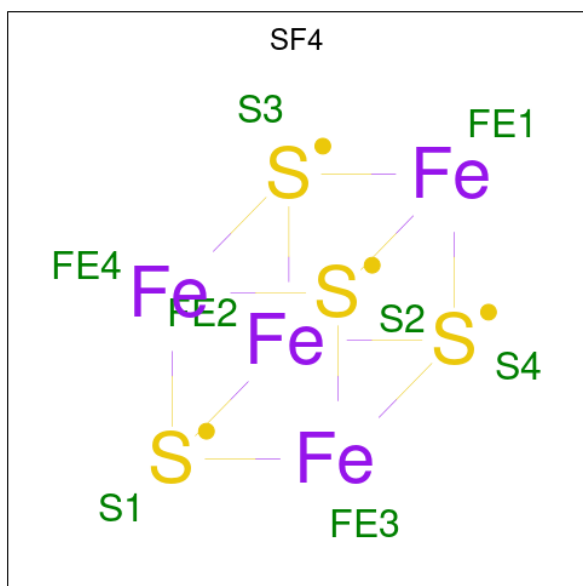
- Molecule 46 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	y	263	Total	C	N	O	S	0	0
			2001	1251	357	386	7		

- Molecule 47 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	z	232	Total	C	N	O	S	0	0
			1763	1105	323	329	6		

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



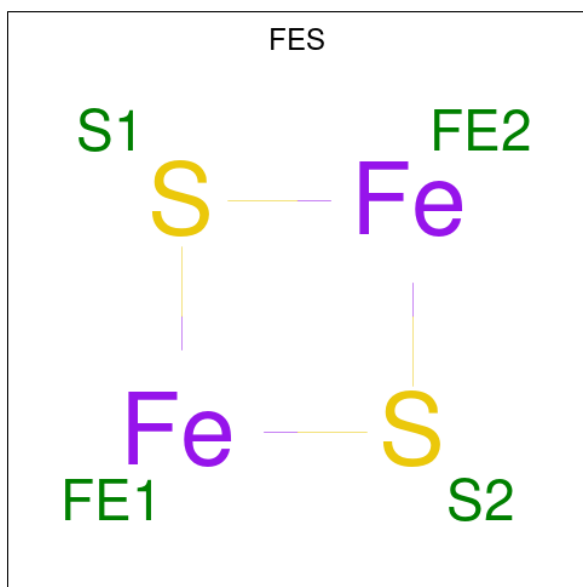
Mol	Chain	Residues	Atoms			AltConf
48	B	1	Total	Fe	S	0
			8	4	4	
48	F	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	
48	G	1	Total	Fe	S	0
			8	4	4	

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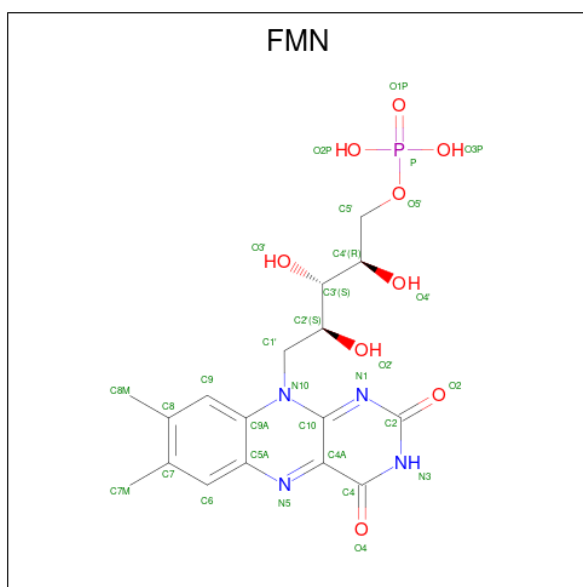
Mol	Chain	Residues	Atoms			AltConf
48	I	1	Total	Fe	S	0
			8	4	4	
48	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 49 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



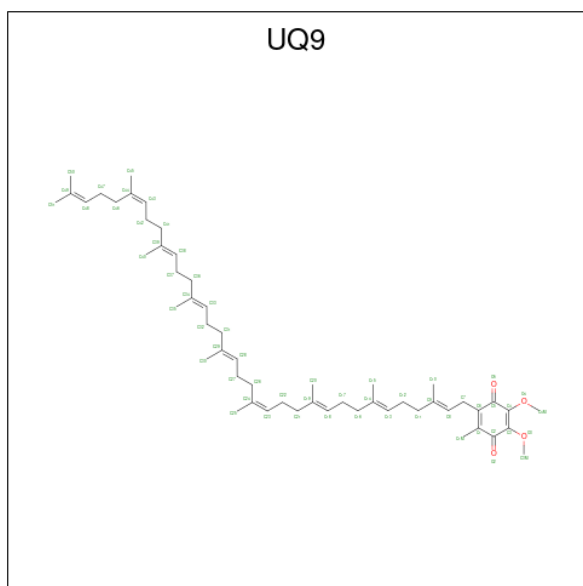
Mol	Chain	Residues	Atoms			AltConf
49	E	1	Total	Fe	S	0
			4	2	2	
49	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 50 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



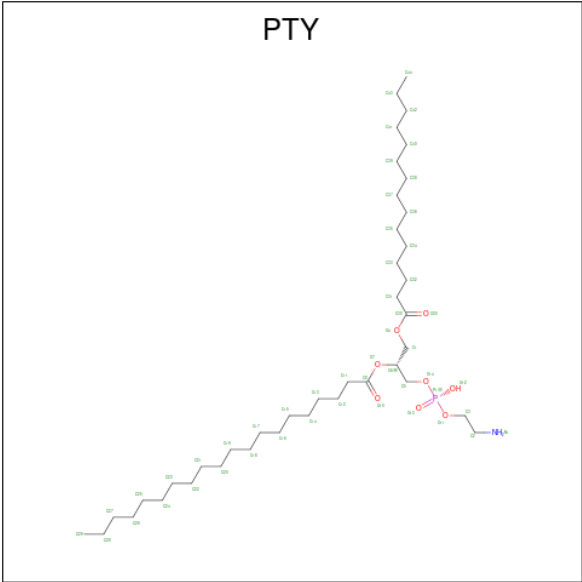
Mol	Chain	Residues	Atoms					AltConf
50	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 51 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).



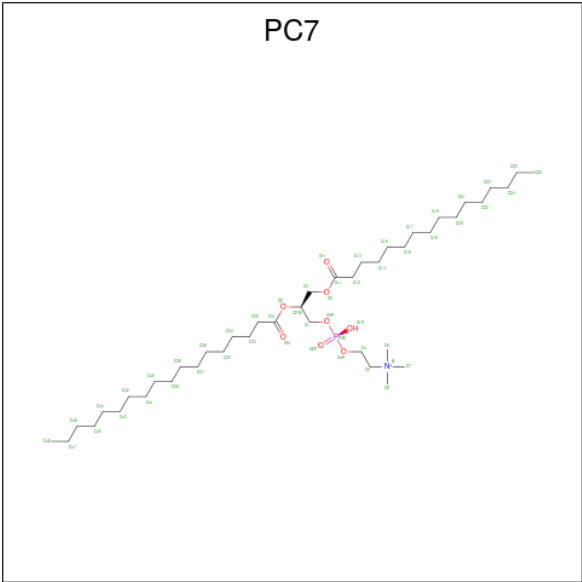
Mol	Chain	Residues	Atoms			AltConf
51	H	1	Total	C	O	0
			35	31	4	

- Molecule 52 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



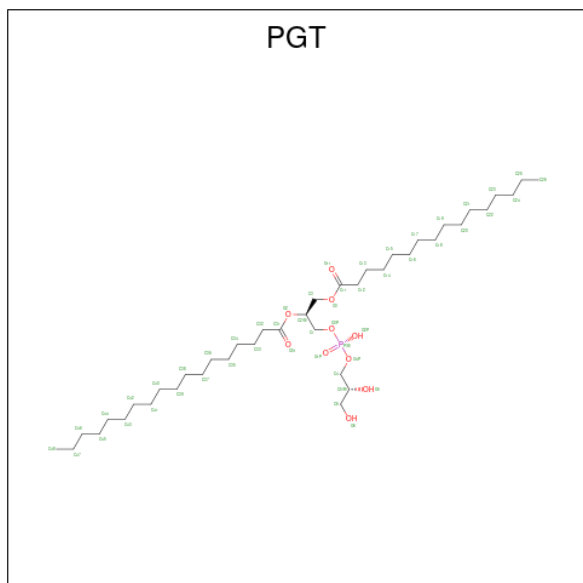
Mol	Chain	Residues	Atoms					AltConf
52	H	1	Total	C	N	O	P	0
			50	40	1	8	1	
52	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
52	N	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 53 is (7S)-4-HYDROXY-N,N,N-TRIMETHYL-9-OXO-7-[(PALMITOYLOXY) METHYL]-3,5,8-TRIOXA-4-PHOSPHAHEXACOSAN-1-AMINIUM 4-OXIDE (CCD ID: PC7) (formula: C₄₂H₈₅NO₈P).



Mol	Chain	Residues	Atoms					AltConf
53	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
53	v	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 54 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
54	N	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 55 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 56 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

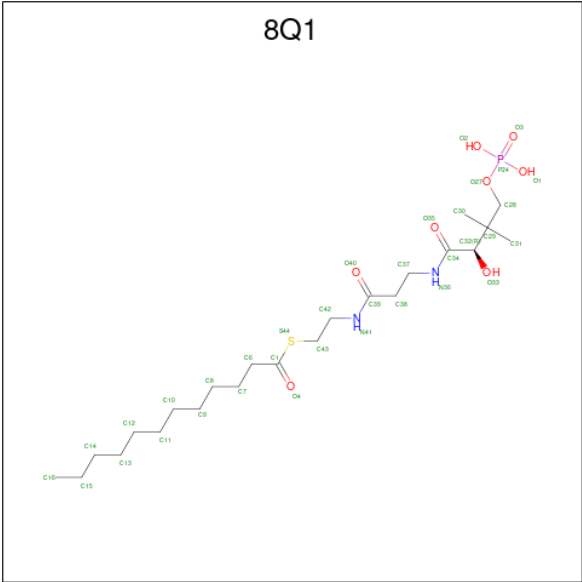


Mol	Chain	Residues	Atoms					AltConf
56	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

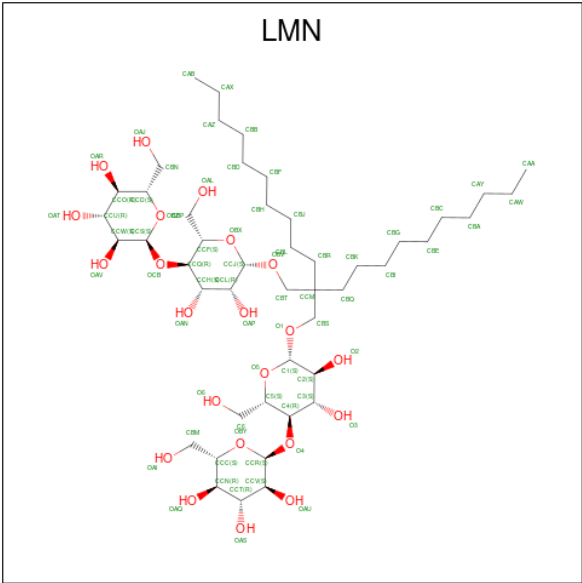
Mol	Chain	Residues	Atoms		AltConf
57	R	1	Total 1	Zn 1	0
57	y	1	Total 1	Zn 1	0

- Molecule 58 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



Mol	Chain	Residues	Atoms						AltConf
58	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
58	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

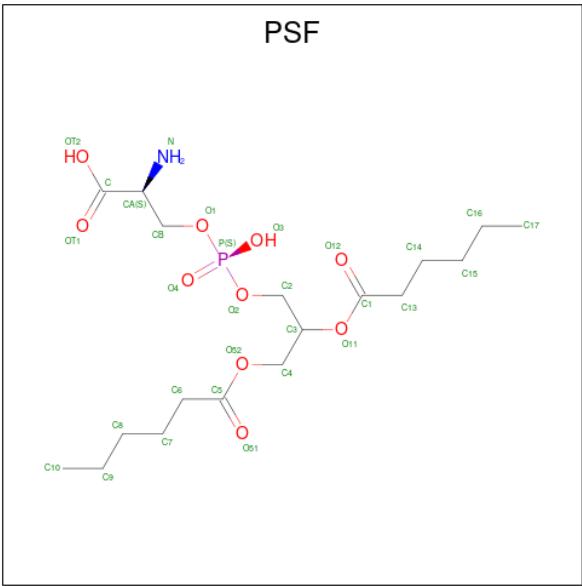
- Molecule 59 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			AltConf
59	d	1	Total	C	O	0
			69	47	22	

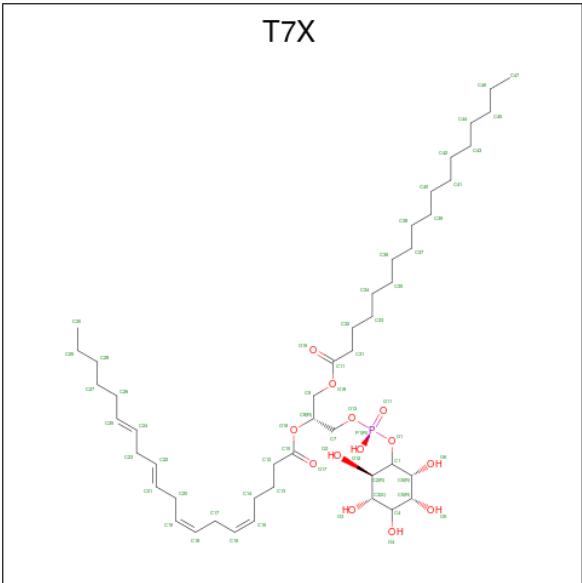
- Molecule 60 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF)

(formula: C₁₈H₃₄NO₁₀P).



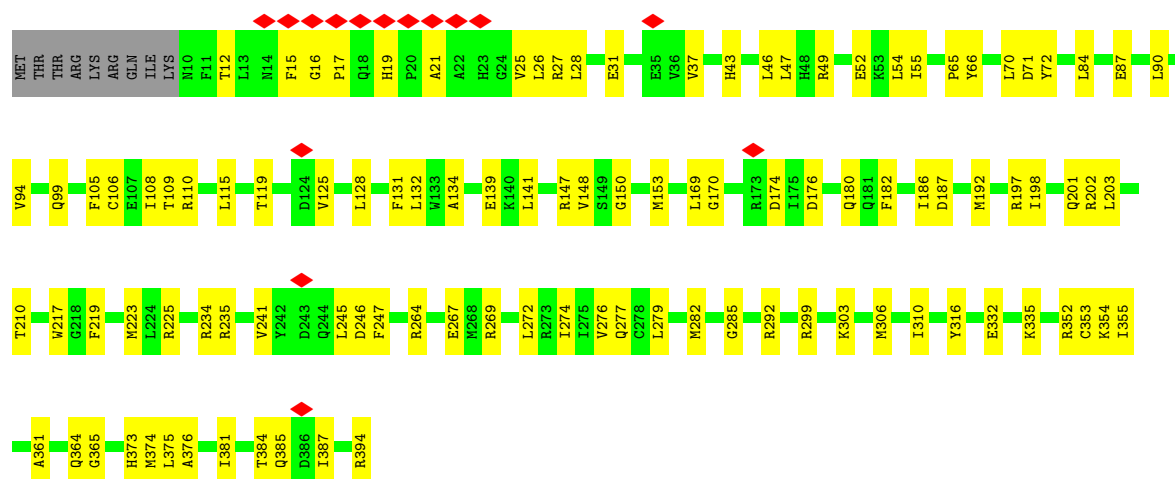
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
60	z	1	30	18	1	10	1	0

- Molecule 61 is Phosphatidylinositol (CCD ID: T7X) (formula: C₄₇H₈₃O₁₃P).



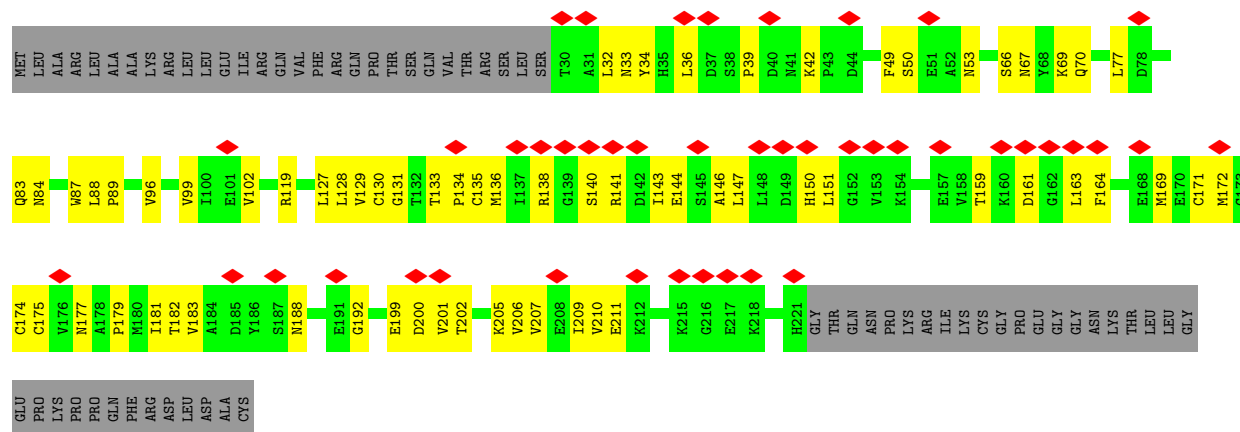
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
61	z	1	61	47	13	1	0

Chain D: 



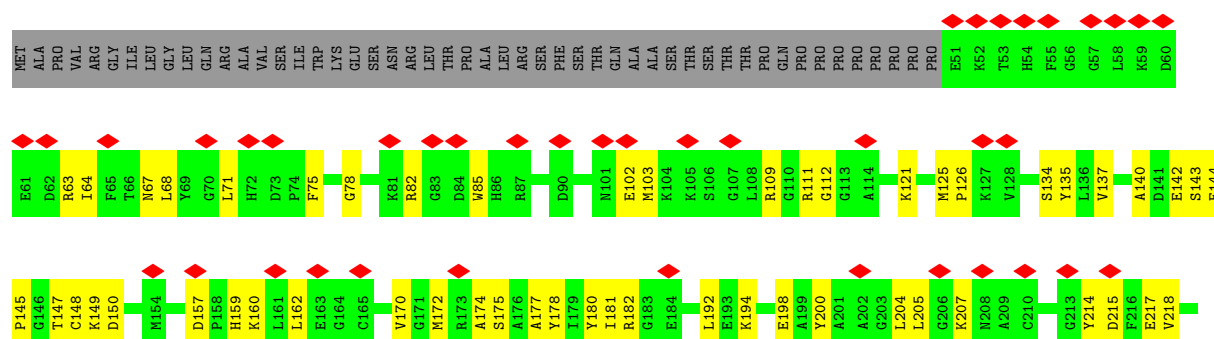
• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

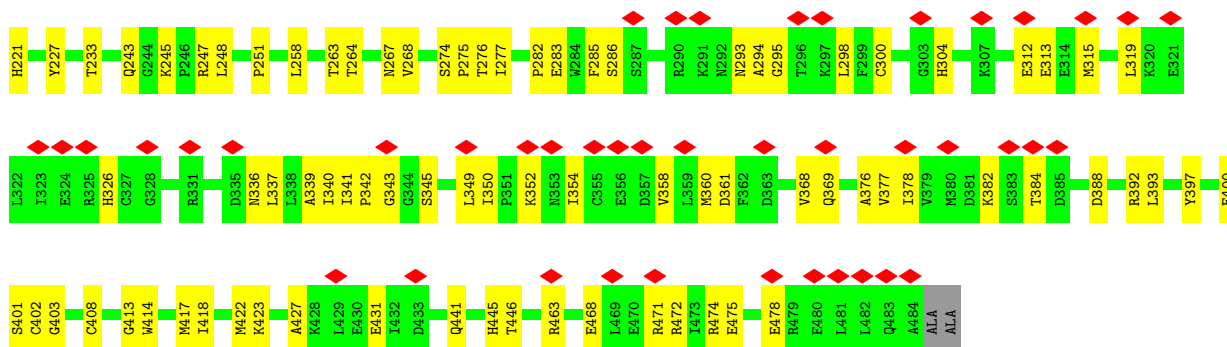
Chain E: 



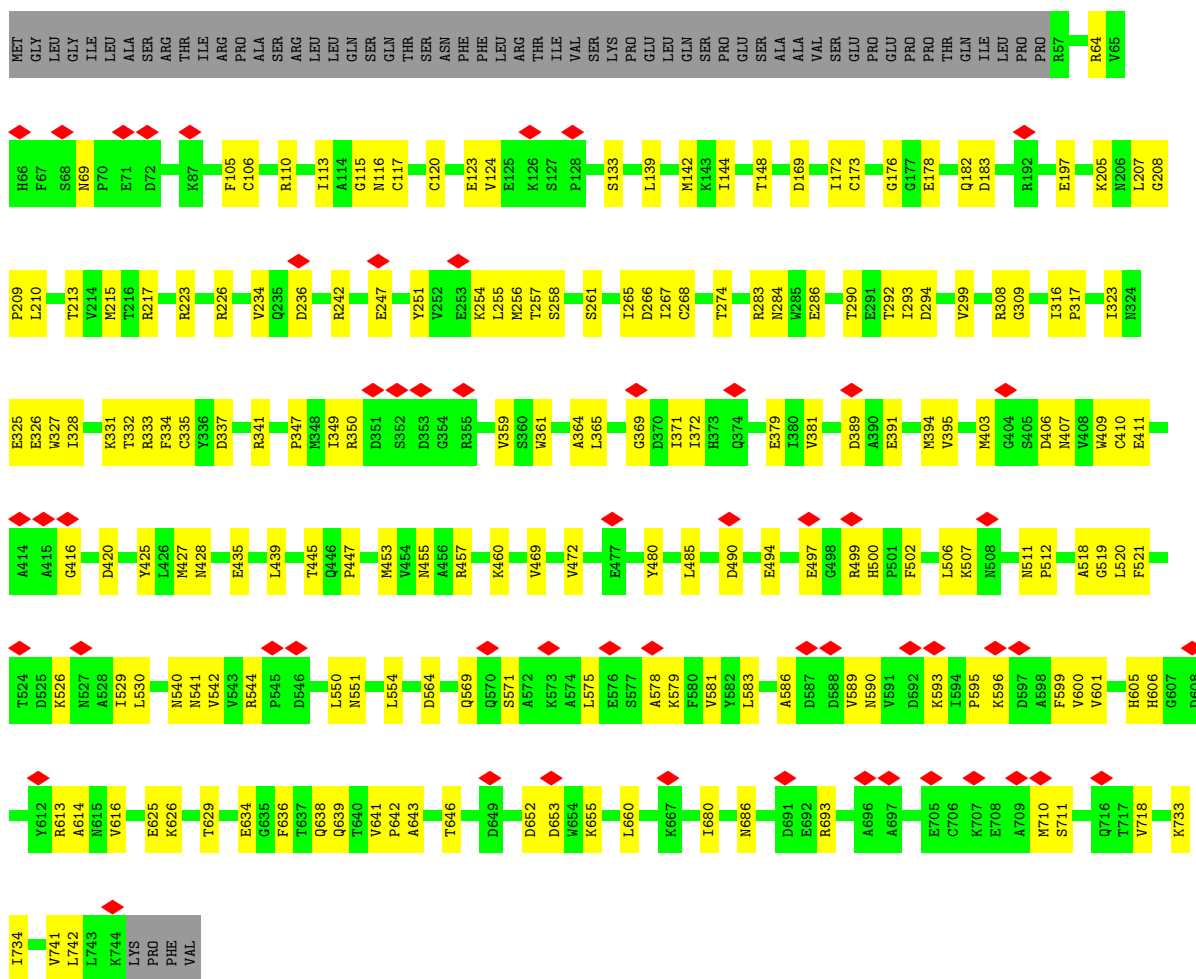
• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 

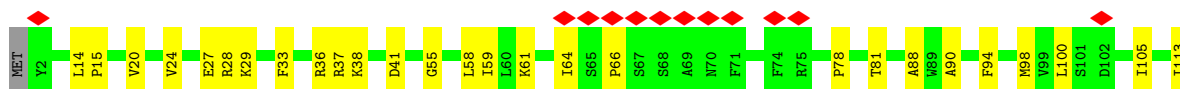
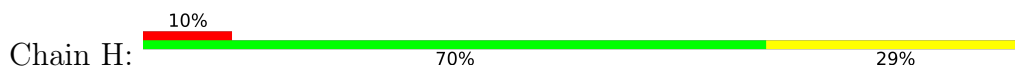


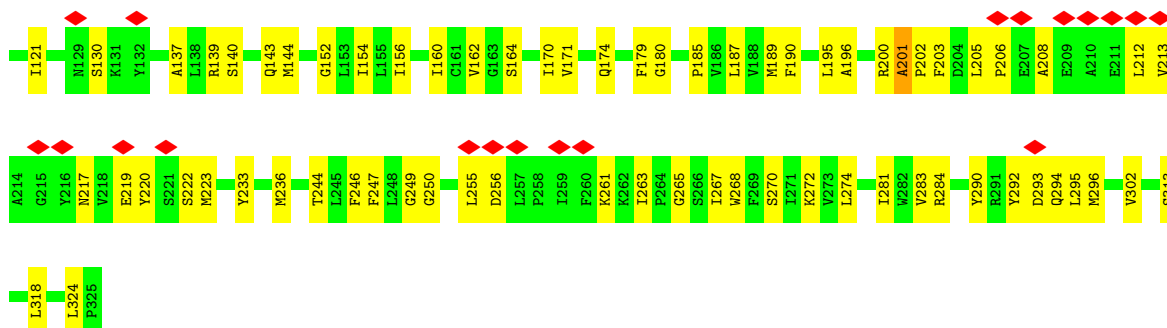


• Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial



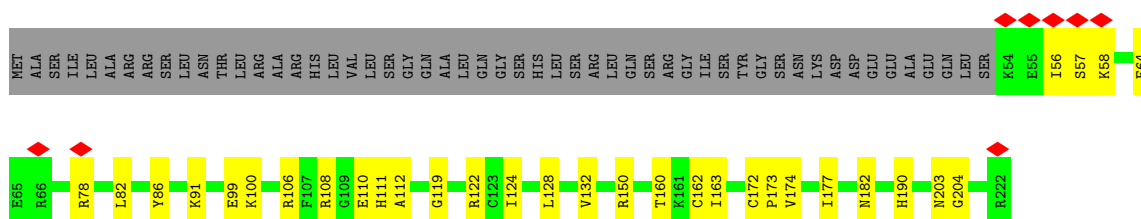
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1





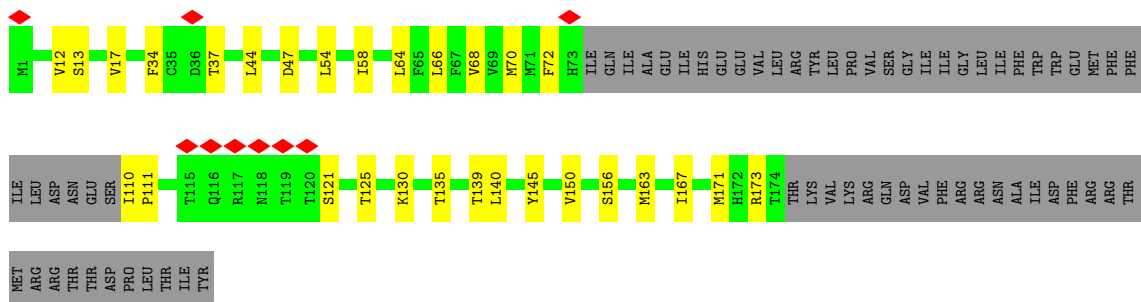
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

Chain I: 62% 14% 24%



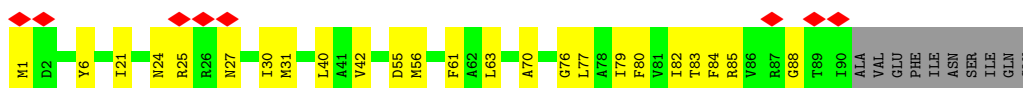
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 53% 14% 33%



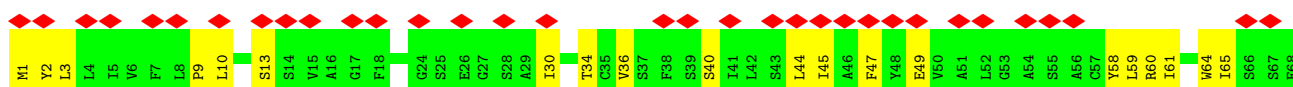
- Molecule 11: NADH dehydrogenase subunit 4L

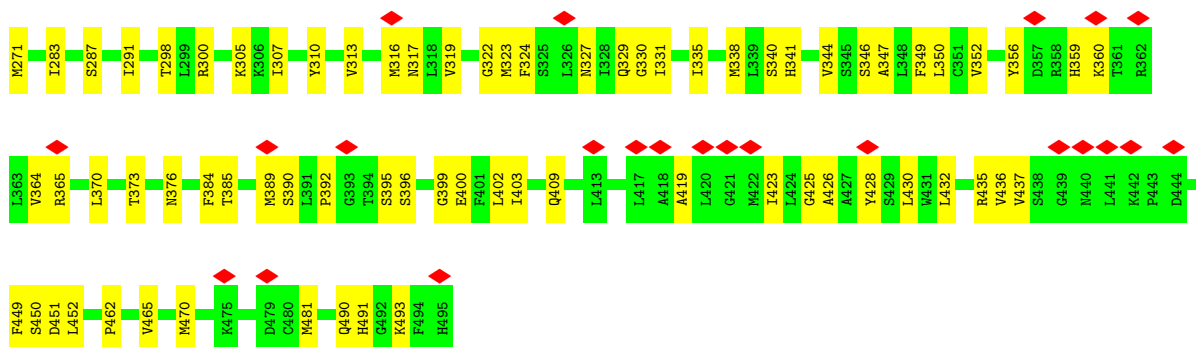
Chain K: 8% 66% 24% 10%



- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

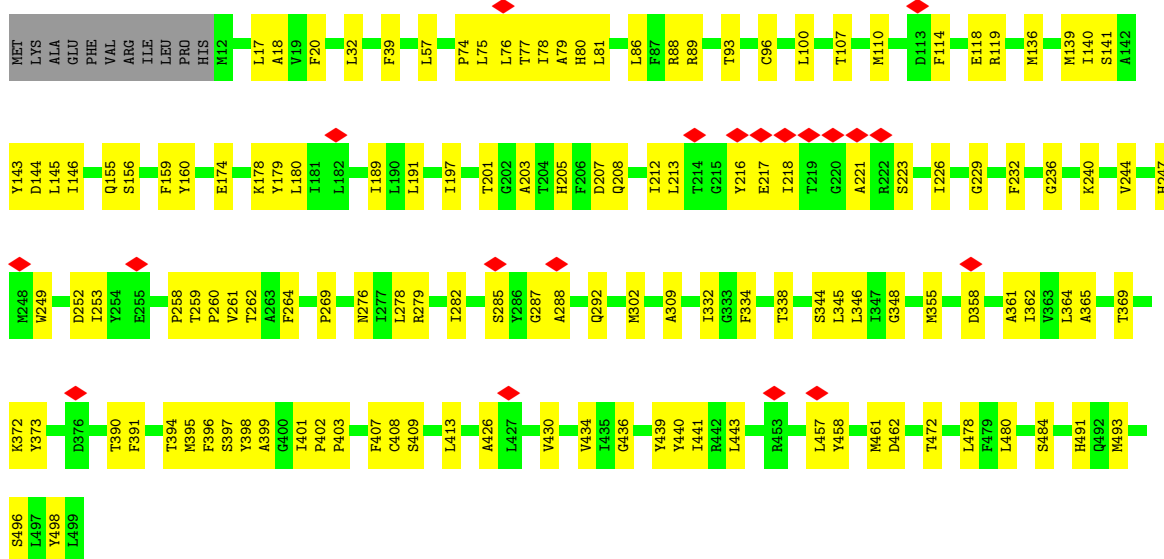
Chain L: 57% 55% 37% 8%





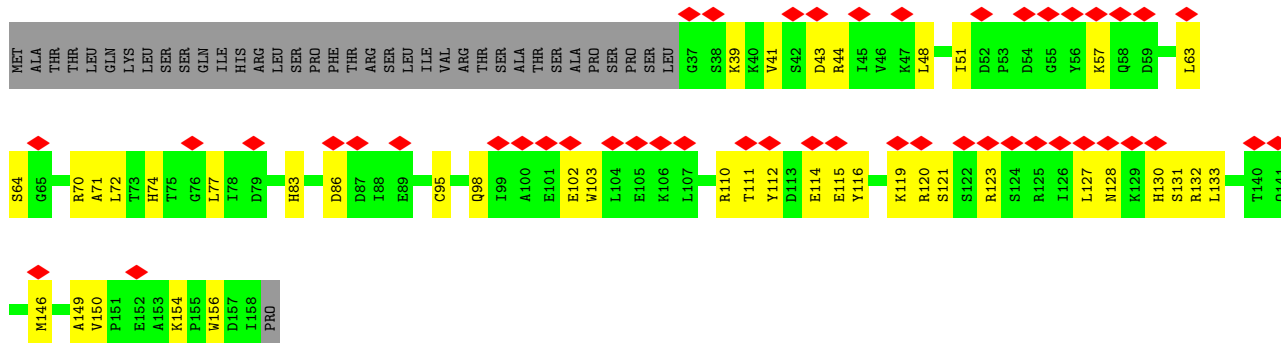
• Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 71% 27% .

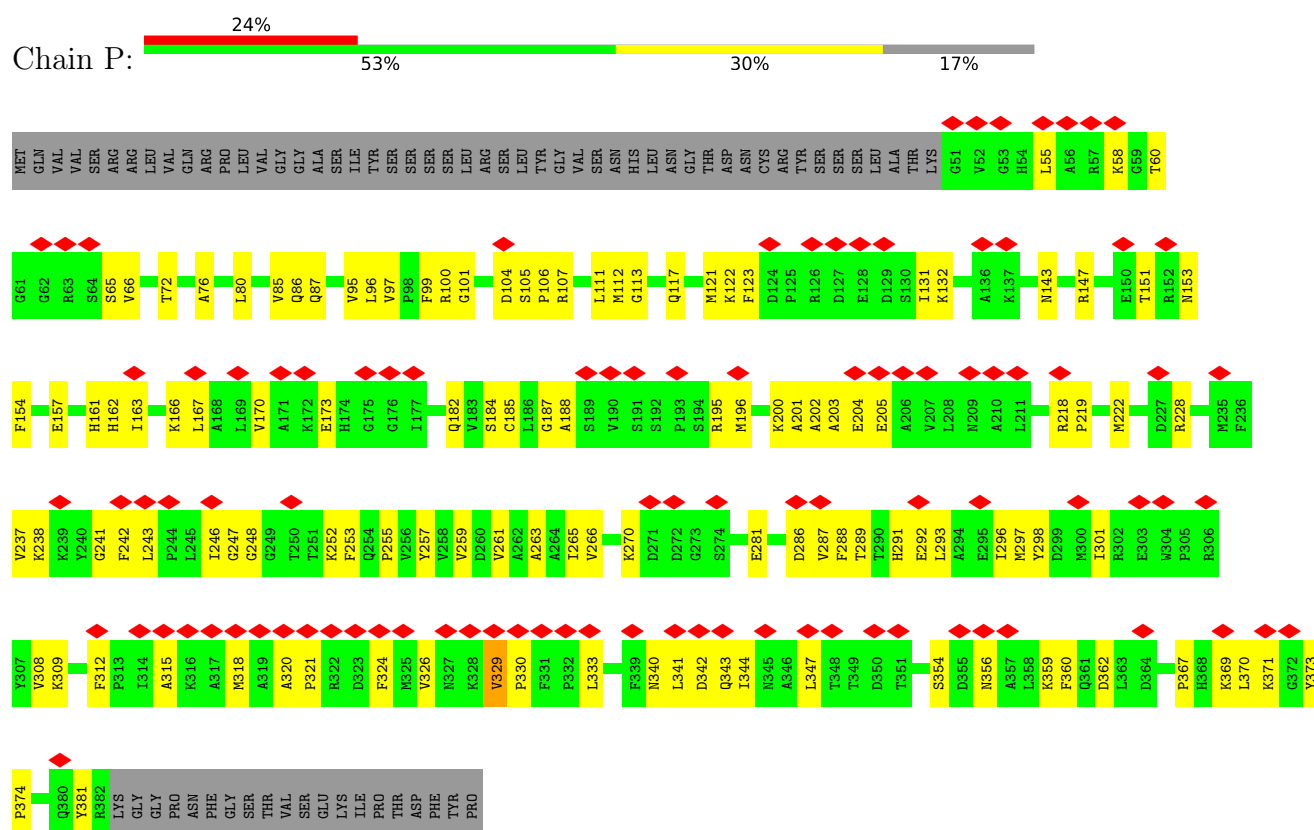


• Molecule 15: AT3G07480.1

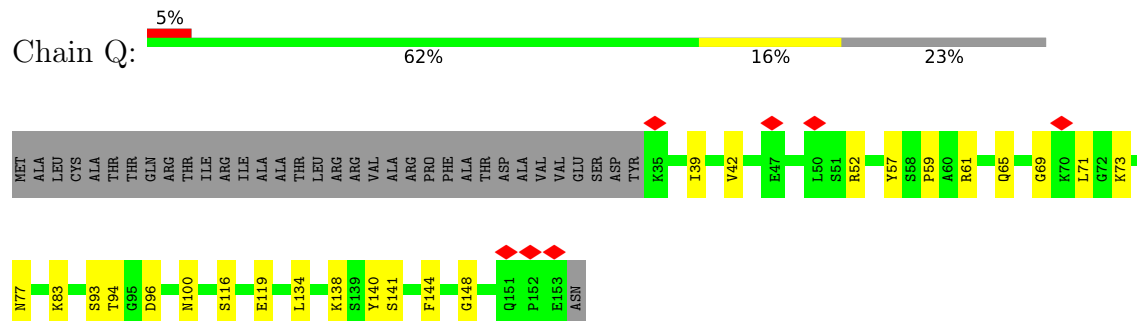
Chain O: 30% 51% 26% 23%



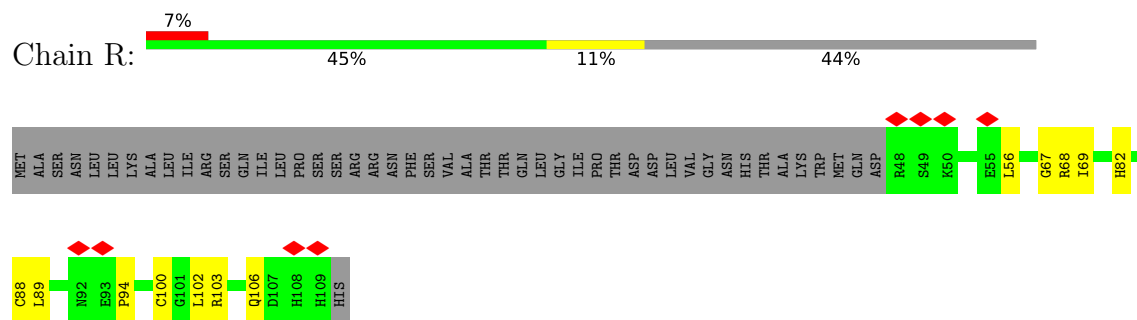
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



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

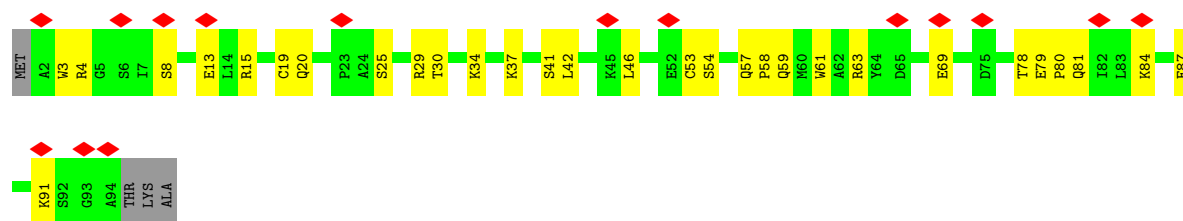


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

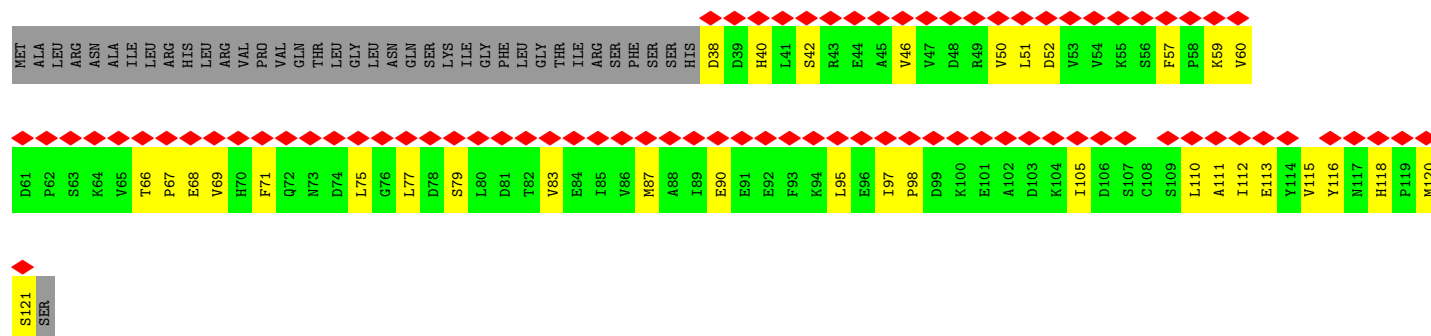


- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

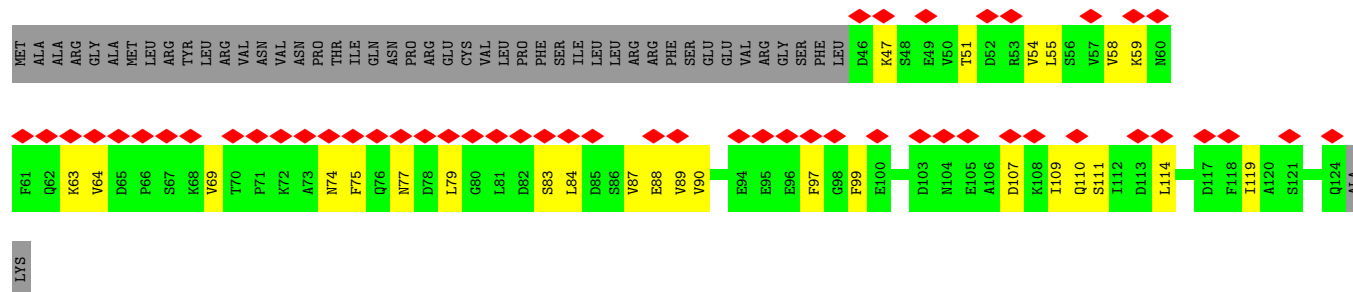




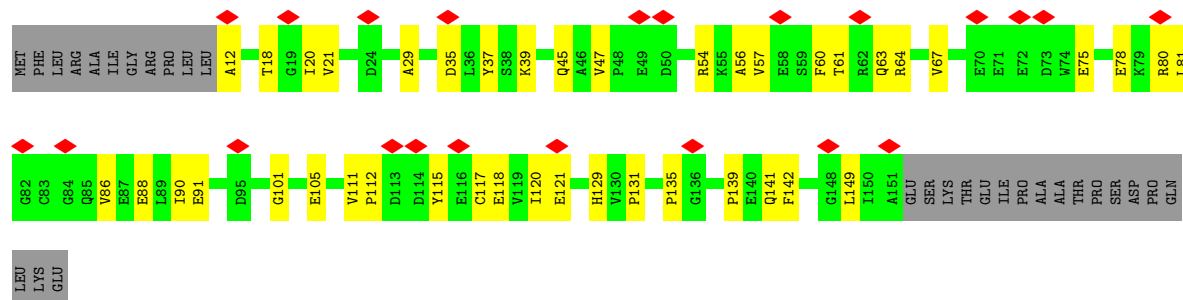
- Molecule 20: Acyl carrier protein 1, mitochondrial



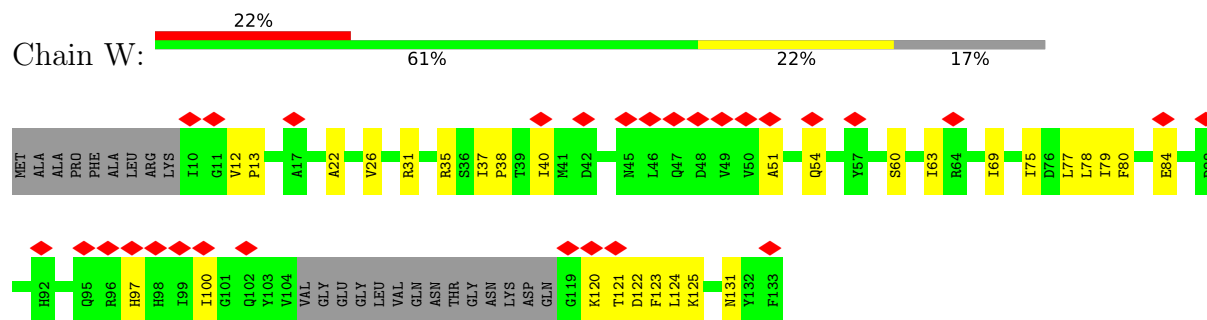
- Molecule 21: Acyl carrier protein 2, mitochondrial



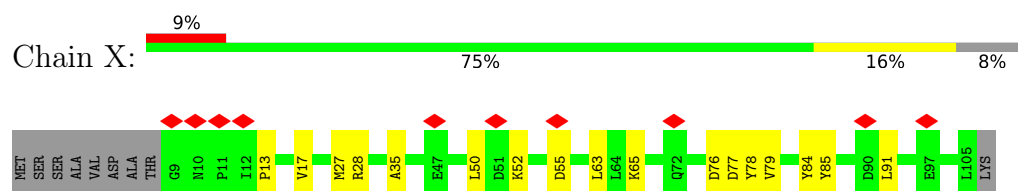
- Molecule 22: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



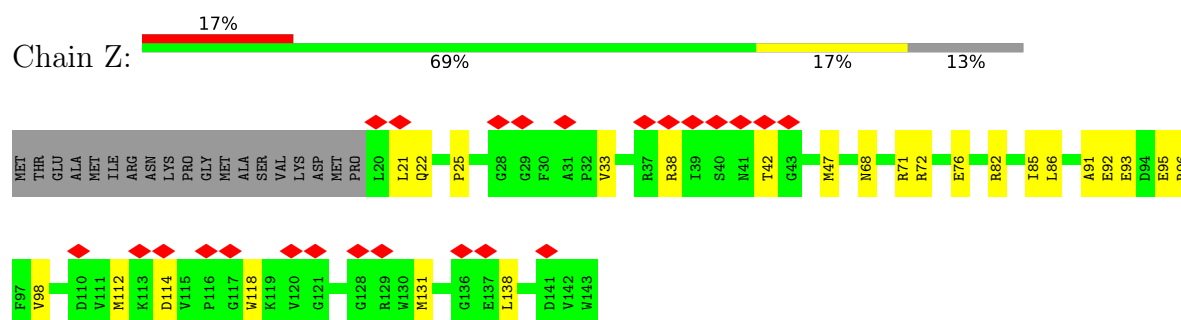
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



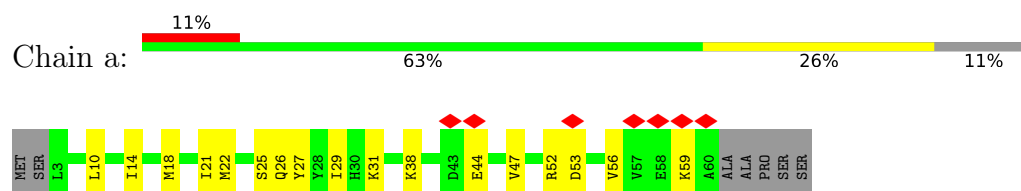
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



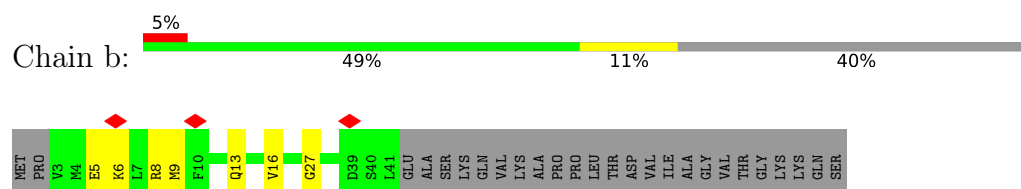
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



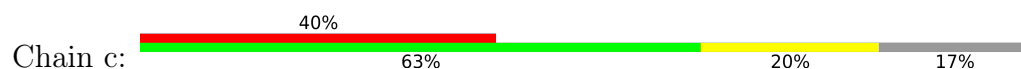
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

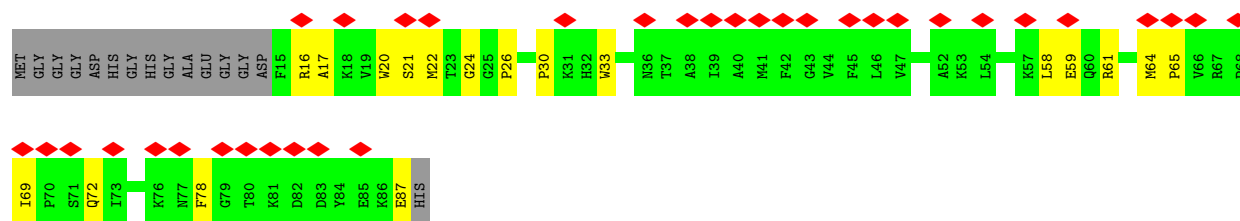


- Molecule 27: At2g46540/F11C10.23



- Molecule 28: Transmembrane protein

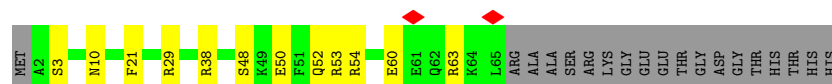




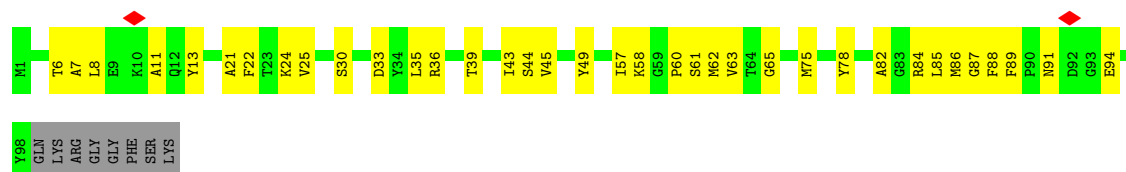
- Molecule 29: Excitatory amino acid transporter



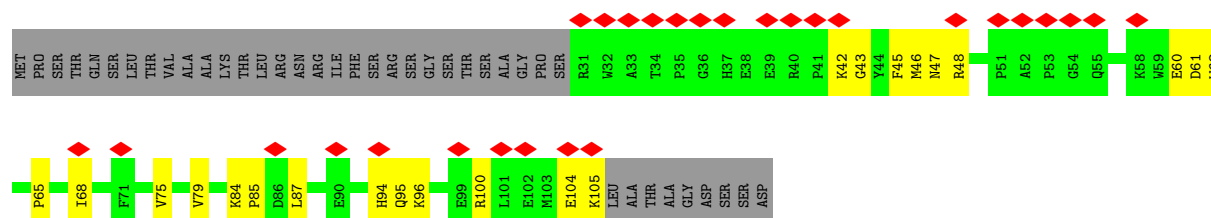
- Molecule 30: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-B



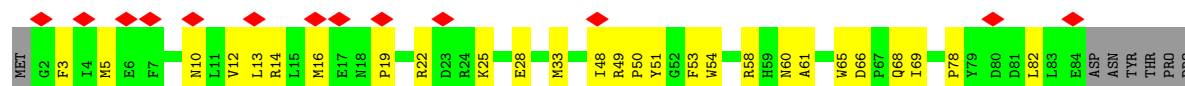
- Molecule 31: At4g16450

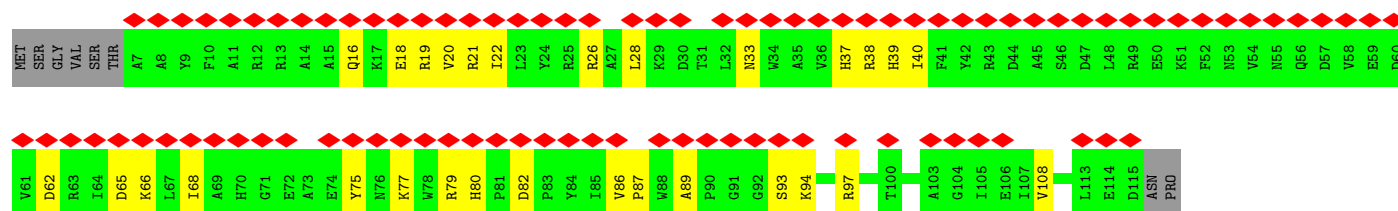


- Molecule 32: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein

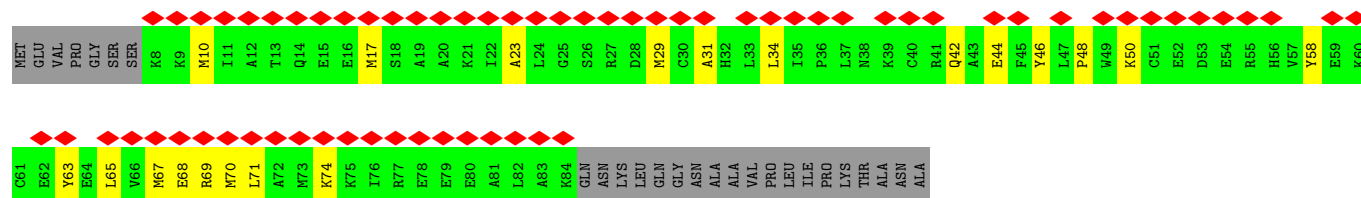


- Molecule 33: P1

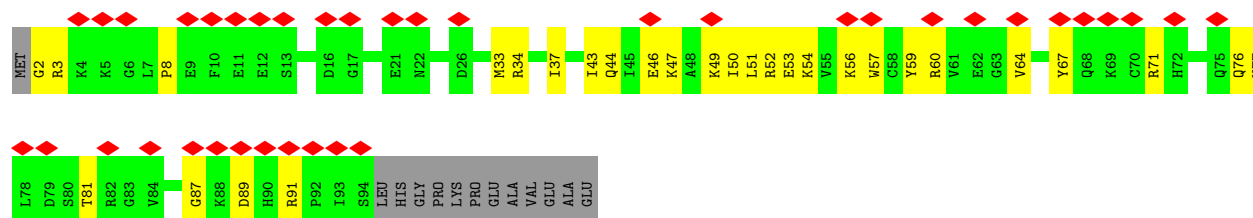




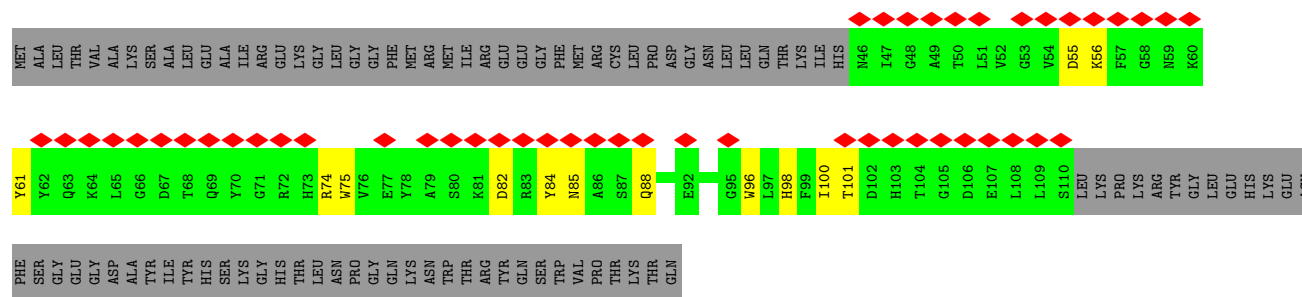
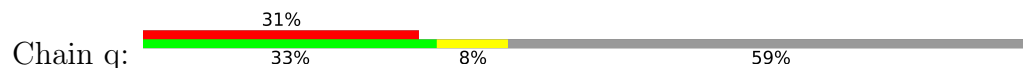
• Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



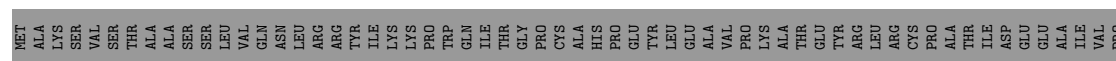
• Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B

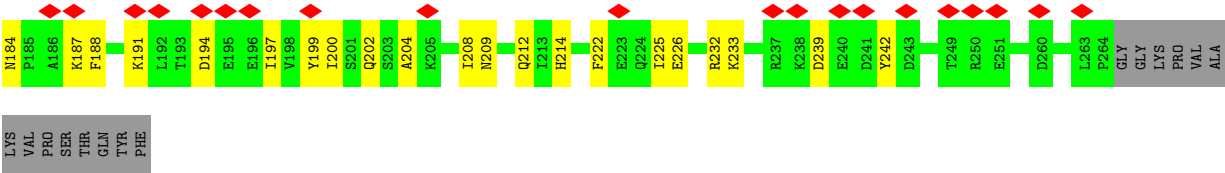


• Molecule 41: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

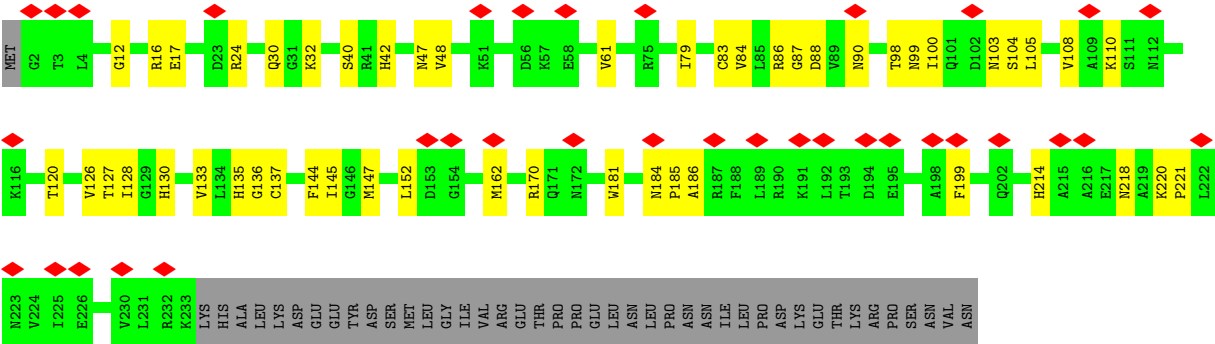


• Molecule 42: Furry





● Molecule 47: Gamma carbonic anhydrase 1, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42096	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 ($e^-/\text{\AA}^2$)	43	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.119	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size (Å)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.837, 0.837, 0.837	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FE, T7X, FES, PTY, PC7, PGT, UQ9, 8Q1, ZN, LMN, PSF, SF4, FMN, NDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/813	0.35	0/1103
2	B	0.18	0/1279	0.35	0/1734
3	C	0.17	0/1629	0.36	0/2207
4	D	0.17	0/3147	0.35	0/4256
5	E	0.14	0/1535	0.39	0/2084
6	F	0.13	0/3441	0.32	0/4641
7	G	0.14	0/5347	0.31	0/7242
8	H	0.18	0/2609	0.39	0/3553
9	I	0.17	0/1410	0.29	0/1904
10	J	0.16	0/1118	0.32	0/1523
11	K	0.16	0/717	0.33	0/969
12	L	0.14	0/4938	0.38	0/6706
13	M	0.15	0/3996	0.33	0/5431
14	N	0.16	0/3924	0.34	0/5327
15	O	0.11	0/971	0.30	0/1314
16	P	0.13	0/2617	0.33	0/3544
17	Q	0.13	0/966	0.26	0/1305
18	R	0.12	0/493	0.26	0/668
19	S	0.11	0/739	0.30	0/996
20	T	0.10	0/679	0.28	0/922
21	U	0.11	0/625	0.29	0/847
22	V	0.13	0/1146	0.32	0/1555
23	W	0.14	0/912	0.39	0/1234
24	X	0.12	0/781	0.30	0/1049
25	Z	0.15	0/1019	0.34	0/1381
26	a	0.14	0/481	0.36	0/646
27	b	0.13	0/292	0.28	0/396
28	c	0.11	0/614	0.31	0/829
29	d	0.16	0/585	0.35	0/788
30	e	0.15	0/559	0.28	0/745
31	f	0.16	0/750	0.34	0/1015
32	g	0.14	0/635	0.38	0/863

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	i	0.14	0/741	0.36	0/997
34	j	0.11	0/433	0.29	0/592
35	k	0.11	0/384	0.32	0/515
36	l	0.11	0/395	0.32	0/538
37	m	0.10	0/584	0.25	0/782
38	n	0.12	0/938	0.32	0/1273
39	o	0.12	0/640	0.35	0/852
40	p	0.12	0/799	0.30	0/1074
41	q	0.11	0/553	0.29	0/750
42	r	1.62	1/89 (1.1%)	3.40	4/118 (3.4%)
44	v	0.12	0/230	0.30	0/311
45	x	0.15	0/1677	0.33	0/2290
46	y	0.12	0/2034	0.31	0/2757
47	z	0.13	0/1795	0.31	0/2430
All	All	0.16	1/62059 (0.0%)	0.36	4/84056 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
42	r	83	PRO	C-N	14.79	1.51	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	r	83	PRO	CA-C-N	-24.16	90.97	123.10
42	r	83	PRO	C-N-CA	-24.16	90.97	123.10
42	r	83	PRO	O-C-N	9.49	138.18	123.00
42	r	83	PRO	CA-N-CD	-8.92	99.51	112.00

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	A	785	0	807	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1244	0	1231	54	0
3	C	1581	0	1529	42	0
4	D	3077	0	3043	98	0
5	E	1500	0	1473	49	0
6	F	3368	0	3353	95	0
7	G	5252	0	5241	129	0
8	H	2536	0	2641	80	0
9	I	1381	0	1328	30	0
10	J	1093	0	1171	31	0
11	K	707	0	771	28	0
12	L	4807	0	4847	193	0
13	M	3887	0	4037	135	0
14	N	3820	0	3926	113	0
15	O	956	0	969	30	0
16	P	2560	0	2601	87	0
17	Q	939	0	928	20	0
18	R	482	0	478	7	0
19	S	727	0	759	20	0
20	T	667	0	648	28	0
21	U	616	0	597	17	0
22	V	1123	0	1112	35	0
23	W	893	0	889	24	0
24	X	767	0	764	13	0
25	Z	990	0	971	23	0
26	a	469	0	472	15	0
27	b	288	0	314	7	0
28	c	595	0	605	14	0
29	d	574	0	593	21	0
30	e	546	0	514	10	0
31	f	734	0	733	30	0
32	g	615	0	604	19	0
33	i	721	0	695	25	0
34	j	415	0	406	9	0
35	k	374	0	369	15	0
36	l	384	0	383	21	0
37	m	569	0	553	11	0
38	n	911	0	879	28	0
39	o	631	0	646	18	0
40	p	778	0	768	28	0
41	q	536	0	495	8	0
42	r	88	0	97	6	0
43	u	150	0	33	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	v	226	0	235	6	0
45	x	1637	0	1647	52	0
46	y	2001	0	2009	61	0
47	z	1763	0	1754	38	0
48	B	8	0	0	0	0
48	F	8	0	0	2	0
48	G	16	0	0	1	0
48	I	16	0	0	0	0
49	E	4	0	0	2	0
49	G	4	0	0	0	0
50	F	31	0	19	3	0
51	H	35	0	40	2	0
52	H	50	0	79	3	0
52	M	50	0	79	0	0
52	N	50	0	79	1	0
53	M	52	0	84	6	0
53	v	52	0	84	4	0
54	N	41	0	52	1	0
55	O	1	0	0	0	0
56	P	48	0	22	4	0
57	R	1	0	0	0	0
57	y	1	0	0	0	0
58	W	35	0	0	2	0
58	n	35	0	0	0	0
59	d	69	0	88	7	0
60	z	30	0	32	0	0
61	z	61	0	0	0	0
All	All	61461	0	61576	1574	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 13.

All (1574) 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)
22:V:67:VAL:HG11	22:V:81:LEU:HD21	1.56	0.87
18:R:82:HIS:CD2	18:R:100:CYS:SG	2.67	0.87
3:C:9:TYR:HH	3:C:48:HIS:HE2	1.26	0.84
15:O:110:ARG:HD3	15:O:115:GLU:HB3	1.58	0.83
36:I:107:PHE:HB2	39:O:69:ARG:HG2	1.63	0.81
3:C:129:LEU:HD12	23:W:12:VAL:HG21	1.61	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:30:THR:OG1	19:S:34:LYS:NZ	2.14	0.80
38:n:87:PRO:HB2	38:n:94:LYS:HG2	1.62	0.79
12:L:331:TYR:HB2	12:L:497:LEU:HD21	1.65	0.79
32:g:94:HIS:HA	40:p:46:GLU:HG2	1.63	0.79
11:K:76:GLY:HA2	14:N:180:LEU:HD21	1.64	0.78
12:L:230:VAL:HG13	12:L:235:GLN:HB2	1.65	0.78
46:y:81:TYR:HH	46:y:214:HIS:HD1	1.29	0.78
28:c:64:MET:HE3	28:c:65:PRO:HD2	1.66	0.78
34:j:13:LYS:HG3	35:k:18:TRP:HB3	1.66	0.78
26:a:18:MET:HA	26:a:21:ILE:HG12	1.66	0.78
45:x:106:LEU:HD22	45:x:127:TRP:HE1	1.48	0.77
12:L:310:VAL:HG21	12:L:437:LEU:HD21	1.65	0.77
46:y:90:ASN:HB2	46:y:108:VAL:HG11	1.67	0.77
8:H:139:ARG:HH12	8:H:213:VAL:HB	1.49	0.77
1:A:77:PHE:O	10:J:145:TYR:OH	2.02	0.76
32:g:95:GLN:HE22	32:g:96:LYS:HE2	1.50	0.76
12:L:13:SER:HB3	12:L:118:SER:HB3	1.67	0.76
22:V:117:CYS:HB3	42:r:89:LEU:HD12	1.69	0.75
12:L:77:LEU:HB2	12:L:131:ASP:HB3	1.68	0.75
21:U:107:ASP:O	21:U:110:GLN:NE2	2.20	0.75
15:O:114:GLU:HG3	15:O:133:LEU:HD13	1.69	0.75
14:N:203:ALA:HB1	14:N:208:GLN:HG3	1.68	0.75
12:L:209:ILE:HG23	37:m:58:MET:HE2	1.69	0.74
13:M:242:VAL:HG23	13:M:305:LYS:HB2	1.69	0.74
16:P:187:GLY:H	16:P:218:ARG:HH21	1.32	0.74
7:G:372:ILE:HG13	7:G:403:MET:HE1	1.69	0.74
17:Q:83:LYS:HG2	17:Q:94:THR:HG22	1.70	0.73
8:H:205:LEU:HB2	8:H:213:VAL:HG11	1.71	0.73
4:D:87:GLU:OE1	22:V:129:HIS:NE2	2.22	0.73
3:C:135:ASP:OD1	3:C:136:TYR:N	2.22	0.73
4:D:299:ARG:NH2	9:I:172:CYS:O	2.23	0.72
7:G:139:LEU:H	7:G:142:MET:HE2	1.54	0.72
13:M:77:TYR:OH	14:N:491:HIS:ND1	2.15	0.72
3:C:61:GLY:O	4:D:352:ARG:NH1	2.23	0.72
5:E:179:PRO:HB2	5:E:201:VAL:HG12	1.71	0.72
13:M:150:LEU:HB3	13:M:174:PHE:HE2	1.55	0.72
31:f:25:VAL:HG12	31:f:85:LEU:HD12	1.70	0.72
13:M:101:ILE:HG13	13:M:127:GLU:HG2	1.70	0.71
20:T:97:ILE:HD12	20:T:98:PRO:HD2	1.72	0.71
12:L:302:ILE:HG13	12:L:303:LEU:HD12	1.71	0.71
8:H:263:ILE:HD12	8:H:267:ILE:HD11	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:187:ASP:OD1	4:D:269:ARG:NH2	2.23	0.71
12:L:262:VAL:HG13	12:L:319:LEU:HD21	1.72	0.71
12:L:548:THR:O	38:n:77:LYS:NZ	2.24	0.71
3:C:173:GLN:OE1	3:C:176:ARG:NH1	2.24	0.71
6:F:258:LEU:HB3	6:F:263:THR:HG21	1.73	0.70
15:O:110:ARG:NH2	15:O:131:SER:O	2.24	0.70
7:G:258:SER:HB3	7:G:261:SER:HB3	1.73	0.70
14:N:213:LEU:HD22	14:N:226:ILE:HD11	1.73	0.70
2:B:166:HIS:O	2:B:166:HIS:ND1	2.24	0.70
20:T:79:SER:O	38:n:21:ARG:NH1	2.24	0.70
15:O:41:VAL:HG22	45:x:191:ARG:HB3	1.72	0.70
7:G:710:MET:HE3	7:G:711:SER:H	1.57	0.70
44:v:79:ASP:O	44:v:83:ASN:ND2	2.24	0.70
45:x:148:TYR:OH	47:z:103:ASN:O	2.10	0.70
4:D:198:ILE:HG12	8:H:290:TYR:HE1	1.57	0.69
8:H:88:ALA:HB2	8:H:113:ILE:HG21	1.73	0.69
14:N:107:THR:HG21	14:N:264:PHE:HB2	1.75	0.69
36:l:105:VAL:HG22	36:l:107:PHE:H	1.56	0.69
3:C:60:CYS:HB2	3:C:74:VAL:HB	1.73	0.69
14:N:355:MET:SD	14:N:397:SER:OG	2.50	0.69
33:i:66:ASP:HA	33:i:69:ILE:HG22	1.73	0.69
40:p:51:LEU:HD11	40:p:76:GLN:HB3	1.75	0.69
12:L:366:ARG:NH1	38:n:82:ASP:O	2.25	0.69
33:i:13:LEU:O	40:p:2:GLY:N	2.26	0.68
9:I:128:LEU:HD12	9:I:173:PRO:HD3	1.75	0.68
5:E:39:PRO:HA	5:E:42:LYS:HE3	1.75	0.68
6:F:248:LEU:HD21	7:G:115:GLY:HA3	1.76	0.68
7:G:341:ARG:HH12	7:G:733:LYS:HB2	1.58	0.68
11:K:21:ILE:HG13	11:K:31:MET:HG3	1.75	0.68
10:J:64:LEU:HG	11:K:77:LEU:HD12	1.74	0.68
12:L:240:THR:HA	12:L:562:ARG:HH22	1.59	0.67
14:N:344:SER:HB2	14:N:413:LEU:HD23	1.77	0.67
16:P:101:GLY:O	16:P:122:LYS:NZ	2.27	0.67
16:P:185:CYS:H	16:P:200:LYS:HD3	1.59	0.67
8:H:143:GLN:NE2	8:H:196:ALA:O	2.27	0.67
3:C:1:MET:HE2	22:V:135:PRO:HB2	1.77	0.67
7:G:350:ARG:NH2	7:G:614:ALA:O	2.28	0.67
14:N:75:LEU:HD22	31:f:88:PHE:HE2	1.59	0.67
7:G:541:ASN:O	7:G:544:ARG:NH1	2.28	0.67
24:X:77:ASP:OD1	24:X:78:TYR:N	2.28	0.67
7:G:445:THR:HG23	7:G:447:PRO:HD3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:56:ILE:HD12	9:I:58:LYS:HE3	1.77	0.67
12:L:178:LEU:O	12:L:182:ILE:HD12	1.94	0.67
16:P:132:LYS:HE3	16:P:170:VAL:HB	1.75	0.67
2:B:100:HIS:NE2	4:D:139:GLU:OE2	2.28	0.67
13:M:396:SER:O	13:M:399:GLY:N	2.28	0.67
14:N:18:ALA:O	14:N:89:ARG:NH1	2.28	0.67
4:D:355:ILE:HB	4:D:394:ARG:HD2	1.75	0.66
40:p:3:ARG:HH22	40:p:8:PRO:HB3	1.60	0.66
13:M:147:GLU:HB2	14:N:402:PRO:HG2	1.77	0.66
28:c:20:TRP:HA	32:g:43:GLY:HA3	1.78	0.66
5:E:50:SER:HB3	5:E:53:ASN:HB2	1.77	0.66
12:L:130:GLY:O	12:L:271:ARG:NH2	2.29	0.66
12:L:218:ILE:HG22	12:L:279:SER:HB3	1.78	0.66
15:O:48:LEU:HD22	15:O:146:MET:HB3	1.78	0.66
12:L:59:LEU:HD21	12:L:76:PHE:HB2	1.77	0.66
13:M:228:VAL:HG23	13:M:316:MET:HB3	1.78	0.66
20:T:60:VAL:HB	20:T:77:LEU:HD11	1.78	0.66
4:D:235:ARG:NH2	4:D:247:PHE:O	2.29	0.66
16:P:72:THR:HG22	16:P:96:LEU:HB2	1.77	0.66
53:M:501:PC7:H132	53:M:501:PC7:H372	1.78	0.66
5:E:138:ARG:NH1	5:E:175:CYS:O	2.29	0.65
5:E:70:GLN:HG3	5:E:102:VAL:HG11	1.78	0.65
12:L:266:VAL:HG21	12:L:322:MET:HE3	1.79	0.65
13:M:125:ILE:HA	13:M:128:PHE:CE1	2.31	0.65
4:D:90:LEU:O	4:D:292:ARG:NH1	2.29	0.65
12:L:521:PRO:HA	12:L:524:PHE:HD1	1.61	0.65
13:M:237:LEU:O	13:M:241:HIS:CB	2.45	0.65
12:L:188:LEU:HD11	12:L:217:ALA:HB1	1.78	0.65
46:y:140:GLU:OE2	46:y:159:LYS:NZ	2.30	0.65
6:F:233:THR:HG21	6:F:247:ARG:HG2	1.79	0.65
12:L:195:SER:HB2	40:p:56:LYS:HG3	1.77	0.65
6:F:181:ILE:HD11	6:F:192:LEU:HD23	1.78	0.65
14:N:355:MET:HB3	14:N:398:TYR:HE1	1.61	0.65
22:V:112:PRO:HG2	22:V:115:TYR:HB2	1.78	0.65
24:X:13:PRO:O	26:a:52:ARG:NH2	2.29	0.65
21:U:84:LEU:O	21:U:88:GLU:HG3	1.97	0.65
47:z:144:PHE:HB3	47:z:162:MET:HG2	1.78	0.65
7:G:294:ASP:OD1	7:G:332:THR:OG1	2.14	0.64
31:f:84:ARG:O	31:f:91:ASN:ND2	2.29	0.64
7:G:634:GLU:OE2	7:G:693:ARG:NH1	2.30	0.64
12:L:197:ILE:O	12:L:201:ALA:HB2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:121:GLU:HB3	42:r:85:ARG:HB2	1.79	0.64
45:x:169:MET:HE2	46:y:165:ALA:HB3	1.80	0.64
13:M:60:ASP:OD2	33:i:22:ARG:NH2	2.30	0.64
19:S:19:CYS:O	19:S:25:SER:OG	2.14	0.64
6:F:121:LYS:NZ	50:F:500:FMN:O3P	2.31	0.64
10:J:66:LEU:O	10:J:70:MET:HG2	1.97	0.64
38:n:62:ASP:O	38:n:66:LYS:NZ	2.30	0.64
47:z:135:HIS:HB3	47:z:152:LEU:HA	1.79	0.64
12:L:60:ARG:H	28:c:58:LEU:HD11	1.62	0.64
14:N:401:ILE:HG22	14:N:403:PRO:HD2	1.80	0.64
2:B:72:VAL:HG12	2:B:76:MET:HE2	1.80	0.64
33:i:19:PRO:HD3	40:p:3:ARG:HG2	1.78	0.64
4:D:119:THR:HG21	4:D:134:ALA:HB3	1.80	0.64
6:F:319:LEU:HD23	6:F:340:ILE:HD13	1.80	0.64
12:L:304:GLN:HB2	12:L:310:VAL:HG12	1.80	0.64
41:q:100:ILE:HG22	41:q:101:THR:HG23	1.80	0.64
14:N:143:TYR:HD1	14:N:279:ARG:HD3	1.63	0.63
6:F:125:MET:SD	6:F:264:THR:OG1	2.55	0.63
6:F:147:THR:HG22	6:F:376:ALA:HB3	1.78	0.63
7:G:349:ILE:HD11	7:G:364:ALA:HA	1.79	0.63
13:M:229:PRO:HB2	13:M:313:VAL:HG13	1.79	0.63
1:A:11:TYR:HD2	8:H:90:ALA:HB2	1.63	0.63
14:N:462:ASP:HB2	52:N:502:PTY:HN12	1.63	0.63
16:P:113:GLY:HA3	16:P:117:GLN:HB2	1.80	0.63
6:F:243:GLN:OE1	6:F:245:LYS:NZ	2.32	0.63
7:G:629:THR:HG22	7:G:639:GLN:HG2	1.80	0.63
14:N:119:ARG:HG3	46:y:239:ASP:HB2	1.81	0.63
45:x:152:ARG:NH1	45:x:170:GLU:OE2	2.32	0.63
12:L:172:ARG:NH2	13:M:390:SER:OG	2.32	0.63
14:N:197:ILE:O	14:N:201:THR:OG1	2.17	0.63
7:G:512:PRO:HG2	7:G:542:VAL:HG12	1.79	0.63
13:M:130:MET:HG2	13:M:259:PHE:HZ	1.64	0.63
14:N:302:MET:SD	14:N:332:ILE:HD11	2.39	0.63
36:l:117:LEU:HG	36:l:120:GLU:HB2	1.81	0.63
4:D:125:VAL:HG13	4:D:202:ARG:HD3	1.80	0.63
4:D:246:ASP:O	4:D:277:GLN:NE2	2.32	0.63
5:E:202:THR:H	5:E:205:LYS:HB2	1.63	0.63
6:F:143:SER:HB2	6:F:227:TYR:HD1	1.64	0.63
14:N:436:GLY:HA2	14:N:439:TYR:CE2	2.34	0.62
19:S:4:ARG:HG2	19:S:42:LEU:HD11	1.80	0.62
4:D:25:VAL:HG13	4:D:46:LEU:HB2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:i:10:ASN:HB3	33:i:14:ARG:NH2	2.15	0.62
29:d:34:GLU:HA	29:d:37:VAL:HG12	1.81	0.62
35:k:19:ARG:HG3	38:n:38:ARG:HH22	1.64	0.62
12:L:373:SER:HB2	35:k:24:LEU:HD13	1.80	0.62
7:G:124:VAL:HG22	7:G:144:ILE:HG22	1.80	0.62
2:B:154:SER:OG	2:B:175:CYS:SG	2.56	0.62
6:F:67:ASN:OD1	6:F:71:LEU:N	2.33	0.62
9:I:78:ARG:HH22	25:Z:42:THR:H	1.48	0.62
13:M:329:GLN:HB2	13:M:402:LEU:HD12	1.82	0.62
7:G:435:GLU:OE1	7:G:460:LYS:NZ	2.29	0.62
20:T:118:HIS:HE1	20:T:120:MET:HB2	1.65	0.62
47:z:86:ARG:NH1	47:z:88:ASP:OD1	2.32	0.62
22:V:57:VAL:HA	22:V:60:PHE:CE1	2.35	0.62
6:F:174:ALA:O	6:F:214:TYR:OH	2.15	0.62
7:G:293:ILE:HD13	7:G:638:GLN:HG3	1.81	0.62
5:E:146:ALA:O	5:E:150:HIS:ND1	2.31	0.61
7:G:626:LYS:NZ	7:G:653:ASP:OD1	2.29	0.61
46:y:168:LEU:HB3	46:y:184:ASN:HA	1.81	0.61
12:L:594:ILE:HG13	13:M:235:ILE:HD11	1.82	0.61
14:N:355:MET:HB3	14:N:398:TYR:CE1	2.35	0.61
15:O:44:ARG:NH2	15:O:64:SER:O	2.34	0.61
46:y:89:VAL:HG11	46:y:110:LYS:HA	1.82	0.61
4:D:225:ARG:NH2	4:D:267:GLU:OE2	2.33	0.61
20:T:66:THR:HB	20:T:69:VAL:HB	1.82	0.61
45:x:161:ILE:HG13	45:x:217:ILE:HG23	1.81	0.61
3:C:4:GLN:HE21	3:C:8:LYS:HE3	1.65	0.61
39:o:71:LEU:HD23	39:o:74:LYS:HD2	1.82	0.61
2:B:164:TYR:HE2	4:D:66:TYR:CD1	2.18	0.61
3:C:24:ARG:NH1	22:V:121:GLU:OE2	2.33	0.61
12:L:120:PHE:HE1	12:L:143:VAL:HG13	1.65	0.61
31:f:33:ASP:OD2	31:f:84:ARG:NH2	2.34	0.61
7:G:317:PRO:HB3	7:G:328:ILE:HB	1.82	0.61
13:M:365:ARG:HD2	37:m:16:TRP:HZ3	1.64	0.61
16:P:289:THR:HG22	16:P:292:GLU:HG2	1.83	0.61
46:y:204:ALA:O	46:y:208:ILE:HG12	2.01	0.61
38:n:75:TYR:OH	38:n:79:ARG:NH1	2.34	0.61
2:B:162:GLY:HA3	2:B:166:HIS:CD2	2.35	0.61
14:N:17:LEU:HB2	14:N:78:ILE:HD11	1.82	0.61
29:d:31:HIS:HB2	29:d:34:GLU:HG2	1.83	0.60
29:d:51:LYS:NZ	59:d:101:LMN:OBZ	2.34	0.60
2:B:164:TYR:CD1	9:I:163:ILE:HD13	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:110:ARG:NH2	4:D:332:GLU:O	2.33	0.60
5:E:67:ASN:ND2	17:Q:148:GLY:O	2.34	0.60
12:L:372:ALA:HB2	12:L:442:PHE:HB3	1.83	0.60
46:y:113:ILE:HG22	46:y:117:VAL:HG22	1.83	0.60
7:G:411:GLU:HG3	7:G:589:VAL:HG13	1.83	0.60
21:U:74:ASN:ND2	21:U:77:ASN:OD1	2.34	0.60
1:A:2:MET:HE1	10:J:47:ASP:HB3	1.81	0.60
1:A:113:ARG:NH2	46:y:242:TYR:OH	2.34	0.60
4:D:376:ALA:H	8:H:212:LEU:HD23	1.66	0.60
6:F:63:ARG:NH1	6:F:312:GLU:O	2.35	0.60
39:o:23:ALA:HA	40:p:64:VAL:HG21	1.82	0.60
47:z:30:GLN:OE1	47:z:32:LYS:NZ	2.33	0.60
7:G:327:TRP:HB2	7:G:453:MET:HE1	1.83	0.60
12:L:302:ILE:HG22	12:L:433:TYR:HB3	1.82	0.60
13:M:237:LEU:O	13:M:241:HIS:HB3	2.01	0.60
28:c:72:GLN:N	28:c:72:GLN:OE1	2.35	0.60
47:z:98:THR:OG1	47:z:126:VAL:O	2.17	0.60
13:M:490:GLN:NE2	13:M:493:LYS:O	2.34	0.60
14:N:288:ALA:HA	14:N:292:GLN:HE22	1.66	0.60
29:d:5:ALA:HB2	59:d:101:LMN:HCJ	1.84	0.60
6:F:337:LEU:HD23	6:F:352:LYS:HG3	1.83	0.60
10:J:110:ILE:HD11	30:e:48:SER:HA	1.81	0.60
12:L:178:LEU:HB2	12:L:228:GLY:HA3	1.83	0.60
16:P:195:ARG:N	16:P:342:ASP:OD1	2.35	0.60
29:d:45:PHE:HD2	59:d:101:LMN:HABA	1.67	0.60
45:x:168:LEU:HD13	45:x:186:LEU:HD21	1.84	0.60
6:F:162:LEU:HD21	6:F:205:LEU:HD11	1.83	0.59
12:L:359:MET:HE2	12:L:368:MET:HG3	1.83	0.59
4:D:27:ARG:HB2	4:D:43:HIS:HB2	1.84	0.59
12:L:311:ILE:HG12	12:L:348:LEU:HD22	1.83	0.59
31:f:44:SER:OG	31:f:65:GLY:O	2.19	0.59
12:L:566:ASP:O	12:L:570:ASN:ND2	2.34	0.59
45:x:203:ALA:O	45:x:204:ARG:NH1	2.35	0.59
16:P:237:VAL:HA	16:P:241:GLY:HA2	1.84	0.59
20:T:105:ILE:HG23	20:T:110:LEU:HB2	1.82	0.59
22:V:18:THR:HG23	22:V:20:ILE:H	1.67	0.59
13:M:78:GLU:OE2	59:d:101:LMN:OAS	2.16	0.59
4:D:150:GLY:HA3	9:I:108:ARG:HG3	1.85	0.59
4:D:306:MET:HE3	4:D:310:ILE:HG13	1.84	0.59
8:H:256:ASP:HA	8:H:261:LYS:HD2	1.84	0.59
29:d:49:LEU:HD23	59:d:101:LMN:HBD	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:78:THR:H	19:S:81:GLN:HB2	1.68	0.59
21:U:90:VAL:HG22	21:U:109:ILE:HD11	1.85	0.59
6:F:137:VAL:HG12	6:F:178:TYR:HB2	1.85	0.59
5:E:159:THR:OG1	5:E:161:ASP:O	2.19	0.59
21:U:111:SER:HB2	21:U:114:LEU:HD13	1.84	0.59
22:V:47:VAL:HG23	22:V:54:ARG:HD2	1.85	0.59
5:E:77:LEU:HD22	5:E:88:LEU:HD21	1.85	0.59
8:H:265:GLY:HA2	8:H:268:TRP:HD1	1.68	0.59
2:B:120:ARG:HG3	8:H:219:GLU:HA	1.85	0.58
8:H:130:SER:OG	8:H:219:GLU:OE1	2.21	0.58
12:L:414:ILE:HD11	36:l:97:VAL:HA	1.84	0.58
16:P:147:ARG:HD3	56:P:500:NDP:H3B	1.85	0.58
4:D:84:LEU:HD13	22:V:131:PRO:HD3	1.85	0.58
12:L:303:LEU:HD22	12:L:559:PHE:HB2	1.84	0.58
14:N:78:ILE:HG22	31:f:7:ALA:HB2	1.84	0.58
14:N:93:THR:OG1	14:N:279:ARG:NH2	2.36	0.58
4:D:245:LEU:HD13	4:D:274:ILE:HG23	1.84	0.58
7:G:105:PHE:O	7:G:223:ARG:NH2	2.34	0.58
7:G:416:GLY:H	7:G:526:LYS:HZ1	1.51	0.58
12:L:541:GLN:HA	38:n:40:ILE:HD12	1.84	0.58
14:N:346:LEU:HD13	14:N:493:MET:HE2	1.84	0.58
19:S:15:ARG:NH2	19:S:69:GLU:OE2	2.33	0.58
23:W:31:ARG:O	23:W:35:ARG:HG2	2.03	0.58
5:E:49:PHE:O	5:E:83:GLN:NE2	2.37	0.58
12:L:64:TRP:N	12:L:72:ALA:O	2.36	0.58
45:x:124:HIS:HB3	45:x:152:ARG:HG3	1.86	0.58
47:z:170:ARG:HB2	47:z:170:ARG:NH1	2.18	0.58
7:G:581:VAL:HG23	7:G:600:VAL:HG23	1.85	0.58
12:L:558:PHE:CE1	36:l:81:TRP:HB3	2.39	0.58
13:M:142:PHE:O	13:M:146:PHE:HB2	2.04	0.58
14:N:390:THR:OG1	29:d:19:TYR:OH	2.21	0.58
45:x:187:PRO:HG2	45:x:190:ARG:HD3	1.84	0.58
1:A:99:PHE:HD2	10:J:156:SER:HB2	1.69	0.58
2:B:189:PRO:HG3	4:D:153:MET:HE2	1.84	0.58
4:D:52:GLU:OE1	4:D:352:ARG:NH2	2.36	0.58
6:F:427:ALA:HB1	6:F:431:GLU:HG3	1.85	0.58
11:K:42:VAL:HG21	14:N:191:LEU:HD23	1.84	0.58
12:L:65:ILE:H	12:L:72:ALA:HB3	1.67	0.58
12:L:292:MET:HE2	36:l:89:PHE:HB3	1.85	0.58
13:M:287:SER:O	13:M:291:ILE:HG13	2.04	0.58
12:L:79:ASP:OD1	12:L:80:SER:N	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:178:GLU:HB3	7:G:284:ASN:HD22	1.67	0.58
7:G:427:MET:HA	7:G:551:ASN:HB2	1.86	0.58
12:L:343:PHE:HB3	12:L:474:SER:HB3	1.86	0.58
12:L:430:THR:HA	12:L:433:TYR:CE1	2.38	0.58
13:M:364:VAL:HG11	13:M:435:ARG:HE	1.69	0.57
3:C:163:ARG:HH11	23:W:97:HIS:HB2	1.68	0.57
6:F:200:TYR:OH	6:F:217:GLU:OE1	2.21	0.57
7:G:365:LEU:HD11	7:G:660:LEU:HA	1.84	0.57
13:M:77:TYR:HH	14:N:491:HIS:HD1	1.49	0.57
12:L:193:ASP:HB3	12:L:196:THR:HG22	1.86	0.57
16:P:60:THR:O	16:P:65:SER:OG	2.14	0.57
46:y:164:ALA:O	46:y:167:SER:OG	2.18	0.57
3:C:23:GLU:HG2	22:V:120:ILE:HB	1.87	0.57
5:E:181:ILE:HG12	5:E:201:VAL:HG11	1.87	0.57
13:M:10:PHE:HD2	13:M:54:VAL:HG11	1.69	0.57
17:Q:52:ARG:NH1	17:Q:96:ASP:OD1	2.37	0.57
4:D:16:GLY:HA2	4:D:26:LEU:O	2.05	0.57
16:P:261:VAL:O	16:P:265:ILE:HD12	2.04	0.57
24:X:76:ASP:OD1	24:X:77:ASP:N	2.37	0.57
12:L:268:MET:HE3	12:L:268:MET:O	2.04	0.57
14:N:18:ALA:HA	14:N:76:LEU:HA	1.87	0.57
14:N:212:ILE:HG22	30:e:21:PHE:HE2	1.69	0.57
40:p:49:LYS:HG2	40:p:52:ARG:HH12	1.69	0.57
7:G:600:VAL:HG13	7:G:614:ALA:HA	1.85	0.57
12:L:72:ALA:HB1	12:L:134:LEU:HD11	1.86	0.57
45:x:167:ILE:HB	45:x:185:VAL:HG13	1.87	0.57
12:L:278:TYR:OH	40:p:67:TYR:OH	2.23	0.57
4:D:54:LEU:HB3	4:D:66:TYR:OH	2.05	0.57
15:O:98:GLN:HB2	15:O:149:ALA:HB3	1.87	0.57
7:G:178:GLU:HB3	7:G:284:ASN:ND2	2.19	0.56
16:P:151:THR:HG23	16:P:154:PHE:H	1.70	0.56
16:P:163:ILE:O	16:P:167:LEU:HG	2.05	0.56
47:z:214:HIS:O	47:z:218:ASN:N	2.32	0.56
1:A:114:GLY:HA3	10:J:173:ARG:HE	1.70	0.56
13:M:83:TYR:HE2	13:M:201:GLN:HE22	1.53	0.56
15:O:111:THR:HG23	15:O:112:TYR:H	1.69	0.56
46:y:68:ILE:HD11	46:y:86:ARG:HG3	1.87	0.56
10:J:34:PHE:HA	10:J:37:THR:HG22	1.87	0.56
12:L:45:ILE:O	12:L:49:GLU:HG2	2.06	0.56
14:N:88:ARG:NH2	14:N:207:ASP:OD2	2.38	0.56
20:T:87:MET:HG3	38:n:28:LEU:HD23	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:71:ASP:OD1	4:D:335:LYS:NZ	2.38	0.56
8:H:64:ILE:HG23	8:H:66:PRO:HD3	1.88	0.56
7:G:371:ILE:HG21	7:G:599:PHE:CE1	2.40	0.56
8:H:174:GLN:NE2	8:H:246:PHE:O	2.39	0.56
10:J:68:VAL:HG21	11:K:77:LEU:HD13	1.88	0.56
12:L:346:ALA:O	12:L:350:LEU:HG	2.06	0.56
12:L:410:THR:HG21	12:L:509:SER:HA	1.88	0.56
3:C:175:PHE:HD2	17:Q:100:ASN:HD21	1.51	0.56
13:M:149:VAL:HG21	13:M:259:PHE:HE2	1.70	0.56
47:z:130:HIS:HB2	47:z:147:MET:HG3	1.88	0.56
25:Z:112:MET:HE1	25:Z:118:TRP:H	1.71	0.56
28:c:58:LEU:HG	28:c:59:GLU:H	1.71	0.56
8:H:29:LYS:NZ	8:H:41:ASP:OD1	2.39	0.56
3:C:72:GLU:OE2	3:C:89:GLN:NE2	2.39	0.56
6:F:251:PRO:HB3	17:Q:141:SER:HB3	1.88	0.56
16:P:340:ASN:HB3	16:P:343:GLN:HB2	1.87	0.56
7:G:292:THR:HG22	7:G:641:VAL:HB	1.88	0.55
8:H:296:MET:HE3	8:H:296:MET:HA	1.88	0.55
12:L:256:ILE:HG23	12:L:257:HIS:CD2	2.41	0.55
13:M:26:LEU:HD11	13:M:40:ILE:HG23	1.87	0.55
14:N:189:ILE:HG23	14:N:232:PHE:HD2	1.70	0.55
16:P:289:THR:HG23	16:P:291:HIS:H	1.70	0.55
2:B:149:PRO:O	16:P:107:ARG:NH2	2.39	0.55
3:C:99:SER:HA	3:C:124:ILE:HG12	1.87	0.55
6:F:423:LYS:O	6:F:472:ARG:NH1	2.40	0.55
8:H:24:VAL:HG12	8:H:28:ARG:HE	1.71	0.55
16:P:257:TYR:CD2	16:P:259:VAL:HG22	2.41	0.55
4:D:27:ARG:HG2	4:D:46:LEU:HD11	1.88	0.55
5:E:143:ILE:O	5:E:147:LEU:HD12	2.06	0.55
9:I:172:CYS:SG	9:I:177:ILE:HG22	2.46	0.55
34:j:42:ARG:NH1	34:j:46:ASP:OD2	2.39	0.55
39:o:10:MET:H	39:o:29:MET:HE3	1.70	0.55
45:x:87:GLN:HG3	45:x:108:LYS:HA	1.89	0.55
1:A:62:TYR:CZ	1:A:66:ILE:HD11	2.41	0.55
14:N:159:PHE:CE2	14:N:269:PRO:HG3	2.42	0.55
20:T:38:ASP:OD1	20:T:40:HIS:NE2	2.39	0.55
25:Z:68:ASN:OD1	25:Z:71:ARG:NH1	2.39	0.55
2:B:180:PRO:HD3	16:P:111:LEU:HD11	1.88	0.55
7:G:207:LEU:HD12	7:G:256:MET:HG3	1.87	0.55
29:d:27:PRO:HG2	29:d:30:ARG:HD3	1.89	0.55
37:m:16:TRP:HE1	37:m:20:ARG:HE	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:219:PHE:HZ	4:D:365:GLY:HA3	1.72	0.55
5:E:84:ASN:ND2	5:E:87:TRP:O	2.38	0.55
20:T:71:PHE:HB2	20:T:77:LEU:HB2	1.89	0.55
26:a:18:MET:HG3	26:a:21:ILE:HD11	1.89	0.55
36:l:124:GLU:CD	36:l:125:PRO:HD2	2.31	0.55
46:y:48:VAL:HG23	46:y:49:PHE:H	1.72	0.55
1:A:23:LEU:HA	8:H:223:MET:HG2	1.89	0.55
8:H:55:GLY:O	8:H:59:ILE:HG12	2.07	0.55
29:d:21:ASN:ND2	29:d:28:TYR:O	2.40	0.55
5:E:49:PHE:HE2	5:E:99:VAL:HG21	1.72	0.55
12:L:332:SER:HB2	12:L:486:ILE:HG22	1.89	0.55
23:W:75:ILE:O	23:W:79:ILE:HG12	2.07	0.55
4:D:210:THR:HA	22:V:21:VAL:HG13	1.89	0.55
14:N:110:MET:HG2	14:N:364:LEU:HD12	1.88	0.55
14:N:457:LEU:HD21	45:x:113:PHE:HB2	1.88	0.55
44:v:76:VAL:HG12	44:v:78:GLU:H	1.70	0.55
4:D:55:ILE:HG12	4:D:66:TYR:HD2	1.72	0.55
7:G:169:ASP:OD1	7:G:217:ARG:NH2	2.37	0.54
12:L:392:PHE:HB3	12:L:395:LEU:HD13	1.88	0.54
14:N:396:PHE:HE1	14:N:441:ILE:HG22	1.72	0.54
16:P:257:TYR:HB2	16:P:370:LEU:HD21	1.90	0.54
40:p:89:ASP:O	40:p:91:ARG:NH1	2.39	0.54
1:A:69:LEU:HD11	11:K:70:ALA:HB1	1.90	0.54
2:B:160:ASN:HB2	2:B:184:TYR:HD1	1.72	0.54
7:G:439:LEU:HD22	7:G:506:LEU:HD13	1.88	0.54
12:L:3:LEU:HD11	12:L:61:ILE:HD11	1.88	0.54
16:P:293:LEU:HA	16:P:296:ILE:HG22	1.88	0.54
22:V:56:ALA:HB2	22:V:149:LEU:HD21	1.89	0.54
24:X:50:LEU:HD11	25:Z:98:VAL:HG21	1.89	0.54
28:c:17:ALA:HA	32:g:42:LYS:HB2	1.89	0.54
12:L:520:ILE:HG23	12:L:524:PHE:HE1	1.72	0.54
16:P:329:VAL:HB	16:P:330:PRO:HD3	1.89	0.54
2:B:164:TYR:CD1	9:I:163:ILE:HG21	2.43	0.54
5:E:34:TYR:CD2	5:E:36:LEU:HD13	2.42	0.54
7:G:741:VAL:HG23	7:G:742:LEU:HD12	1.88	0.54
29:d:17:GLN:HG2	29:d:35:HIS:HA	1.89	0.54
46:y:188:PHE:HZ	46:y:191:LYS:HD3	1.72	0.54
4:D:25:VAL:HG11	4:D:47:LEU:HB2	1.89	0.54
5:E:177:ASN:HD21	5:E:200:ASP:CG	2.15	0.54
7:G:110:ARG:HD2	7:G:325:GLU:OE2	2.08	0.54
7:G:425:TYR:OH	7:G:564:ASP:OD1	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:51:ALA:H	23:W:54:GLN:HE22	1.55	0.54
12:L:316:CYS:HA	12:L:319:LEU:HD12	1.89	0.54
13:M:37:ILE:HD13	13:M:117:LYS:HB3	1.90	0.54
46:y:30:GLN:HG3	47:z:12:GLY:HA3	1.89	0.54
46:y:90:ASN:HB3	46:y:119:PRO:HB3	1.89	0.54
6:F:342:PRO:HG3	6:F:350:ILE:HD12	1.88	0.54
14:N:408:CYS:HB2	14:N:480:LEU:HD21	1.89	0.54
20:T:57:PHE:HB3	20:T:60:VAL:HG12	1.90	0.54
1:A:2:MET:HE3	1:A:2:MET:HA	1.89	0.54
1:A:11:TYR:CD2	8:H:90:ALA:HB2	2.41	0.54
4:D:115:LEU:O	4:D:119:THR:HG23	2.08	0.54
14:N:174:GLU:OE2	14:N:178:LYS:HD2	2.08	0.54
47:z:220:LYS:HE3	47:z:221:PRO:HD2	1.89	0.54
2:B:218:LYS:HG3	16:P:100:ARG:HH12	1.73	0.54
13:M:90:SER:HB2	13:M:134:PHE:HB3	1.88	0.54
13:M:436:VAL:HG12	13:M:437:VAL:HG13	1.89	0.54
44:v:87:VAL:HA	44:v:90:VAL:HG22	1.90	0.54
3:C:160:PRO:HD3	16:P:86:GLN:HG3	1.89	0.54
6:F:75:PHE:O	6:F:159:HIS:NE2	2.41	0.54
46:y:111:THR:HA	46:y:117:VAL:HB	1.88	0.54
7:G:266:ASP:OD2	7:G:333:ARG:NH2	2.26	0.53
7:G:472:VAL:HG22	7:G:485:LEU:HB2	1.89	0.53
7:G:494:GLU:HG2	7:G:500:HIS:HD2	1.73	0.53
8:H:255:LEU:HD23	8:H:261:LYS:HE3	1.89	0.53
16:P:248:GLY:HA2	16:P:309:LYS:HG3	1.90	0.53
45:x:102:LEU:HD23	45:x:123:VAL:HB	1.89	0.53
4:D:119:THR:HB	4:D:131:PHE:HA	1.90	0.53
7:G:686:ASN:ND2	19:S:53:CYS:SG	2.82	0.53
8:H:33:PHE:O	9:I:91:LYS:NZ	2.41	0.53
9:I:110:GLU:OE2	9:I:203:ASN:ND2	2.41	0.53
13:M:74:TRP:HZ2	14:N:480:LEU:HD22	1.73	0.53
16:P:161:HIS:HA	16:P:203:ALA:HB2	1.90	0.53
12:L:501:PRO:HB3	36:l:112:TYR:CE2	2.43	0.53
1:A:88:ILE:HD12	1:A:92:GLY:HA3	1.91	0.53
4:D:276:VAL:HG21	25:Z:33:VAL:HG21	1.89	0.53
7:G:519:GLY:HA3	7:G:718:VAL:HG11	1.90	0.53
9:I:111:HIS:NE2	9:I:162:CYS:SG	2.79	0.53
10:J:13:SER:O	10:J:17:VAL:HG23	2.09	0.53
16:P:170:VAL:HA	16:P:173:GLU:HG2	1.91	0.53
25:Z:91:ALA:O	25:Z:95:GLU:HG2	2.08	0.53
6:F:298:LEU:HG	6:F:312:GLU:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:309:GLY:O	17:Q:83:LYS:NZ	2.35	0.53
4:D:70:LEU:HD11	4:D:355:ILE:HD13	1.91	0.53
5:E:171:CYS:HB3	6:F:145:PRO:HB3	1.90	0.53
8:H:324:LEU:O	25:Z:72:ARG:NH1	2.41	0.53
13:M:451:ASP:OD1	13:M:452:LEU:N	2.34	0.53
14:N:362:ILE:HG21	14:N:391:PHE:CD1	2.43	0.53
15:O:115:GLU:HB2	15:O:127:LEU:HD21	1.90	0.53
45:x:51:ARG:NH2	46:y:59:VAL:O	2.31	0.53
5:E:134:PRO:HG2	49:E:500:FES:S2	2.49	0.53
18:R:67:GLY:O	18:R:106:GLN:NE2	2.40	0.53
24:X:17:VAL:HG23	24:X:79:VAL:HG11	1.90	0.53
30:e:60:GLU:HA	30:e:63:ARG:HG2	1.91	0.53
36:l:92:LEU:HA	36:l:95:LEU:HD12	1.89	0.53
7:G:590:ASN:HD21	7:G:593:LYS:HE2	1.74	0.53
14:N:358:ASP:HB2	14:N:472:THR:HG21	1.91	0.53
22:V:54:ARG:HA	22:V:57:VAL:HG12	1.90	0.53
25:Z:92:GLU:OE1	26:a:52:ARG:NH1	2.42	0.53
7:G:110:ARG:NE	7:G:326:GLU:OE2	2.42	0.53
7:G:172:ILE:HG23	9:I:124:ILE:HD12	1.91	0.53
12:L:150:LEU:HB3	12:L:252:VAL:HG21	1.91	0.53
16:P:104:ASP:OD1	16:P:107:ARG:NH1	2.41	0.53
8:H:154:ILE:HG21	8:H:190:PHE:HB2	1.91	0.53
8:H:302:VAL:HG13	27:b:16:VAL:HG11	1.91	0.53
12:L:409:TYR:O	36:l:101:LYS:NZ	2.32	0.53
28:c:30:PRO:HG2	28:c:33:TRP:HB3	1.91	0.53
29:d:26:LEU:HD23	29:d:30:ARG:HG3	1.91	0.53
38:n:26:ARG:HH21	38:n:75:TYR:HE2	1.55	0.53
5:E:131:GLY:N	49:E:500:FES:S1	2.76	0.52
16:P:246:ILE:HD13	16:P:344:ILE:HG22	1.91	0.52
16:P:263:ALA:HA	16:P:266:VAL:HG22	1.91	0.52
2:B:164:TYR:HE2	4:D:66:TYR:HD1	1.57	0.52
4:D:285:GLY:O	25:Z:22:GLN:NE2	2.42	0.52
6:F:350:ILE:HG23	6:F:354:ILE:HG13	1.91	0.52
7:G:381:VAL:HG13	7:G:581:VAL:HG12	1.90	0.52
26:a:25:SER:O	26:a:29:ILE:HG12	2.08	0.52
33:i:65:TRP:HE3	33:i:68:GLN:HE21	1.57	0.52
7:G:323:ILE:HD11	7:G:636:PHE:HD2	1.73	0.52
8:H:201:ALA:HB1	8:H:283:VAL:HG12	1.90	0.52
15:O:43:ASP:OD1	15:O:44:ARG:N	2.41	0.52
16:P:326:VAL:HG12	16:P:333:LEU:HD13	1.91	0.52
4:D:385:GLN:HG3	4:D:387:ILE:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:212:ILE:O	30:e:38:ARG:NE	2.33	0.52
41:q:55:ASP:OD1	41:q:56:LYS:N	2.43	0.52
46:y:86:ARG:HD2	46:y:107:HIS:CD2	2.44	0.52
46:y:160:HIS:CD2	46:y:197:ILE:HG13	2.45	0.52
3:C:110:TRP:HB2	4:D:364:GLN:OE1	2.08	0.52
3:C:118:MET:HB3	3:C:143:LEU:HB2	1.92	0.52
6:F:468:GLU:OE1	6:F:471:ARG:NH2	2.42	0.52
12:L:36:VAL:HG21	12:L:97:HIS:CE1	2.44	0.52
16:P:252:LYS:HG2	16:P:289:THR:HB	1.90	0.52
23:W:51:ALA:H	23:W:54:GLN:NE2	2.07	0.52
33:i:10:ASN:HB3	33:i:14:ARG:HH21	1.74	0.52
1:A:1:MET:SD	1:A:1:MET:N	2.78	0.52
2:B:176:ASP:OD2	2:B:184:TYR:OH	2.28	0.52
6:F:194:LYS:O	6:F:198:GLU:HG2	2.09	0.52
12:L:115:CYS:O	12:L:119:ILE:HG12	2.10	0.52
16:P:85:VAL:HG13	16:P:95:VAL:HG11	1.91	0.52
20:T:71:PHE:HA	20:T:75:LEU:HB2	1.91	0.52
4:D:147:ARG:NH1	4:D:170:GLY:O	2.42	0.52
9:I:64:PHE:HE2	25:Z:47:MET:HG2	1.75	0.52
13:M:169:ALA:HB1	13:M:240:ALA:HA	1.91	0.52
13:M:390:SER:HB2	13:M:400:GLU:OE2	2.10	0.52
19:S:59:GLN:OE1	19:S:61:TRP:NE1	2.37	0.52
39:o:63:TYR:O	39:o:67:MET:HG2	2.08	0.52
5:E:136:MET:SD	5:E:141:ARG:HG2	2.50	0.52
8:H:185:PRO:HB3	52:H:402:PTY:H351	1.92	0.52
33:i:60:ASN:OD1	33:i:61:ALA:N	2.38	0.52
37:m:16:TRP:HE1	37:m:20:ARG:HH21	1.58	0.52
45:x:238:TYR:HD1	47:z:24:ARG:HD3	1.74	0.52
4:D:12:THR:OG1	4:D:31:GLU:OE2	2.21	0.52
6:F:274:SER:O	6:F:277:ILE:HG22	2.10	0.52
7:G:575:LEU:HA	7:G:578:ALA:HB2	1.92	0.52
14:N:17:LEU:HA	14:N:20:PHE:HB2	1.92	0.52
41:q:85:ASN:HB2	41:q:88:GLN:HE21	1.75	0.52
2:B:118:SER:OG	2:B:121:GLN:OE1	2.23	0.52
3:C:97:ARG:NH1	23:W:13:PRO:O	2.42	0.52
6:F:248:LEU:HB2	17:Q:140:TYR:CE2	2.45	0.52
12:L:166:LYS:NZ	12:L:240:THR:O	2.42	0.52
12:L:170:VAL:HG21	12:L:241:TRP:HB3	1.91	0.52
12:L:284:ILE:HG22	12:L:288:PHE:CE2	2.45	0.52
13:M:340:SER:O	13:M:344:VAL:HG22	2.10	0.52
15:O:102:GLU:HG2	21:U:47:LYS:HE2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:16:LYS:O	3:C:17:LYS:HG2	2.10	0.51
6:F:142:GLU:O	6:F:182:ARG:NH1	2.43	0.51
16:P:167:LEU:HA	16:P:170:VAL:HG22	1.93	0.51
21:U:58:VAL:HG12	21:U:64:VAL:HG11	1.92	0.51
45:x:177:ARG:HH21	45:x:214:THR:HG23	1.75	0.51
1:A:78:PHE:HZ	1:A:100:LEU:HD11	1.75	0.51
4:D:375:LEU:HD22	8:H:212:LEU:HB3	1.92	0.51
7:G:144:ILE:HG13	7:G:144:ILE:O	2.09	0.51
12:L:258:ALA:HB1	12:L:345:LYS:HG2	1.91	0.51
12:L:505:ILE:HG23	12:L:508:GLU:HG2	1.92	0.51
20:T:50:VAL:HG11	20:T:112:ILE:HB	1.91	0.51
20:T:118:HIS:CE1	20:T:120:MET:HB2	2.44	0.51
23:W:26:VAL:HG22	23:W:79:ILE:HD11	1.91	0.51
31:f:11:ALA:HA	31:f:88:PHE:HB3	1.91	0.51
9:I:112:ALA:HB1	9:I:204:GLY:HA2	1.92	0.51
13:M:174:PHE:CD1	14:N:441:ILE:HD13	2.44	0.51
13:M:244:ALA:HB3	13:M:249:SER:HB2	1.92	0.51
45:x:177:ARG:NH2	45:x:214:THR:O	2.43	0.51
1:A:99:PHE:CD2	10:J:156:SER:HB2	2.44	0.51
10:J:34:PHE:CE1	11:K:40:LEU:HD13	2.46	0.51
12:L:590:ASP:OD1	12:L:591:LYS:N	2.43	0.51
46:y:137:CYS:SG	46:y:138:THR:N	2.84	0.51
8:H:152:GLY:O	8:H:156:ILE:HG12	2.10	0.51
15:O:116:TYR:HA	15:O:119:LYS:HG2	1.92	0.51
25:Z:118:TRP:HB3	30:e:53:ARG:HH12	1.76	0.51
35:k:21:HIS:O	35:k:24:LEU:N	2.42	0.51
46:y:194:ASP:HA	46:y:197:ILE:HG22	1.93	0.51
7:G:569:GLN:NE2	7:G:571:SER:O	2.42	0.51
12:L:124:MET:SD	12:L:260:THR:HB	2.50	0.51
13:M:349:PHE:HA	13:M:352:VAL:HG22	1.92	0.51
14:N:76:LEU:HD22	14:N:89:ARG:HH11	1.75	0.51
4:D:219:PHE:HB3	4:D:223:MET:HB2	1.92	0.51
12:L:520:ILE:HG12	12:L:524:PHE:CE1	2.45	0.51
14:N:100:LEU:HD11	14:N:136:MET:HB3	1.93	0.51
46:y:27:SER:HB2	47:z:16:ARG:HH11	1.75	0.51
47:z:181:TRP:HB3	47:z:186:ALA:HB1	1.91	0.51
2:B:164:TYR:OH	4:D:65:PRO:HG2	2.11	0.51
12:L:571:ASP:HA	12:L:575:ARG:HG3	1.93	0.51
13:M:126:CYS:SG	13:M:153:MET:HE3	2.51	0.51
14:N:96:CYS:HB3	14:N:140:ILE:HD13	1.91	0.51
4:D:264:ARG:NH2	4:D:384:THR:O	2.34	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:99:GLU:HB3	41:q:75:TRP:HB3	1.93	0.51
12:L:299:THR:HG23	12:L:563:TRP:HH2	1.76	0.51
13:M:150:LEU:HB3	13:M:174:PHE:CE2	2.42	0.51
13:M:450:SER:OG	13:M:451:ASP:N	2.43	0.51
14:N:32:LEU:HD21	14:N:57:LEU:HB3	1.92	0.51
14:N:139:MET:HE1	14:N:155:GLN:CD	2.35	0.51
16:P:354:SER:OG	16:P:356:ASN:OD1	2.29	0.51
8:H:244:THR:OG1	8:H:272:LYS:HB3	2.11	0.50
9:I:119:GLY:HA3	18:R:56:LEU:HD22	1.93	0.50
12:L:69:MET:HE2	12:L:190:GLN:HB2	1.93	0.50
12:L:226:PHE:O	12:L:230:VAL:HG23	2.11	0.50
12:L:570:ASN:HA	12:L:574:VAL:HG22	1.93	0.50
13:M:237:LEU:O	13:M:241:HIS:HB2	2.10	0.50
24:X:35:ALA:O	24:X:52:LYS:NZ	2.44	0.50
2:B:164:TYR:HB2	9:I:163:ILE:HG21	1.93	0.50
8:H:187:LEU:HD21	52:H:402:PTY:H261	1.93	0.50
13:M:67:GLN:OE1	33:i:22:ARG:NH1	2.44	0.50
13:M:322:GLY:HA3	13:M:403:ILE:HG23	1.92	0.50
46:y:24:ARG:O	46:y:28:LEU:HG	2.11	0.50
5:E:163:LEU:HB3	5:E:164:PHE:CD2	2.47	0.50
8:H:15:PRO:HB2	26:a:22:MET:HB2	1.94	0.50
8:H:105:ILE:HD13	10:J:47:ASP:HB2	1.93	0.50
12:L:584:VAL:HG22	37:m:36:LEU:HD22	1.93	0.50
15:O:63:LEU:HD11	45:x:133:LEU:HD11	1.93	0.50
15:O:116:TYR:HA	15:O:119:LYS:HE2	1.93	0.50
16:P:320:ALA:HA	16:P:341:LEU:HG	1.93	0.50
11:K:6:TYR:HE1	25:Z:138:LEU:HD21	1.76	0.50
12:L:361:ASP:OD2	38:n:97:ARG:NH1	2.42	0.50
12:L:448:SER:O	35:k:19:ARG:NH2	2.45	0.50
23:W:22:ALA:O	23:W:26:VAL:HG23	2.11	0.50
31:f:13:TYR:HB2	31:f:87:GLY:O	2.11	0.50
47:z:87:GLY:HA2	47:z:108:VAL:HG21	1.92	0.50
13:M:184:MET:HE3	13:M:223:SER:OG	2.11	0.50
19:S:8:SER:HA	19:S:46:LEU:HD13	1.93	0.50
19:S:25:SER:OG	19:S:29:ARG:NH2	2.38	0.50
29:d:17:GLN:NE2	29:d:34:GLU:OE2	2.45	0.50
9:I:110:GLU:OE1	9:I:182:ASN:ND2	2.44	0.50
12:L:483:ASP:HB3	39:o:48:PRO:HB3	1.94	0.50
45:x:214:THR:HG23	45:x:215:LEU:HD12	1.93	0.50
7:G:183:ASP:OD2	17:Q:65:GLN:NE2	2.41	0.50
7:G:406:ASP:OD2	19:S:63:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:311:ILE:HD12	12:L:314:SER:HB3	1.92	0.50
13:M:224:PHE:O	13:M:228:VAL:HG12	2.11	0.50
14:N:74:PRO:HB2	31:f:88:PHE:HD2	1.77	0.50
14:N:144:ASP:OD1	14:N:145:LEU:N	2.44	0.50
20:T:79:SER:OG	38:n:21:ARG:NH2	2.44	0.50
29:d:14:LEU:HG	29:d:18:MET:HE2	1.93	0.50
3:C:114:GLU:OE2	4:D:354:LYS:NZ	2.45	0.50
6:F:125:MET:HG3	6:F:172:MET:HB2	1.94	0.50
13:M:252:LEU:HA	13:M:256:LEU:HB2	1.93	0.50
14:N:478:LEU:HB3	59:d:101:LMN:HAWA	1.93	0.50
5:E:207:VAL:O	5:E:210:VAL:HG22	2.12	0.50
6:F:112:GLY:HA3	6:F:267:ASN:ND2	2.27	0.50
6:F:134:SER:O	6:F:175:SER:N	2.43	0.50
13:M:385:THR:O	13:M:389:MET:N	2.42	0.50
14:N:136:MET:HA	14:N:139:MET:HE3	1.94	0.50
14:N:201:THR:HB	14:N:212:ILE:HD11	1.94	0.50
14:N:372:LYS:HD3	14:N:373:TYR:CZ	2.47	0.50
19:S:57:GLN:OE1	19:S:58:PRO:HD2	2.12	0.50
31:f:36:ARG:HA	31:f:39:THR:HG22	1.93	0.50
38:n:87:PRO:HA	38:n:93:SER:H	1.77	0.50
45:x:101:VAL:HG12	45:x:101:VAL:O	2.11	0.50
47:z:47:ASN:ND2	47:z:48:VAL:O	2.45	0.50
4:D:375:LEU:HB3	8:H:212:LEU:HD23	1.93	0.49
8:H:36:ARG:HD3	9:I:86:TYR:CD2	2.46	0.49
10:J:130:LYS:HD2	26:a:44:GLU:HB3	1.93	0.49
12:L:533:TYR:HD1	12:L:537:LEU:HD22	1.77	0.49
13:M:161:GLY:HA3	13:M:166:LYS:HD3	1.94	0.49
23:W:120:LYS:HD2	23:W:124:LEU:HD23	1.94	0.49
46:y:107:HIS:HB3	46:y:135:HIS:CD2	2.47	0.49
3:C:183:PRO:HB3	17:Q:69:GLY:H	1.76	0.49
12:L:460:PRO:HD2	12:L:463:MET:SD	2.52	0.49
20:T:90:GLU:HG2	20:T:95:LEU:O	2.12	0.49
4:D:361:ALA:HA	4:D:364:GLN:HG2	1.93	0.49
5:E:127:LEU:HD23	5:E:183:VAL:HG12	1.94	0.49
5:E:128:LEU:HB2	5:E:182:THR:HB	1.93	0.49
10:J:54:LEU:HD22	10:J:58:ILE:HD11	1.93	0.49
12:L:2:TYR:HB3	12:L:78:PHE:CE2	2.46	0.49
13:M:229:PRO:O	13:M:317:ASN:ND2	2.37	0.49
37:m:16:TRP:NE1	37:m:20:ARG:HE	2.10	0.49
46:y:153:ASP:OD1	46:y:153:ASP:N	2.45	0.49
5:E:128:LEU:HB3	5:E:169:MET:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:78:GLY:O	6:F:82:ARG:NE	2.31	0.49
13:M:86:ILE:HD12	13:M:91:LEU:HB2	1.93	0.49
13:M:117:LYS:O	13:M:121:ILE:HG12	2.12	0.49
14:N:110:MET:HE2	14:N:361:ALA:HB2	1.93	0.49
16:P:296:ILE:HD11	16:P:371:LYS:HA	1.95	0.49
31:f:84:ARG:NH1	31:f:94:GLU:OE2	2.45	0.49
34:j:56:PRO:HG2	34:j:57:TRP:CE3	2.47	0.49
21:U:55:LEU:O	21:U:59:LYS:HE2	2.11	0.49
4:D:17:PRO:HB2	4:D:19:HIS:CE1	2.47	0.49
12:L:243:PRO:O	12:L:309:ARG:NH1	2.46	0.49
15:O:39:LYS:HD2	45:x:193:PRO:HG3	1.94	0.49
16:P:80:LEU:HB2	16:P:222:MET:HE1	1.95	0.49
19:S:84:LYS:HA	19:S:87:GLU:HG2	1.94	0.49
22:V:118:GLU:N	22:V:118:GLU:OE1	2.45	0.49
31:f:35:LEU:HD11	44:v:95:GLY:HA2	1.95	0.49
4:D:182:PHE:HD2	4:D:272:LEU:HD13	1.77	0.49
7:G:257:THR:OG1	7:G:742:LEU:O	2.24	0.49
7:G:349:ILE:HG12	7:G:616:VAL:HG22	1.94	0.49
8:H:162:VAL:HG11	8:H:170:ILE:HG12	1.93	0.49
22:V:139:PRO:HG2	22:V:142:PHE:CD1	2.48	0.49
46:y:113:ILE:H	46:y:117:VAL:HG21	1.76	0.49
2:B:164:TYR:CE1	9:I:163:ILE:HD13	2.48	0.49
4:D:105:PHE:HZ	4:D:148:VAL:HG11	1.77	0.49
5:E:133:THR:HG23	5:E:134:PRO:HD3	1.94	0.49
6:F:111:ARG:HH21	6:F:295:GLY:HA3	1.78	0.49
7:G:349:ILE:HD12	7:G:359:VAL:HG21	1.94	0.49
8:H:100:LEU:O	26:a:38:LYS:NZ	2.45	0.49
13:M:67:GLN:O	13:M:69:VAL:HG13	2.13	0.49
13:M:395:SER:HB2	13:M:470:MET:SD	2.53	0.49
14:N:365:ALA:HB1	14:N:461:MET:HE2	1.94	0.49
22:V:78:GLU:HB3	22:V:86:VAL:HG13	1.94	0.49
22:V:111:VAL:HG11	42:r:91:LYS:HD2	1.94	0.49
2:B:218:LYS:HG3	16:P:100:ARG:HH22	1.77	0.49
6:F:177:ALA:HB3	6:F:218:VAL:HG22	1.95	0.49
7:G:520:LEU:HD11	7:G:529:ILE:HG21	1.95	0.49
12:L:442:PHE:O	35:k:27:GLN:HG3	2.13	0.49
20:T:60:VAL:HG21	20:T:75:LEU:HD13	1.95	0.49
32:g:45:PHE:CD2	32:g:46:MET:HE2	2.47	0.49
38:n:86:VAL:HB	38:n:89:ALA:HB2	1.95	0.49
4:D:375:LEU:HB3	8:H:212:LEU:HB3	1.94	0.48
50:F:500:FMN:O4'	50:F:500:FMN:O2'	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:389:ASP:OD2	7:G:389:ASP:N	2.45	0.48
7:G:625:GLU:OE1	7:G:646:THR:HA	2.13	0.48
11:K:80:PHE:O	11:K:83:THR:HG22	2.13	0.48
14:N:369:THR:HG21	14:N:458:TYR:HA	1.95	0.48
27:b:9:MET:O	27:b:13:GLN:HG2	2.12	0.48
47:z:128:ILE:HD13	47:z:145:ILE:HG13	1.95	0.48
3:C:132:ILE:HG23	3:C:133:LEU:HG	1.95	0.48
6:F:339:ALA:HB1	6:F:349:LEU:HD11	1.94	0.48
12:L:299:THR:HG23	12:L:563:TRP:CH2	2.47	0.48
13:M:126:CYS:O	13:M:130:MET:HE2	2.13	0.48
22:V:12:ALA:N	22:V:75:GLU:OE2	2.46	0.48
38:n:37:HIS:HB3	38:n:39:HIS:CE1	2.48	0.48
3:C:123:PHE:HB2	3:C:129:LEU:HD11	1.95	0.48
8:H:61:LYS:NZ	8:H:222:SER:HB3	2.29	0.48
11:K:61:PHE:CD1	14:N:146:ILE:HG12	2.48	0.48
12:L:294:SER:HB3	12:L:320:GLY:HA3	1.95	0.48
15:O:103:TRP:CE2	15:O:146:MET:HA	2.47	0.48
27:b:8:ARG:HG3	27:b:9:MET:HE2	1.96	0.48
45:x:109:ILE:HG22	45:x:137:THR:HG22	1.95	0.48
5:E:119:ARG:HD2	7:G:251:TYR:OH	2.13	0.48
12:L:44:LEU:HD22	12:L:87:ILE:HD12	1.95	0.48
28:c:87:GLU:H	40:p:54:LYS:HE3	1.78	0.48
32:g:60:GLU:HG2	32:g:62:TRP:CD1	2.47	0.48
40:p:44:GLN:HA	40:p:47:LYS:HG2	1.95	0.48
6:F:267:ASN:OD1	6:F:268:VAL:N	2.46	0.48
12:L:10:LEU:HB2	12:L:122:PHE:CG	2.48	0.48
13:M:227:LYS:HB2	13:M:260:GLY:HA3	1.95	0.48
13:M:261:THR:HG22	13:M:323:MET:HE1	1.95	0.48
16:P:320:ALA:HB3	16:P:321:PRO:HD3	1.95	0.48
26:a:10:LEU:O	26:a:14:ILE:HG12	2.13	0.48
33:i:3:PHE:CE2	33:i:5:MET:HE2	2.49	0.48
46:y:128:VAL:HA	46:y:145:VAL:HB	1.95	0.48
2:B:104:ALA:HA	8:H:37:ARG:HG2	1.95	0.48
4:D:316:TYR:HD1	9:I:132:VAL:HG21	1.79	0.48
12:L:168:MET:HG2	13:M:430:LEU:HD22	1.95	0.48
13:M:43:CYS:O	13:M:47:ILE:HG12	2.14	0.48
16:P:188:ALA:HB1	16:P:201:ALA:HB2	1.96	0.48
2:B:132:THR:OG1	4:D:46:LEU:O	2.29	0.48
4:D:381:ILE:O	4:D:385:GLN:HG2	2.14	0.48
7:G:578:ALA:HB3	7:G:595:PRO:HD2	1.96	0.48
12:L:85:MET:HE2	12:L:85:MET:HB3	1.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:485:MET:HA	12:L:490:THR:HG21	1.94	0.48
12:L:562:ARG:HH11	12:L:565:PHE:HD2	1.62	0.48
14:N:402:PRO:HA	14:N:407:PHE:CG	2.48	0.48
16:P:76:ALA:HB3	16:P:97:VAL:HG13	1.95	0.48
20:T:95:LEU:HD13	20:T:121:SER:HB3	1.96	0.48
38:n:82:ASP:OD1	38:n:82:ASP:N	2.47	0.48
3:C:4:GLN:NE2	3:C:8:LYS:HE3	2.27	0.48
6:F:157:ASP:HB3	6:F:160:LYS:HG3	1.94	0.48
13:M:146:PHE:CE1	13:M:259:PHE:HB3	2.49	0.48
14:N:139:MET:CG	14:N:276:ASN:HD21	2.27	0.48
22:V:29:ALA:HB1	22:V:90:ILE:HD11	1.94	0.48
23:W:35:ARG:HG3	23:W:35:ARG:HH11	1.79	0.48
24:X:55:ASP:OD1	24:X:55:ASP:N	2.47	0.48
45:x:56:TYR:OH	45:x:245:VAL:HG13	2.13	0.48
45:x:116:ASN:ND2	45:x:224:ILE:HG21	2.29	0.48
6:F:285:PHE:CD2	6:F:295:GLY:HA2	2.48	0.48
8:H:38:LYS:HB3	8:H:41:ASP:OD2	2.14	0.48
13:M:73:ARG:NH1	13:M:76:PRO:HA	2.29	0.48
16:P:343:GLN:O	16:P:347:LEU:HG	2.14	0.48
21:U:99:PHE:CZ	21:U:119:ILE:HG23	2.49	0.48
2:B:76:MET:HE1	2:B:212:PHE:HB2	1.96	0.48
2:B:135:MET:O	2:B:135:MET:HG3	2.13	0.48
4:D:128:LEU:HD23	4:D:128:LEU:H	1.78	0.48
5:E:174:CYS:HB3	6:F:300:CYS:SG	2.54	0.48
6:F:125:MET:HE3	6:F:126:PRO:HD2	1.95	0.48
6:F:446:THR:HB	48:F:501:SF4:S3	2.54	0.48
8:H:200:ARG:NH1	8:H:236:MET:SD	2.87	0.48
12:L:446:THR:O	35:k:19:ARG:NE	2.43	0.48
38:n:19:ARG:HD2	38:n:20:VAL:N	2.29	0.48
2:B:165:TYR:OH	4:D:49:ARG:NE	2.47	0.47
5:E:136:MET:HE2	5:E:140:SER:HB3	1.96	0.47
7:G:596:LYS:O	7:G:613:ARG:NH2	2.46	0.47
12:L:304:GLN:HG3	12:L:313:TYR:HE2	1.79	0.47
14:N:249:TRP:O	14:N:253:ILE:HG12	2.13	0.47
21:U:51:THR:HA	21:U:54:VAL:HG22	1.95	0.47
23:W:37:ILE:N	23:W:38:PRO:HD2	2.29	0.47
23:W:122:ASP:OD1	23:W:123:PHE:N	2.47	0.47
45:x:217:ILE:HB	45:x:218:PRO:HD3	1.96	0.47
47:z:84:VAL:HG12	47:z:84:VAL:O	2.14	0.47
2:B:111:PHE:HE2	2:B:196:LEU:HD22	1.78	0.47
2:B:162:GLY:H	2:B:173:ARG:C	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:111:PRO:HB3	11:K:1:MET:HB3	1.95	0.47
13:M:180:GLY:C	13:M:223:SER:HB3	2.39	0.47
22:V:111:VAL:HB	42:r:91:LYS:NZ	2.29	0.47
31:f:63:VAL:HG11	53:v:201:PC7:H351	1.97	0.47
5:E:129:VAL:O	5:E:169:MET:HB3	2.13	0.47
7:G:655:LYS:NZ	23:W:131:ASN:O	2.47	0.47
16:P:370:LEU:HD23	16:P:374:PRO:HG2	1.96	0.47
38:n:65:ASP:OD1	38:n:65:ASP:N	2.46	0.47
40:p:52:ARG:HB2	40:p:77:TYR:CE2	2.49	0.47
46:y:67:VAL:HG22	46:y:85:LEU:HB2	1.94	0.47
46:y:137:CYS:SG	46:y:155:VAL:HG23	2.55	0.47
6:F:247:ARG:HD3	17:Q:144:PHE:CE2	2.48	0.47
12:L:250:THR:HG23	12:L:308:LYS:HE2	1.96	0.47
12:L:533:TYR:CD1	12:L:537:LEU:HD22	2.49	0.47
13:M:66:PHE:CD1	13:M:87:ASP:HB2	2.49	0.47
14:N:20:PHE:HE2	31:f:75:MET:HB3	1.78	0.47
28:c:69:ILE:H	28:c:72:GLN:HE22	1.62	0.47
47:z:61:VAL:HA	47:z:79:ILE:HB	1.96	0.47
4:D:55:ILE:HA	4:D:66:TYR:HE2	1.80	0.47
8:H:208:ALA:HB3	8:H:213:VAL:HG13	1.97	0.47
12:L:233:SER:O	12:L:319:LEU:HD13	2.15	0.47
12:L:354:SER:HA	12:L:357:HIS:CE1	2.49	0.47
12:L:568:VAL:HG11	36:l:82:LEU:HD22	1.95	0.47
14:N:156:SER:HB3	14:N:160:TYR:CZ	2.50	0.47
16:P:105:SER:OG	16:P:106:PRO:HD3	2.13	0.47
16:P:242:PHE:HD2	16:P:308:VAL:HG11	1.79	0.47
16:P:324:PHE:HB2	16:P:341:LEU:HD21	1.96	0.47
20:T:112:ILE:HA	20:T:115:VAL:HG22	1.95	0.47
29:d:21:ASN:HD21	29:d:30:ARG:H	1.61	0.47
31:f:45:VAL:HG13	31:f:62:MET:HG3	1.95	0.47
6:F:304:HIS:HE2	6:F:384:THR:HG21	1.80	0.47
6:F:341:ILE:O	6:F:341:ILE:HG13	2.13	0.47
7:G:518:ALA:HB2	7:G:554:LEU:HA	1.96	0.47
8:H:78:PRO:HA	8:H:81:THR:HG22	1.95	0.47
12:L:361:ASP:O	38:n:94:LYS:NZ	2.48	0.47
12:L:508:GLU:CD	12:L:508:GLU:H	2.22	0.47
16:P:218:ARG:NH1	16:P:281:GLU:OE2	2.48	0.47
16:P:243:LEU:HD22	16:P:298:TYR:HE1	1.78	0.47
39:o:17:MET:HE2	39:o:17:MET:HA	1.95	0.47
45:x:56:TYR:HE1	46:y:39:LEU:HD21	1.79	0.47
3:C:30:ARG:NE	3:C:89:GLN:OE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:147:LEU:HG	5:E:206:VAL:HG21	1.96	0.47
6:F:103:MET:HE1	6:F:277:ILE:HG21	1.97	0.47
6:F:135:TYR:HB2	6:F:263:THR:HG22	1.95	0.47
6:F:170:VAL:HG12	6:F:214:TYR:CE2	2.49	0.47
6:F:368:VAL:HG12	6:F:368:VAL:O	2.15	0.47
7:G:428:ASN:ND2	7:G:550:LEU:O	2.29	0.47
13:M:203:LEU:HD22	13:M:271:MET:SD	2.54	0.47
13:M:346:SER:O	13:M:350:LEU:HG	2.15	0.47
13:M:365:ARG:HD2	37:m:16:TRP:CZ3	2.47	0.47
15:O:111:THR:HG23	15:O:112:TYR:N	2.29	0.47
16:P:360:PHE:CD2	16:P:367:PRO:HG3	2.49	0.47
19:S:87:GLU:HB2	19:S:91:LYS:NZ	2.30	0.47
28:c:21:SER:OG	28:c:24:GLY:O	2.32	0.47
31:f:30:SER:OG	31:f:33:ASP:OD2	2.30	0.47
33:i:3:PHE:HE2	33:i:5:MET:HE2	1.80	0.47
33:i:19:PRO:HG3	40:p:3:ARG:NH2	2.30	0.47
35:k:13:ARG:NH1	35:k:17:GLU:OE2	2.48	0.47
36:l:123:GLY:O	40:p:71:ARG:NH1	2.47	0.47
45:x:163:GLY:O	45:x:166:SER:OG	2.31	0.47
47:z:100:ILE:HG22	47:z:104:SER:OG	2.14	0.47
4:D:106:CYS:O	4:D:109:THR:OG1	2.27	0.47
7:G:172:ILE:HG22	9:I:150:ARG:HD3	1.97	0.47
12:L:381:MET:HE1	12:L:468:ILE:HA	1.96	0.47
14:N:139:MET:SD	14:N:276:ASN:ND2	2.83	0.47
16:P:286:ASP:N	16:P:286:ASP:OD1	2.46	0.47
31:f:8:LEU:HD21	33:i:58:ARG:HB3	1.95	0.47
2:B:155:MET:HE3	2:B:195:LEU:HB2	1.96	0.47
5:E:84:ASN:ND2	5:E:89:PRO:HD3	2.30	0.47
6:F:112:GLY:HA3	6:F:267:ASN:HD22	1.80	0.47
7:G:337:ASP:HB2	7:G:734:ILE:HD12	1.95	0.47
7:G:494:GLU:HG2	7:G:500:HIS:CD2	2.50	0.47
12:L:371:LEU:HA	35:k:24:LEU:HD21	1.97	0.47
13:M:19:PRO:HB2	13:M:128:PHE:HB3	1.97	0.47
13:M:229:PRO:HG2	13:M:313:VAL:HG22	1.97	0.47
13:M:319:VAL:HG21	13:M:338:MET:HG3	1.97	0.47
14:N:279:ARG:O	14:N:282:ILE:HG12	2.15	0.47
14:N:399:ALA:HB3	14:N:401:ILE:HG12	1.96	0.47
16:P:228:ARG:NH1	56:P:500:NDP:O1A	2.47	0.47
22:V:64:ARG:HA	22:V:67:VAL:HG12	1.96	0.47
46:y:44:THR:HG22	46:y:65:ALA:O	2.15	0.47
3:C:6:ILE:HG21	3:C:86:ILE:HD11	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:374:MET:HG3	8:H:293:ASP:OD2	2.15	0.47
6:F:149:LYS:HG3	6:F:150:ASP:OD2	2.15	0.47
12:L:183:LEU:HD23	12:L:183:LEU:H	1.80	0.47
13:M:38:ARG:HG2	13:M:112:MET:HG2	1.96	0.47
13:M:283:ILE:HG13	13:M:324:PHE:CE2	2.50	0.47
14:N:17:LEU:HD23	14:N:20:PHE:CD1	2.50	0.47
22:V:67:VAL:HG23	22:V:80:ARG:NH1	2.29	0.47
46:y:138:THR:HB	46:y:156:VAL:HG22	1.97	0.47
4:D:55:ILE:HG21	4:D:353:CYS:HB3	1.96	0.46
6:F:102:GLU:OE1	6:F:282:PRO:HB3	2.15	0.46
6:F:361:ASP:OD1	6:F:361:ASP:N	2.43	0.46
7:G:120:CYS:O	7:G:133:SER:OG	2.29	0.46
7:G:299:VAL:HG21	7:G:453:MET:HB2	1.97	0.46
7:G:500:HIS:HD1	7:G:502:PHE:HB3	1.79	0.46
8:H:20:VAL:O	8:H:24:VAL:HG23	2.16	0.46
12:L:384:ILE:HD13	12:L:475:LEU:HD11	1.97	0.46
16:P:238:LYS:HA	16:P:238:LYS:HD3	1.68	0.46
17:Q:61:ARG:HB2	17:Q:71:LEU:HD11	1.96	0.46
24:X:27:MET:SD	24:X:28:ARG:HG3	2.55	0.46
6:F:68:LEU:HD23	6:F:68:LEU:H	1.79	0.46
7:G:210:LEU:HD12	7:G:334:PHE:CE2	2.49	0.46
7:G:601:VAL:O	7:G:601:VAL:HG13	2.15	0.46
10:J:72:PHE:HB3	11:K:84:PHE:HE2	1.78	0.46
13:M:258:LYS:O	13:M:262:TYR:HB3	2.16	0.46
13:M:341:HIS:HA	13:M:344:VAL:HG22	1.96	0.46
13:M:462:PRO:HA	13:M:465:VAL:HG12	1.96	0.46
4:D:182:PHE:CE2	4:D:186:ILE:HD11	2.49	0.46
5:E:206:VAL:HA	5:E:209:ILE:HG22	1.98	0.46
6:F:474:ARG:NH1	6:F:474:ARG:HB2	2.31	0.46
12:L:272:CYS:HB3	12:L:275:LEU:HD12	1.97	0.46
13:M:147:GLU:HG3	13:M:181:SER:HB2	1.97	0.46
13:M:184:MET:HE1	13:M:224:PHE:CE1	2.49	0.46
54:N:501:PGT:H122	54:N:501:PGT:H151	1.71	0.46
21:U:83:SER:OG	58:W:200:8Q1:O3	2.23	0.46
32:g:84:LYS:HA	33:i:12:VAL:HG11	1.97	0.46
7:G:106:CYS:O	7:G:226:ARG:NH2	2.41	0.46
7:G:369:GLY:O	7:G:372:ILE:HG22	2.15	0.46
7:G:420:ASP:OD1	7:G:420:ASP:N	2.48	0.46
12:L:369:GLY:HA3	12:L:446:THR:HA	1.96	0.46
15:O:110:ARG:N	15:O:132:ARG:HH12	2.14	0.46
20:T:83:VAL:O	20:T:87:MET:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:f:85:LEU:HD23	31:f:85:LEU:HA	1.70	0.46
46:y:70:ASP:OD1	46:y:70:ASP:N	2.47	0.46
6:F:441:GLN:O	6:F:445:HIS:ND1	2.43	0.46
7:G:64:ARG:HH12	17:Q:134:LEU:HD12	1.81	0.46
7:G:518:ALA:HB2	7:G:554:LEU:HD23	1.97	0.46
12:L:1:MET:HE1	12:L:45:ILE:HG21	1.96	0.46
12:L:243:PRO:HB3	12:L:313:TYR:CE1	2.51	0.46
12:L:295:PHE:O	12:L:299:THR:HG22	2.15	0.46
16:P:257:TYR:HD2	16:P:259:VAL:HG22	1.81	0.46
17:Q:39:ILE:HA	17:Q:42:VAL:HG22	1.97	0.46
45:x:97:TRP:CD1	45:x:118:GLN:HA	2.50	0.46
1:A:70:ILE:HG21	10:J:163:MET:HE2	1.97	0.46
4:D:15:PHE:HD2	4:D:28:LEU:HB3	1.80	0.46
8:H:59:ILE:HD13	8:H:223:MET:HE1	1.97	0.46
8:H:180:GLY:N	8:H:247:PHE:O	2.48	0.46
10:J:44:LEU:HD12	11:K:6:TYR:CZ	2.50	0.46
12:L:9:PRO:O	12:L:118:SER:OG	2.34	0.46
45:x:227:LEU:HD13	47:z:110:LYS:HB2	1.98	0.46
46:y:194:ASP:O	46:y:197:ILE:HG22	2.16	0.46
46:y:233:LYS:HB2	46:y:233:LYS:HE2	1.70	0.46
4:D:94:VAL:HG12	22:V:129:HIS:CE1	2.50	0.46
7:G:290:THR:HG21	7:G:643:ALA:HB2	1.97	0.46
7:G:379:GLU:OE2	7:G:578:ALA:HA	2.16	0.46
7:G:447:PRO:O	7:G:455:ASN:HB2	2.14	0.46
7:G:583:LEU:HD12	7:G:586:ALA:HB3	1.97	0.46
13:M:129:LEU:O	13:M:133:VAL:HG23	2.15	0.46
16:P:166:LYS:HD3	16:P:166:LYS:HA	1.69	0.46
18:R:69:ILE:HG22	18:R:88:CYS:HA	1.98	0.46
2:B:93:CYS:HB2	4:D:153:MET:HE3	1.98	0.46
12:L:174:GLY:HA3	12:L:231:GLY:HA3	1.97	0.46
14:N:205:HIS:HB3	14:N:208:GLN:HG2	1.98	0.46
14:N:259:THR:HA	14:N:262:THR:HG22	1.97	0.46
17:Q:42:VAL:HB	23:W:77:LEU:HD22	1.98	0.46
33:i:16:MET:HB3	40:p:3:ARG:HD2	1.98	0.46
8:H:14:LEU:HB2	8:H:15:PRO:HD3	1.98	0.46
8:H:58:LEU:HD22	8:H:222:SER:HB2	1.97	0.46
8:H:203:PHE:HD1	8:H:295:LEU:HD13	1.81	0.46
13:M:73:ARG:NH1	14:N:484:SER:OG	2.48	0.46
39:o:31:ALA:HA	39:o:34:LEU:HD23	1.97	0.46
45:x:236:LEU:HD23	45:x:236:LEU:H	1.80	0.46
4:D:148:VAL:O	9:I:106:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:413:GLY:O	6:F:417:MET:HG3	2.15	0.46
6:F:475:GLU:HA	6:F:478:GLU:HG2	1.98	0.46
12:L:486:ILE:O	12:L:486:ILE:HG13	2.16	0.46
41:q:55:ASP:HB2	41:q:61:TYR:HE1	1.80	0.46
4:D:219:PHE:CZ	4:D:365:GLY:HA3	2.50	0.45
6:F:422:MET:HE3	6:F:422:MET:HB2	1.80	0.45
8:H:162:VAL:HG21	8:H:170:ILE:HG12	1.97	0.45
8:H:200:ARG:NH2	8:H:284:ARG:HD3	2.31	0.45
12:L:187:THR:HG22	13:M:409:GLN:HG2	1.98	0.45
13:M:370:LEU:HB2	13:M:437:VAL:HG12	1.97	0.45
25:Z:86:LEU:HD21	33:i:82:LEU:HD21	1.97	0.45
31:f:57:ILE:HG22	31:f:61:SER:H	1.81	0.45
47:z:83:CYS:HA	47:z:104:SER:O	2.16	0.45
47:z:105:LEU:HD11	47:z:133:VAL:HG13	1.97	0.45
8:H:171:VAL:HG13	8:H:250:GLY:H	1.82	0.45
12:L:172:ARG:NH2	13:M:390:SER:HG	2.14	0.45
13:M:399:GLY:O	13:M:403:ILE:HG12	2.16	0.45
16:P:87:GLN:HB3	16:P:266:VAL:HG11	1.98	0.45
53:v:201:PC7:H152	53:v:201:PC7:H182	1.59	0.45
47:z:137:CYS:HB3	47:z:152:LEU:O	2.15	0.45
2:B:135:MET:HE3	4:D:25:VAL:HG22	1.98	0.45
6:F:343:GLY:H	6:F:377:VAL:HG12	1.81	0.45
10:J:139:THR:HG23	11:K:56:MET:HE1	1.98	0.45
12:L:10:LEU:HD11	53:M:501:PC7:H232	1.99	0.45
12:L:199:ALA:HB2	40:p:59:TYR:HB2	1.97	0.45
12:L:412:TYR:CD1	36:l:101:LYS:HE2	2.51	0.45
13:M:184:MET:O	13:M:188:ILE:HG13	2.16	0.45
16:P:196:MET:HG2	16:P:342:ASP:CG	2.41	0.45
16:P:257:TYR:CD1	16:P:374:PRO:HB3	2.52	0.45
45:x:59:GLN:H	47:z:40:SER:HB2	1.80	0.45
11:K:84:PHE:CB	11:K:85:ARG:HH21	2.29	0.45
12:L:69:MET:HE1	40:p:81:THR:HG22	1.99	0.45
12:L:262:VAL:HG13	12:L:319:LEU:CD2	2.43	0.45
12:L:280:PRO:O	12:L:284:ILE:HG12	2.17	0.45
13:M:283:ILE:HG13	13:M:324:PHE:CD2	2.51	0.45
15:O:70:ARG:NH2	15:O:86:ASP:OD1	2.44	0.45
22:V:120:ILE:HG12	42:r:86:ARG:HG2	1.97	0.45
23:W:80:PHE:O	23:W:84:GLU:HG2	2.15	0.45
4:D:17:PRO:HB2	4:D:19:HIS:NE2	2.32	0.45
6:F:293:ASN:HB3	6:F:315:MET:HE2	1.99	0.45
7:G:116:ASN:O	7:G:117:CYS:SG	2.75	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:270:SER:O	8:H:274:LEU:HD13	2.17	0.45
10:J:121:SER:O	25:Z:96:ARG:NH1	2.48	0.45
12:L:40:SER:HA	12:L:90:THR:HB	1.97	0.45
12:L:223:ILE:O	12:L:227:ILE:HG12	2.17	0.45
12:L:412:TYR:OH	36:l:106:PRO:HD2	2.16	0.45
19:S:3:TRP:CZ2	19:S:87:GLU:HB3	2.51	0.45
22:V:37:TYR:CE2	22:V:64:ARG:HB3	2.52	0.45
46:y:126:VAL:HG22	46:y:143:ALA:H	1.82	0.45
4:D:147:ARG:NH1	4:D:174:ASP:OD2	2.50	0.45
6:F:408:CYS:HB2	48:F:501:SF4:S3	2.56	0.45
7:G:499:ARG:HD3	7:G:499:ARG:HA	1.74	0.45
13:M:17:LEU:O	13:M:21:LEU:HG	2.16	0.45
13:M:179:LEU:HD23	14:N:434:VAL:HG21	1.99	0.45
14:N:372:LYS:NZ	15:O:156:TRP:O	2.46	0.45
24:X:65:LYS:HB3	24:X:65:LYS:HE3	1.73	0.45
30:e:50:GLU:OE2	30:e:54:ARG:NH1	2.50	0.45
47:z:120:THR:OG1	47:z:136:GLY:HA2	2.17	0.45
2:B:143:TYR:CD1	2:B:179:VAL:HG23	2.52	0.45
5:E:206:VAL:O	5:E:210:VAL:HG13	2.16	0.45
6:F:402:CYS:HA	7:G:242:ARG:HG3	1.99	0.45
8:H:249:GLY:O	8:H:272:LYS:NZ	2.43	0.45
12:L:47:PHE:HE1	12:L:84:VAL:HG22	1.81	0.45
22:V:57:VAL:O	22:V:61:THR:OG1	2.34	0.45
35:k:22:PRO:HA	35:k:25:SER:HB2	1.99	0.45
3:C:97:ARG:HB3	3:C:124:ILE:HG23	1.99	0.45
4:D:19:HIS:ND1	4:D:21:ALA:HB3	2.32	0.45
4:D:37:VAL:HG12	4:D:373:HIS:O	2.17	0.45
6:F:274:SER:N	6:F:275:PRO:HD2	2.31	0.45
10:J:150:VAL:HB	14:N:86:LEU:HD23	1.98	0.45
12:L:58:TYR:CG	40:p:60:ARG:HD3	2.51	0.45
31:f:22:PHE:HD1	31:f:78:TYR:HE2	1.64	0.45
5:E:130:CYS:HB3	5:E:135:CYS:SG	2.57	0.45
11:K:55:ASP:OD2	30:e:3:SER:OG	2.34	0.45
13:M:153:MET:HE1	13:M:251:ILE:HD11	1.99	0.45
13:M:491:HIS:CD2	40:p:34:ARG:HH11	2.34	0.45
14:N:178:LYS:NZ	14:N:252:ASP:OD2	2.49	0.45
14:N:216:TYR:OH	14:N:221:ALA:N	2.50	0.45
16:P:184:SER:O	16:P:219:PRO:HD2	2.17	0.45
21:U:84:LEU:O	21:U:87:VAL:HG12	2.17	0.45
32:g:104:GLU:HG2	32:g:105:LYS:N	2.32	0.45
3:C:38:LEU:HD21	3:C:75:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:169:LEU:HD11	25:Z:21:LEU:HG	1.98	0.45
7:G:197:GLU:OE1	7:G:197:GLU:N	2.48	0.45
7:G:208:GLY:H	7:G:255:LEU:HD22	1.82	0.45
12:L:296:LEU:O	12:L:300:THR:OG1	2.26	0.45
12:L:315:THR:O	12:L:319:LEU:HG	2.17	0.45
13:M:22:GLY:O	13:M:26:LEU:HD13	2.16	0.45
13:M:115:TYR:HB3	13:M:119:TYR:HB2	1.98	0.45
15:O:123:ARG:HA	15:O:123:ARG:HD2	1.79	0.45
46:y:124:ASP:O	46:y:142:ASP:N	2.41	0.45
7:G:123:GLU:HG3	7:G:148:THR:OG1	2.17	0.44
7:G:331:LYS:O	7:G:335:CYS:HB3	2.16	0.44
8:H:179:PHE:HB2	8:H:247:PHE:HA	1.99	0.44
9:I:100:LYS:HD2	41:q:98:HIS:NE2	2.31	0.44
12:L:565:PHE:O	12:L:569:LEU:HB3	2.17	0.44
13:M:217:TRP:HZ2	13:M:324:PHE:HE2	1.63	0.44
22:V:111:VAL:HB	42:r:91:LYS:HZ3	1.82	0.44
38:n:18:GLU:O	38:n:22:ILE:HG12	2.17	0.44
7:G:439:LEU:HD21	7:G:502:PHE:CZ	2.52	0.44
8:H:217:ASN:HA	8:H:220:TYR:HD2	1.81	0.44
12:L:178:LEU:HD23	12:L:182:ILE:HD11	1.98	0.44
12:L:341:HIS:NE2	12:L:345:LYS:HD2	2.33	0.44
12:L:409:TYR:HB2	12:L:420:PHE:CE1	2.51	0.44
16:P:147:ARG:HH11	16:P:147:ARG:HA	1.82	0.44
21:U:97:PHE:HB3	21:U:99:PHE:CE2	2.52	0.44
32:g:46:MET:HE3	32:g:48:ARG:HD2	1.99	0.44
45:x:167:ILE:O	45:x:169:MET:HG3	2.18	0.44
5:E:32:LEU:HD22	5:E:34:TYR:CE1	2.52	0.44
6:F:180:TYR:HA	6:F:221:HIS:O	2.17	0.44
7:G:236:ASP:HB2	7:G:254:LYS:HD2	1.99	0.44
14:N:178:LYS:HE2	14:N:249:TRP:CD2	2.52	0.44
19:S:37:LYS:O	19:S:41:SER:OG	2.27	0.44
8:H:162:VAL:HG12	8:H:164:SER:H	1.82	0.44
12:L:518:LYS:HE2	34:j:50:VAL:HB	2.00	0.44
16:P:315:ALA:HA	16:P:318:MET:HG2	1.98	0.44
20:T:42:SER:HA	20:T:116:TYR:HE1	1.83	0.44
38:n:26:ARG:HB3	38:n:75:TYR:OH	2.18	0.44
1:A:1:MET:HE1	26:a:47:VAL:HG21	1.99	0.44
4:D:376:ALA:N	8:H:212:LEU:HD23	2.32	0.44
6:F:207:LYS:NZ	6:F:215:ASP:OD2	2.37	0.44
7:G:381:VAL:HG23	7:G:407:ASN:O	2.18	0.44
11:K:76:GLY:HA2	14:N:180:LEU:CD2	2.43	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:84:PHE:HA	11:K:88:GLY:H	1.82	0.44
12:L:13:SER:HB3	12:L:118:SER:CB	2.44	0.44
12:L:263:THR:HB	12:L:338:LEU:HD11	1.99	0.44
13:M:72:LEU:O	13:M:81:ASN:HB2	2.18	0.44
20:T:57:PHE:CE2	20:T:59:LYS:HB2	2.53	0.44
25:Z:38:ARG:HA	25:Z:38:ARG:NE	2.32	0.44
31:f:39:THR:O	31:f:43:ILE:HG12	2.17	0.44
31:f:82:ALA:HB1	31:f:86:MET:HE1	1.99	0.44
41:q:74:ARG:NH1	41:q:96:TRP:O	2.39	0.44
45:x:59:GLN:CD	46:y:64:SER:HB3	2.43	0.44
6:F:336:ASN:HB3	6:F:382:LYS:H	1.81	0.44
12:L:370:GLY:O	12:L:446:THR:OG1	2.36	0.44
12:L:401:LYS:HA	12:L:404:ILE:HG22	1.99	0.44
14:N:398:TYR:HB3	14:N:440:TYR:CE2	2.52	0.44
19:S:79:GLU:HB2	19:S:80:PRO:HD3	2.00	0.44
20:T:42:SER:O	20:T:46:VAL:HG23	2.17	0.44
32:g:105:LYS:N	32:g:105:LYS:HD3	2.33	0.44
4:D:192:MET:HG3	9:I:82:LEU:HD23	1.99	0.44
4:D:282:MET:HB3	25:Z:25:PRO:HD3	1.98	0.44
6:F:388:ASP:OD1	6:F:392:ARG:NH1	2.51	0.44
6:F:414:TRP:O	6:F:418:ILE:HG12	2.18	0.44
8:H:185:PRO:O	8:H:189:MET:HG3	2.18	0.44
12:L:241:TRP:CH2	12:L:261:MET:HE2	2.53	0.44
13:M:174:PHE:CE1	14:N:441:ILE:HG21	2.52	0.44
53:M:501:PC7:H442	53:M:501:PC7:H472	1.76	0.44
14:N:197:ILE:HG23	14:N:229:GLY:HA3	2.00	0.44
14:N:395:MET:SD	14:N:443:LEU:HD22	2.58	0.44
16:P:85:VAL:HG12	16:P:112:MET:HG3	1.99	0.44
19:S:13:GLU:OE1	19:S:15:ARG:NH2	2.50	0.44
30:e:29:ARG:HB3	33:i:51:TYR:CE2	2.53	0.44
32:g:96:LYS:HB3	40:p:43:ILE:HD12	1.98	0.44
35:k:19:ARG:HG3	38:n:38:ARG:NH2	2.31	0.44
45:x:66:GLY:O	46:y:232:ARG:NE	2.49	0.44
46:y:209:ASN:O	46:y:212:GLN:NE2	2.51	0.44
6:F:140:ALA:HB3	6:F:180:TYR:O	2.18	0.44
6:F:345:SER:O	6:F:397:TYR:OH	2.34	0.44
7:G:409:TRP:HD1	7:G:410:CYS:O	2.01	0.44
10:J:140:LEU:HD21	11:K:63:LEU:HD13	2.00	0.44
12:L:77:LEU:HB3	12:L:271:ARG:NH2	2.33	0.44
16:P:99:PHE:CG	16:P:106:PRO:HG3	2.53	0.44
29:d:31:HIS:HB3	29:d:33:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:k:18:TRP:CZ3	35:k:19:ARG:HD3	2.53	0.44
38:n:65:ASP:HA	38:n:68:ILE:HG12	2.00	0.44
45:x:52:VAL:HG12	45:x:54:TRP:H	1.83	0.44
46:y:99:ASN:OD1	46:y:127:THR:HA	2.17	0.44
8:H:202:PRO:HG3	52:H:402:PTY:H152	2.00	0.44
12:L:484:MET:HB3	39:o:46:TYR:HB3	2.00	0.44
14:N:79:ALA:H	31:f:6:THR:H	1.66	0.44
14:N:282:ILE:HA	14:N:498:TYR:OH	2.18	0.44
39:o:34:LEU:HD21	39:o:58:TYR:CE1	2.53	0.44
46:y:46:MET:HG2	46:y:68:ILE:HG22	1.99	0.44
46:y:164:ALA:HB3	46:y:182:GLY:HA3	1.99	0.44
1:A:118:TRP:HZ3	8:H:292:TYR:CE2	2.35	0.43
4:D:234:ARG:HH11	4:D:332:GLU:HG2	1.83	0.43
5:E:177:ASN:ND2	5:E:199:GLU:HB2	2.33	0.43
5:E:188:ASN:HB3	5:E:192:GLY:HA3	1.99	0.43
7:G:485:LEU:HD11	7:G:502:PHE:CD2	2.53	0.43
7:G:494:GLU:HG3	7:G:499:ARG:HB2	2.00	0.43
12:L:246:MET:SD	12:L:246:MET:N	2.91	0.43
14:N:496:SER:HA	29:d:63:MET:HE1	2.00	0.43
16:P:252:LYS:HB3	16:P:287:VAL:HG12	2.00	0.43
22:V:45:GLN:HA	22:V:54:ARG:NH2	2.33	0.43
29:d:21:ASN:HD21	29:d:30:ARG:HB2	1.83	0.43
36:l:109:PRO:O	39:o:69:ARG:NH1	2.51	0.43
39:o:70:MET:SD	39:o:74:LYS:HE2	2.57	0.43
47:z:108:VAL:HG12	47:z:108:VAL:O	2.18	0.43
7:G:265:ILE:HG23	7:G:274:THR:HA	2.00	0.43
8:H:61:LYS:HZ1	8:H:222:SER:HB3	1.83	0.43
53:M:501:PC7:H182	53:M:501:PC7:H412	2.01	0.43
16:P:132:LYS:NZ	16:P:173:GLU:OE2	2.49	0.43
22:V:35:ASP:OD1	22:V:39:LYS:HE2	2.17	0.43
39:o:44:GLU:HB3	39:o:50:LYS:HD3	1.98	0.43
12:L:226:PHE:CG	12:L:286:ILE:HG12	2.54	0.43
13:M:331:ILE:O	13:M:335:ILE:HG13	2.18	0.43
23:W:60:SER:HA	23:W:63:ILE:HG22	2.01	0.43
23:W:121:THR:HG23	23:W:123:PHE:N	2.34	0.43
24:X:84:TYR:OH	26:a:31:LYS:NZ	2.40	0.43
34:j:47:GLY:N	34:j:48:PRO:HD2	2.34	0.43
38:n:16:GLN:O	38:n:19:ARG:HG3	2.19	0.43
1:A:118:TRP:HZ3	8:H:292:TYR:HE2	1.65	0.43
5:E:77:LEU:HD23	5:E:96:VAL:HG21	2.01	0.43
6:F:67:ASN:HB3	6:F:82:ARG:NH1	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:111:ARG:NH2	6:F:294:ALA:O	2.51	0.43
6:F:369:GLN:HE21	6:F:463:ARG:HH12	1.66	0.43
6:F:401:SER:C	6:F:403:GLY:H	2.26	0.43
7:G:601:VAL:HG23	7:G:616:VAL:HB	1.99	0.43
9:I:57:SER:O	9:I:58:LYS:HD3	2.17	0.43
16:P:359:LYS:N	16:P:362:ASP:OD2	2.41	0.43
29:d:14:LEU:HG	29:d:18:MET:CE	2.47	0.43
35:k:10:GLU:HG2	35:k:11:PHE:N	2.33	0.43
2:B:93:CYS:HB3	4:D:72:TYR:CB	2.49	0.43
10:J:135:THR:O	10:J:139:THR:HG22	2.18	0.43
14:N:358:ASP:OD2	14:N:394:THR:OG1	2.26	0.43
16:P:253:PHE:CE2	16:P:255:PRO:HG3	2.53	0.43
20:T:105:ILE:HG12	20:T:110:LEU:HB3	2.01	0.43
22:V:45:GLN:OE1	22:V:54:ARG:NH2	2.51	0.43
24:X:91:LEU:HD23	24:X:91:LEU:HA	1.89	0.43
28:c:16:ARG:HH11	28:c:26:PRO:HG3	1.83	0.43
31:f:21:ALA:H	31:f:24:LYS:HE2	1.83	0.43
2:B:164:TYR:CE2	4:D:66:TYR:CE1	3.06	0.43
3:C:171:MET:HB3	3:C:171:MET:HE2	1.77	0.43
7:G:469:VAL:HG21	7:G:480:TYR:CE2	2.53	0.43
8:H:160:ILE:HG22	8:H:318:LEU:HD12	2.01	0.43
11:K:84:PHE:HB3	11:K:85:ARG:HH21	1.83	0.43
12:L:423:GLY:O	12:L:427:VAL:HG23	2.19	0.43
13:M:180:GLY:O	13:M:223:SER:HB3	2.18	0.43
14:N:334:PHE:HB2	14:N:345:LEU:HD22	2.01	0.43
45:x:108:LYS:HE3	45:x:108:LYS:HB3	1.89	0.43
11:K:79:ILE:HA	11:K:82:ILE:HG12	2.00	0.43
12:L:10:LEU:HD22	12:L:122:PHE:CZ	2.53	0.43
17:Q:116:SER:HA	17:Q:119:GLU:HG2	2.00	0.43
21:U:59:LYS:NZ	21:U:69:VAL:HG11	2.34	0.43
23:W:69:ILE:HB	23:W:75:ILE:HD11	2.01	0.43
39:o:65:LEU:O	39:o:68:GLU:HG3	2.19	0.43
45:x:88:VAL:HG23	45:x:109:ILE:HG13	2.01	0.43
46:y:155:VAL:HG12	46:y:173:THR:H	1.83	0.43
2:B:85:TRP:HB3	2:B:116:ARG:HG2	2.01	0.43
4:D:202:ARG:O	4:D:203:LEU:HD23	2.18	0.43
10:J:125:THR:HG22	25:Z:93:GLU:OE1	2.18	0.43
11:K:24:ASN:HD22	11:K:27:ASN:HB3	1.84	0.43
16:P:297:MET:O	16:P:301:ILE:HG13	2.19	0.43
23:W:97:HIS:CD2	23:W:100:ILE:HD11	2.54	0.43
46:y:113:ILE:HD12	47:z:199:PHE:HZ	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:y:144:PHE:HD2	46:y:200:ILE:HG12	1.83	0.43
1:A:58:ASP:OD1	1:A:59:ILE:N	2.48	0.43
1:A:103:LEU:HD23	1:A:103:LEU:HA	1.84	0.43
3:C:118:MET:HA	3:C:118:MET:HE2	2.01	0.43
6:F:360:MET:SD	6:F:360:MET:N	2.91	0.43
7:G:213:THR:OG1	7:G:215:MET:HE2	2.19	0.43
51:H:401:UQ9:H10B	51:H:401:UQ9:H12A	1.82	0.43
9:I:58:LYS:HD3	9:I:58:LYS:HA	1.83	0.43
9:I:160:THR:HG21	9:I:190:HIS:CE1	2.53	0.43
15:O:72:LEU:HD22	15:O:77:LEU:HD21	2.01	0.43
16:P:369:LYS:CD	16:P:371:LYS:HB2	2.49	0.43
25:Z:72:ARG:O	25:Z:76:GLU:HG2	2.19	0.43
6:F:85:TRP:CD2	6:F:204:LEU:HD13	2.54	0.43
12:L:97:HIS:NE2	12:L:117:LEU:HB3	2.33	0.43
13:M:298:THR:OG1	13:M:310:TYR:HB3	2.19	0.43
15:O:71:ALA:HA	15:O:74:HIS:CE1	2.54	0.43
23:W:125:LYS:HD2	23:W:125:LYS:O	2.19	0.43
46:y:140:GLU:CD	46:y:158:GLU:HA	2.43	0.43
2:B:162:GLY:H	2:B:174:GLY:N	2.17	0.42
4:D:105:PHE:O	4:D:109:THR:HG23	2.19	0.42
7:G:521:PHE:CE1	7:G:530:LEU:HD11	2.53	0.42
12:L:139:GLY:O	12:L:143:VAL:HG23	2.19	0.42
12:L:278:TYR:CZ	12:L:500:LEU:HD21	2.54	0.42
14:N:223:SER:HB3	14:N:226:ILE:HG22	2.01	0.42
16:P:288:PHE:HA	16:P:292:GLU:OE2	2.18	0.42
16:P:373:TYR:HB3	16:P:374:PRO:HD3	2.01	0.42
22:V:63:GLN:HG3	22:V:141:GLN:NE2	2.34	0.42
32:g:60:GLU:HG3	32:g:61:ASP:H	1.83	0.42
45:x:204:ARG:HA	45:x:204:ARG:HD3	1.66	0.42
46:y:33:HIS:O	47:z:47:ASN:ND2	2.52	0.42
2:B:93:CYS:HB3	4:D:72:TYR:CG	2.53	0.42
2:B:178:ILE:HG22	2:B:179:VAL:N	2.35	0.42
3:C:9:TYR:CE1	3:C:50:TYR:HD2	2.37	0.42
7:G:511:ASN:N	7:G:512:PRO:HD3	2.34	0.42
8:H:293:ASP:OD1	8:H:294:GLN:N	2.52	0.42
13:M:359:HIS:NE2	13:M:449:PHE:HB3	2.35	0.42
14:N:285:SER:HA	33:i:49:ARG:HH21	1.84	0.42
16:P:143:ASN:HB3	16:P:182:GLN:HG2	2.01	0.42
31:f:84:ARG:HA	31:f:89:PHE:HB2	2.01	0.42
32:g:96:LYS:HG3	32:g:100:ARG:HD3	2.02	0.42
53:v:201:PC7:H421	53:v:201:PC7:H392	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:x:81:ASN:HB2	45:x:98:ASN:HB2	2.00	0.42
7:G:497:GLU:N	7:G:497:GLU:OE1	2.52	0.42
51:H:401:UQ9:H20	51:H:401:UQ9:H17	1.65	0.42
11:K:24:ASN:ND2	11:K:27:ASN:HB3	2.34	0.42
12:L:326:CYS:HA	12:L:331:TYR:HD1	1.85	0.42
13:M:450:SER:HB2	38:n:108:VAL:HG23	2.02	0.42
19:S:87:GLU:HB2	19:S:91:LYS:HZ1	1.85	0.42
20:T:105:ILE:HD13	20:T:111:ALA:HA	2.01	0.42
36:l:108:THR:OG1	39:o:69:ARG:HG3	2.20	0.42
37:m:20:ARG:HA	37:m:23:LEU:HD21	2.02	0.42
46:y:64:SER:OG	46:y:82:GLY:N	2.40	0.42
3:C:172:THR:O	17:Q:93:SER:OG	2.29	0.42
11:K:25:ARG:HD3	11:K:25:ARG:HA	1.78	0.42
12:L:284:ILE:O	12:L:287:THR:OG1	2.32	0.42
12:L:580:PHE:O	12:L:584:VAL:HB	2.19	0.42
16:P:123:PHE:HD2	16:P:131:ILE:HG12	1.84	0.42
38:n:33:ASN:HB3	38:n:80:HIS:ND1	2.34	0.42
40:p:50:ILE:HA	40:p:53:GLU:HG2	2.02	0.42
45:x:71:LYS:HE2	45:x:71:LYS:HB2	1.90	0.42
47:z:133:VAL:HG12	47:z:133:VAL:O	2.18	0.42
2:B:165:TYR:O	2:B:167:TYR:N	2.52	0.42
2:B:179:VAL:O	2:B:179:VAL:HG13	2.19	0.42
8:H:121:ILE:O	8:H:137:ALA:HB1	2.19	0.42
12:L:79:ASP:CG	12:L:496:SER:HG	2.28	0.42
12:L:133:PHE:HB2	12:L:192:VAL:HG22	2.01	0.42
12:L:138:LEU:HA	13:M:392:PRO:CG	2.50	0.42
12:L:311:ILE:HD11	12:L:345:LYS:HE2	2.02	0.42
12:L:470:LEU:HD23	12:L:470:LEU:HA	1.85	0.42
13:M:165:ARG:HB3	13:M:243:GLU:OE1	2.20	0.42
13:M:451:ASP:HB3	32:g:47:ASN:ND2	2.34	0.42
14:N:93:THR:HG21	14:N:141:SER:HB3	2.02	0.42
21:U:63:LYS:NZ	21:U:79:LEU:O	2.53	0.42
25:Z:82:ARG:O	25:Z:85:ILE:HG22	2.20	0.42
28:c:72:GLN:HG3	28:c:78:PHE:CZ	2.54	0.42
45:x:179:ILE:HD11	45:x:217:ILE:HD11	2.01	0.42
2:B:71:LYS:HD3	2:B:71:LYS:HA	1.77	0.42
2:B:93:CYS:O	4:D:153:MET:HE1	2.20	0.42
7:G:176:GLY:HA2	48:G:802:SF4:S2	2.60	0.42
8:H:212:LEU:HD12	8:H:213:VAL:N	2.34	0.42
9:I:58:LYS:O	27:b:8:ARG:NH1	2.46	0.42
12:L:148:TYR:CD1	12:L:164:ALA:HB1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:273:SER:OG	12:L:274:PRO:HD3	2.20	0.42
12:L:375:PHE:HA	12:L:376:PRO:HD3	1.83	0.42
12:L:457:HIS:ND1	12:L:457:HIS:C	2.76	0.42
13:M:158:GLY:O	13:M:166:LYS:HD2	2.19	0.42
13:M:233:VAL:O	13:M:233:VAL:HG13	2.20	0.42
13:M:316:MET:HA	13:M:319:VAL:HG12	2.02	0.42
53:M:501:PC7:H72	53:M:501:PC7:H41	1.65	0.42
14:N:114:PHE:O	14:N:118:GLU:HB3	2.20	0.42
14:N:217:GLU:OE2	14:N:218:ILE:HG12	2.18	0.42
16:P:202:ALA:O	16:P:205:GLU:HG3	2.20	0.42
29:d:46:ALA:HB2	59:d:101:LMN:HAX	2.01	0.42
32:g:75:VAL:O	32:g:79:VAL:HG22	2.18	0.42
45:x:175:GLU:OE2	45:x:191:ARG:NH2	2.45	0.42
45:x:201:ASN:HB3	45:x:202:PRO:HD3	2.02	0.42
5:E:174:CYS:H	6:F:148:CYS:HB3	1.84	0.42
6:F:64:ILE:HG23	6:F:276:THR:HG21	2.02	0.42
8:H:187:LEU:HD13	8:H:247:PHE:HB2	2.00	0.42
13:M:74:TRP:NE1	14:N:480:LEU:O	2.49	0.42
53:M:501:PC7:H432	53:M:501:PC7:H401	1.79	0.42
14:N:278:LEU:HD11	14:N:345:LEU:HD21	2.01	0.42
16:P:147:ARG:HD3	56:P:500:NDP:H8A	2.02	0.42
16:P:247:GLY:HA2	16:P:312:PHE:CE1	2.55	0.42
53:v:201:PC7:H222	53:v:201:PC7:H191	1.63	0.42
45:x:169:MET:SD	45:x:188:PRO:HD3	2.59	0.42
46:y:222:PHE:HA	46:y:225:ILE:HG22	2.02	0.42
47:z:184:ASN:HA	47:z:185:PRO:HA	1.88	0.42
4:D:16:GLY:H	4:D:17:PRO:HD3	1.84	0.42
4:D:197:ARG:HG2	4:D:201:GLN:OE1	2.20	0.42
50:F:500:FMN:N1	50:F:500:FMN:O3'	2.39	0.42
7:G:347:PRO:HG2	7:G:361:TRP:HA	2.01	0.42
7:G:381:VAL:O	7:G:581:VAL:HA	2.20	0.42
7:G:394:MET:HG2	7:G:680:ILE:HG13	2.01	0.42
8:H:98:MET:C	26:a:26:GLN:HE21	2.27	0.42
12:L:330:ASN:HB3	12:L:407:LEU:HD13	2.02	0.42
15:O:51:ILE:HG12	15:O:57:LYS:HD3	2.02	0.42
45:x:92:ASP:OD1	45:x:92:ASP:N	2.51	0.42
4:D:99:GLN:HE21	4:D:241:VAL:HG13	1.84	0.42
5:E:134:PRO:HG3	6:F:145:PRO:HB2	2.02	0.42
6:F:313:GLU:OE2	6:F:326:HIS:NE2	2.49	0.42
7:G:652:ASP:HB2	7:G:655:LYS:HE3	2.01	0.42
8:H:313:SER:HA	27:b:27:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:119:TYR:OH	13:M:247:ALA:HB3	2.20	0.42
13:M:202:ILE:HD11	33:i:33:MET:HB3	2.02	0.42
14:N:287:GLY:O	14:N:292:GLN:NE2	2.53	0.42
15:O:77:LEU:HD12	15:O:150:VAL:HG21	2.02	0.42
15:O:128:ASN:C	15:O:130:HIS:H	2.27	0.42
20:T:52:ASP:HB3	35:k:15:ARG:NH1	2.35	0.42
34:j:22:THR:O	34:j:26:VAL:HG22	2.19	0.42
36:l:112:TYR:HB2	36:l:116:ASN:HA	2.01	0.42
46:y:104:THR:HG21	46:y:128:VAL:HG11	2.02	0.42
46:y:134:ILE:HG23	46:y:137:CYS:HB3	2.02	0.42
3:C:107:SER:HB3	4:D:217:TRP:HA	2.00	0.42
4:D:108:ILE:HG23	4:D:141:LEU:HD22	2.01	0.42
6:F:143:SER:O	6:F:144:GLU:HG2	2.19	0.42
6:F:472:ARG:O	6:F:475:GLU:HG3	2.20	0.42
12:L:138:LEU:HA	13:M:392:PRO:HG2	2.02	0.42
12:L:459:ALA:O	34:j:24:HIS:NE2	2.53	0.42
13:M:150:LEU:HD22	13:M:174:PHE:CD2	2.55	0.42
14:N:309:ALA:HB3	14:N:439:TYR:CZ	2.55	0.42
15:O:154:LYS:HE3	15:O:154:LYS:HB3	1.81	0.42
26:a:53:ASP:HA	26:a:56:VAL:HG22	2.01	0.42
31:f:35:LEU:HD21	44:v:98:GLY:HA3	2.01	0.42
36:l:115:ASP:HB3	36:l:118:ARG:HB2	2.02	0.42
2:B:84:ILE:O	2:B:86:PRO:HD3	2.20	0.41
3:C:60:CYS:SG	4:D:354:LYS:HD3	2.60	0.41
5:E:34:TYR:HD2	5:E:36:LEU:HD13	1.82	0.41
6:F:342:PRO:HA	6:F:377:VAL:HG12	2.02	0.41
7:G:316:ILE:HD13	7:G:316:ILE:HA	1.89	0.41
10:J:12:VAL:HG21	43:u:9:UNK:HA	2.02	0.41
10:J:66:LEU:HD23	10:J:66:LEU:HA	1.77	0.41
11:K:76:GLY:CA	14:N:180:LEU:HD21	2.45	0.41
13:M:59:PHE:HZ	13:M:88:GLY:HA2	1.85	0.41
13:M:376:ASN:HD21	28:c:22:MET:HB2	1.84	0.41
13:M:419:ALA:O	13:M:423:ILE:HG12	2.20	0.41
16:P:147:ARG:HG2	56:P:500:NDP:H8A	2.01	0.41
19:S:3:TRP:CE2	19:S:87:GLU:HB3	2.55	0.41
19:S:20:GLN:NE2	19:S:54:SER:HB3	2.35	0.41
21:U:75:PHE:HD1	21:U:110:GLN:O	2.03	0.41
24:X:28:ARG:HD2	24:X:63:LEU:HD13	2.00	0.41
37:m:30:THR:HG23	37:m:33:ASN:HB2	2.02	0.41
44:v:84:TYR:HA	44:v:87:VAL:HG12	2.02	0.41
7:G:176:GLY:O	7:G:182:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:605:HIS:O	7:G:606:HIS:ND1	2.53	0.41
12:L:140:TRP:CE2	12:L:232:LYS:HG3	2.55	0.41
12:L:232:LYS:HE2	12:L:232:LYS:HB3	1.80	0.41
15:O:120:ARG:HH21	15:O:121:SER:HB3	1.85	0.41
20:T:51:LEU:HD21	20:T:67:PRO:HA	2.02	0.41
21:U:75:PHE:CE2	21:U:89:VAL:HG11	2.54	0.41
31:f:49:TYR:OH	31:f:58:LYS:NZ	2.48	0.41
33:i:48:ILE:HG23	33:i:49:ARG:HG3	2.01	0.41
41:q:82:ASP:C	41:q:84:TYR:H	2.28	0.41
45:x:81:ASN:OD1	47:z:42:HIS:ND1	2.53	0.41
2:B:66:GLU:HA	2:B:69:ILE:HG12	2.01	0.41
4:D:176:ASP:O	4:D:180:GLN:HG2	2.20	0.41
5:E:33:ASN:ND2	7:G:247:GLU:OE1	2.54	0.41
5:E:66:SER:O	5:E:69:LYS:HG3	2.20	0.41
5:E:151:LEU:HD12	5:E:151:LEU:HA	1.90	0.41
7:G:113:ILE:HG13	17:Q:138:LYS:HE3	2.02	0.41
8:H:27:GLU:HA	8:H:281:ILE:HD13	2.03	0.41
12:L:135:GLN:O	12:L:138:LEU:HG	2.20	0.41
12:L:147:SER:OG	12:L:256:ILE:HD11	2.21	0.41
12:L:418:PHE:CD1	36:l:93:GLY:HA2	2.55	0.41
13:M:137:LEU:O	13:M:200:LEU:HB2	2.19	0.41
14:N:39:PHE:CZ	31:f:60:PRO:HB3	2.55	0.41
15:O:74:HIS:HB3	45:x:134:PRO:HD3	2.01	0.41
15:O:83:HIS:CD2	15:O:95:CYS:HB3	2.54	0.41
16:P:157:GLU:HB2	16:P:162:HIS:HE1	1.85	0.41
18:R:94:PRO:HB2	18:R:103:ARG:HB3	2.01	0.41
28:c:61:ARG:NH2	28:c:69:ILE:HD11	2.35	0.41
29:d:19:TYR:O	29:d:23:LEU:HB2	2.19	0.41
32:g:65:PRO:HA	32:g:68:ILE:HG12	2.02	0.41
38:n:80:HIS:O	38:n:82:ASP:N	2.53	0.41
2:B:167:TYR:O	3:C:150:SER:HA	2.20	0.41
3:C:21:LYS:HG2	3:C:32:ASP:HB3	2.02	0.41
3:C:145:LYS:HD3	3:C:145:LYS:HA	1.91	0.41
4:D:192:MET:HE2	4:D:192:MET:HB3	1.71	0.41
8:H:140:SER:O	8:H:144:MET:HG3	2.21	0.41
13:M:335:ILE:HB	13:M:481:MET:HE1	2.02	0.41
13:M:356:TYR:O	13:M:360:LYS:HG3	2.20	0.41
16:P:238:LYS:HE3	16:P:381:TYR:HB3	2.02	0.41
16:P:318:MET:HE3	16:P:318:MET:HB2	1.95	0.41
45:x:185:VAL:HB	45:x:201:ASN:O	2.20	0.41
3:C:100:SER:OG	3:C:102:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:126:HIS:ND1	3:C:129:LEU:HG	2.36	0.41
7:G:69:ASN:OD1	7:G:69:ASN:N	2.53	0.41
7:G:209:PRO:HD2	7:G:742:LEU:HD11	2.03	0.41
11:K:24:ASN:ND2	11:K:30:ILE:HD11	2.36	0.41
12:L:236:ILE:N	12:L:293:THR:OG1	2.53	0.41
12:L:427:VAL:HA	12:L:430:THR:HG22	2.03	0.41
13:M:316:MET:O	13:M:319:VAL:HG12	2.20	0.41
16:P:55:LEU:HD21	16:P:270:LYS:NZ	2.36	0.41
16:P:185:CYS:N	16:P:200:LYS:HD3	2.31	0.41
16:P:370:LEU:HA	16:P:374:PRO:HG2	2.02	0.41
17:Q:59:PRO:HD2	17:Q:73:LYS:O	2.20	0.41
32:g:85:PRO:HG2	32:g:87:LEU:HD22	2.03	0.41
33:i:25:LYS:HA	33:i:28:GLU:OE2	2.20	0.41
45:x:236:LEU:HD12	47:z:17:GLU:HG3	2.02	0.41
46:y:45:LEU:HD23	46:y:67:VAL:HB	2.03	0.41
46:y:99:ASN:OD1	46:y:99:ASN:N	2.52	0.41
46:y:226:GLU:OE2	46:y:226:GLU:HA	2.21	0.41
47:z:99:ASN:OD1	47:z:127:THR:HA	2.20	0.41
1:A:112:LYS:HE3	1:A:112:LYS:HB3	1.81	0.41
4:D:279:LEU:HD23	4:D:279:LEU:HA	1.91	0.41
6:F:227:TYR:HB3	6:F:400:GLU:HB3	2.02	0.41
10:J:72:PHE:HB3	11:K:84:PHE:CE2	2.54	0.41
12:L:127:LEU:HD12	12:L:139:GLY:C	2.44	0.41
13:M:143:TYR:HA	13:M:146:PHE:HB3	2.02	0.41
13:M:409:GLN:HB3	40:p:87:GLY:O	2.21	0.41
13:M:425:GLY:HA2	13:M:428:TYR:CE2	2.56	0.41
14:N:498:TYR:HD2	33:i:50:PRO:HD2	1.85	0.41
16:P:201:ALA:HA	16:P:204:GLU:HG2	2.02	0.41
25:Z:131:MET:HE3	25:Z:131:MET:HB3	1.91	0.41
45:x:165:HIS:CE1	47:z:133:VAL:HG21	2.56	0.41
2:B:103:ALA:HA	4:D:132:LEU:HD22	2.02	0.41
6:F:109:ARG:HD2	6:F:109:ARG:HA	1.88	0.41
7:G:578:ALA:O	7:G:579:LYS:HD3	2.20	0.41
8:H:27:GLU:OE2	8:H:233:TYR:OH	2.25	0.41
12:L:61:ILE:HB	12:L:74:TRP:HB2	2.02	0.41
12:L:528:GLY:HA2	12:L:531:VAL:HG12	2.02	0.41
12:L:608:ARG:O	12:L:612:ARG:HG2	2.20	0.41
13:M:470:MET:O	13:M:470:MET:HG2	2.21	0.41
14:N:93:THR:HG23	14:N:140:ILE:HG22	2.03	0.41
14:N:114:PHE:CD2	14:N:260:PRO:HG3	2.56	0.41
14:N:159:PHE:HB3	14:N:179:TYR:HE2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:189:ILE:HG23	14:N:232:PHE:CD2	2.52	0.41
14:N:244:VAL:HG22	14:N:247:HIS:CE1	2.56	0.41
14:N:338:THR:HA	33:i:48:ILE:HB	2.02	0.41
20:T:66:THR:HG22	20:T:68:GLU:H	1.85	0.41
25:Z:118:TRP:HB3	30:e:53:ARG:NH1	2.34	0.41
26:a:59:LYS:HA	26:a:59:LYS:HD3	1.89	0.41
35:k:6:GLY:C	35:k:8:THR:H	2.27	0.41
2:B:113:ILE:HG22	2:B:113:ILE:O	2.21	0.41
2:B:164:TYR:CE2	4:D:66:TYR:CD1	3.05	0.41
2:B:165:TYR:C	2:B:167:TYR:H	2.28	0.41
2:B:217:ASN:O	16:P:153:ASN:ND2	2.52	0.41
7:G:391:GLU:O	7:G:395:VAL:HG23	2.21	0.41
7:G:490:ASP:N	7:G:490:ASP:OD1	2.54	0.41
12:L:126:MET:HE3	12:L:126:MET:HB3	1.89	0.41
12:L:520:ILE:N	12:L:521:PRO:CD	2.84	0.41
13:M:229:PRO:HD3	13:M:257:LEU:HD11	2.02	0.41
13:M:237:LEU:HB3	13:M:238:PRO:HD3	2.02	0.41
14:N:74:PRO:HB2	31:f:88:PHE:CD2	2.54	0.41
17:Q:57:TYR:HE1	17:Q:77:ASN:HB2	1.85	0.41
18:R:68:ARG:O	18:R:89:LEU:HD23	2.21	0.41
22:V:101:GLY:O	22:V:105:GLU:HG2	2.20	0.41
39:o:67:MET:O	39:o:70:MET:HG3	2.20	0.41
46:y:80:TRP:CD1	46:y:101:GLN:HA	2.55	0.41
46:y:199:TYR:HA	46:y:202:GLN:HG3	2.03	0.41
6:F:125:MET:HE3	6:F:125:MET:HB3	1.79	0.41
7:G:205:LYS:HE3	7:G:205:LYS:HB3	1.84	0.41
7:G:286:GLU:OE2	7:G:308:ARG:NH1	2.44	0.41
7:G:341:ARG:HA	7:G:341:ARG:HD3	1.80	0.41
8:H:201:ALA:CB	8:H:202:PRO:HD3	2.51	0.41
12:L:108:PRO:O	12:L:110:SER:N	2.54	0.41
12:L:198:PHE:CD1	12:L:274:PRO:HG2	2.56	0.41
12:L:241:TRP:CZ3	12:L:261:MET:HE2	2.56	0.41
12:L:325:ALA:HB1	12:L:333:VAL:HG23	2.02	0.41
12:L:382:MET:HE1	12:L:438:LEU:HD23	2.03	0.41
12:L:386:SER:O	12:L:390:ILE:HD12	2.21	0.41
12:L:417:ASN:OD1	12:L:421:TRP:NE1	2.54	0.41
12:L:480:LEU:HG	12:L:484:MET:HE2	2.02	0.41
13:M:109:TRP:CZ2	32:g:62:TRP:HB3	2.56	0.41
13:M:185:LEU:O	13:M:189:LEU:HG	2.21	0.41
13:M:347:ALA:HB1	13:M:384:PHE:CE2	2.56	0.41
13:M:389:MET:HE2	13:M:389:MET:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:278:LEU:HD11	14:N:345:LEU:CD2	2.51	0.41
14:N:348:GLY:HA2	14:N:409:SER:HB2	2.02	0.41
22:V:88:GLU:HA	22:V:91:GLU:OE2	2.20	0.41
30:e:10:ASN:HB3	33:i:78:PRO:HG3	2.02	0.41
36:l:113:PRO:HG3	39:o:10:MET:SD	2.61	0.41
39:o:42:GLN:HA	39:o:46:TYR:CE2	2.56	0.41
46:y:13:ASN:OD1	47:z:30:GLN:NE2	2.53	0.41
2:B:97:GLU:HG3	2:B:189:PRO:HB2	2.03	0.41
2:B:168:SER:HB3	4:D:54:LEU:HD11	2.02	0.41
4:D:182:PHE:O	4:D:186:ILE:HG13	2.21	0.41
6:F:319:LEU:HD13	6:F:358:VAL:HG23	2.02	0.41
10:J:167:ILE:HG13	10:J:171:MET:HG3	2.03	0.41
12:L:120:PHE:CE1	12:L:143:VAL:HG13	2.50	0.41
13:M:36:LEU:O	13:M:40:ILE:HG22	2.20	0.41
16:P:96:LEU:HD13	16:P:121:MET:HE1	2.02	0.41
18:R:102:LEU:HD23	18:R:102:LEU:HA	1.97	0.41
23:W:40:ILE:H	23:W:40:ILE:HD12	1.86	0.41
46:y:187:LYS:HD2	46:y:187:LYS:O	2.20	0.41
3:C:72:GLU:HG3	3:C:90:THR:O	2.21	0.40
3:C:174:GLU:HB3	17:Q:94:THR:HG23	2.04	0.40
5:E:143:ILE:HG13	5:E:144:GLU:N	2.36	0.40
5:E:207:VAL:O	5:E:211:GLU:OE1	2.39	0.40
6:F:283:GLU:HA	6:F:286:SER:OG	2.21	0.40
6:F:345:SER:HB2	6:F:393:LEU:HD21	2.02	0.40
7:G:173:CYS:O	7:G:283:ARG:NH1	2.47	0.40
7:G:234:VAL:HG11	7:G:258:SER:HB2	2.03	0.40
7:G:550:LEU:HD12	7:G:551:ASN:N	2.36	0.40
12:L:294:SER:HA	12:L:317:SER:HA	2.03	0.40
12:L:384:ILE:HG23	12:L:475:LEU:HD21	2.02	0.40
14:N:80:HIS:CE1	14:N:81:LEU:HG	2.57	0.40
14:N:236:GLY:O	14:N:240:LYS:HG2	2.22	0.40
24:X:85:TYR:CD2	24:X:91:LEU:HB3	2.56	0.40
33:i:53:PHE:HB3	33:i:54:TRP:CE3	2.56	0.40
34:j:56:PRO:HG2	34:j:57:TRP:CZ3	2.56	0.40
37:m:65:ARG:HH22	40:p:91:ARG:NH1	2.18	0.40
40:p:53:GLU:O	40:p:57:TRP:HD1	2.04	0.40
47:z:32:LYS:HE2	47:z:32:LYS:HB2	1.79	0.40
3:C:9:TYR:OH	3:C:48:HIS:NE2	2.29	0.40
6:F:341:ILE:HD11	6:F:378:ILE:HD12	2.02	0.40
8:H:195:LEU:HD22	8:H:201:ALA:HB3	2.03	0.40
8:H:205:LEU:HD23	8:H:206:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:30:ILE:O	12:L:34:THR:OG1	2.34	0.40
12:L:314:SER:O	12:L:318:GLN:HG2	2.21	0.40
12:L:435:PHE:HD1	12:L:438:LEU:HD12	1.87	0.40
12:L:495:ASN:HD21	40:p:64:VAL:HA	1.86	0.40
12:L:587:GLU:HG3	37:m:27:PHE:CD2	2.56	0.40
23:W:78:LEU:HB3	58:W:200:8Q1:S44	2.61	0.40
47:z:90:ASN:H	47:z:108:VAL:HG11	1.86	0.40
6:F:349:LEU:HD12	6:F:350:ILE:H	1.86	0.40
7:G:507:LYS:HG2	7:G:540:ASN:OD1	2.21	0.40
7:G:641:VAL:HA	7:G:642:PRO:HD3	1.97	0.40
7:G:646:THR:HG21	23:W:131:ASN:HD22	1.86	0.40
8:H:94:PHE:HB2	8:H:98:MET:HB2	2.03	0.40
8:H:98:MET:HG2	26:a:27:TYR:HB2	2.03	0.40
12:L:276:PHE:HB3	12:L:283:LEU:HD21	2.03	0.40
13:M:70:GLU:H	13:M:84:LEU:HB2	1.85	0.40
13:M:327:ASN:HB2	13:M:330:GLY:H	1.86	0.40
13:M:373:THR:HG21	13:M:449:PHE:HE1	1.86	0.40
13:M:389:MET:SD	13:M:426:ALA:HA	2.61	0.40
14:N:258:PRO:HB2	14:N:261:VAL:HG23	2.02	0.40
27:b:5:GLU:HG2	27:b:6:LYS:N	2.37	0.40
27:b:6:LYS:H	27:b:6:LYS:HG2	1.72	0.40
32:g:46:MET:HE3	32:g:46:MET:HB2	1.85	0.40
38:n:94:LYS:HB2	38:n:97:ARG:HB2	2.03	0.40
46:y:153:ASP:OD1	46:y:171:GLN:HG3	2.21	0.40
2:B:158:CYS:HA	2:B:163:GLY:HA3	2.02	0.40
4:D:299:ARG:O	4:D:303:LYS:HD2	2.21	0.40
6:F:207:LYS:HA	6:F:207:LYS:HD2	1.85	0.40
7:G:267:ILE:HG13	7:G:268:CYS:N	2.37	0.40
7:G:341:ARG:HH22	7:G:733:LYS:CB	2.34	0.40
10:J:34:PHE:HE1	11:K:40:LEU:HD13	1.83	0.40
13:M:174:PHE:HD1	14:N:441:ILE:HD13	1.85	0.40
16:P:58:LYS:CB	16:P:66:VAL:HB	2.51	0.40
25:Z:114:ASP:OD1	25:Z:114:ASP:N	2.43	0.40
29:d:19:TYR:CE1	29:d:23:LEU:HD12	2.56	0.40
34:j:35:MET:HE3	34:j:35:MET:HB3	1.90	0.40
1:A:100:LEU:HA	1:A:100:LEU:HD23	1.85	0.40
2:B:182:ASP:HB3	2:B:205:LYS:HE2	2.03	0.40
5:E:172:MET:O	6:F:182:ARG:NH1	2.52	0.40
7:G:325:GLU:HB2	7:G:457:ARG:HH12	1.86	0.40
9:I:122:ARG:HD3	9:I:174:VAL:O	2.22	0.40
10:J:171:MET:HE1	10:J:173:ARG:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:98:LEU:O	12:L:101:ILE:HG12	2.21	0.40
12:L:582:TYR:HB2	13:M:300:ARG:HG3	2.04	0.40
13:M:105:ILE:HD12	13:M:120:ILE:HD12	2.02	0.40
13:M:307:ILE:HD12	13:M:432:LEU:HD12	2.03	0.40
14:N:77:THR:HG22	31:f:8:LEU:H	1.87	0.40
14:N:426:ALA:O	14:N:430:VAL:HG23	2.22	0.40
20:T:112:ILE:HG23	20:T:113:GLU:OE2	2.20	0.40
36:l:125:PRO:HD3	40:p:71:ARG:HD2	2.03	0.40
40:p:33:MET:HE3	40:p:37:ILE:HD11	2.03	0.40
45:x:94:SER:OG	45:x:95:SER:N	2.54	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	A	88/119 (74%)	86 (98%)	2 (2%)	0	100	100
2	B	155/218 (71%)	136 (88%)	19 (12%)	0	100	100
3	C	183/190 (96%)	164 (90%)	19 (10%)	0	100	100
4	D	383/394 (97%)	354 (92%)	29 (8%)	0	100	100
5	E	190/255 (74%)	172 (90%)	18 (10%)	0	100	100
6	F	432/486 (89%)	399 (92%)	33 (8%)	0	100	100
7	G	686/748 (92%)	618 (90%)	68 (10%)	0	100	100
8	H	322/325 (99%)	290 (90%)	31 (10%)	1 (0%)	36	66
9	I	167/222 (75%)	164 (98%)	3 (2%)	0	100	100
10	J	134/205 (65%)	129 (96%)	5 (4%)	0	100	100
11	K	88/100 (88%)	85 (97%)	3 (3%)	0	100	100
12	L	613/669 (92%)	569 (93%)	44 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	M	485/495 (98%)	466 (96%)	19 (4%)	0	100	100
14	N	486/499 (97%)	469 (96%)	17 (4%)	0	100	100
15	O	120/159 (76%)	113 (94%)	7 (6%)	0	100	100
16	P	330/402 (82%)	299 (91%)	30 (9%)	1 (0%)	36	66
17	Q	117/154 (76%)	111 (95%)	6 (5%)	0	100	100
18	R	60/110 (54%)	60 (100%)	0	0	100	100
19	S	91/97 (94%)	82 (90%)	9 (10%)	0	100	100
20	T	82/122 (67%)	78 (95%)	4 (5%)	0	100	100
21	U	77/126 (61%)	72 (94%)	5 (6%)	0	100	100
22	V	138/169 (82%)	133 (96%)	5 (4%)	0	100	100
23	W	106/133 (80%)	102 (96%)	4 (4%)	0	100	100
24	X	95/106 (90%)	90 (95%)	5 (5%)	0	100	100
25	Z	122/143 (85%)	113 (93%)	9 (7%)	0	100	100
26	a	56/65 (86%)	54 (96%)	2 (4%)	0	100	100
27	b	37/65 (57%)	37 (100%)	0	0	100	100
28	c	71/88 (81%)	62 (87%)	9 (13%)	0	100	100
29	d	71/81 (88%)	68 (96%)	3 (4%)	0	100	100
30	e	62/83 (75%)	58 (94%)	4 (6%)	0	100	100
31	f	96/106 (91%)	86 (90%)	10 (10%)	0	100	100
32	g	73/114 (64%)	67 (92%)	6 (8%)	0	100	100
33	i	81/98 (83%)	75 (93%)	6 (7%)	0	100	100
34	j	49/69 (71%)	40 (82%)	9 (18%)	0	100	100
35	k	45/72 (62%)	38 (84%)	7 (16%)	0	100	100
36	l	48/125 (38%)	47 (98%)	1 (2%)	0	100	100
37	m	67/71 (94%)	63 (94%)	4 (6%)	0	100	100
38	n	107/117 (92%)	97 (91%)	10 (9%)	0	100	100
39	o	75/103 (73%)	69 (92%)	6 (8%)	0	100	100
40	p	91/106 (86%)	81 (89%)	10 (11%)	0	100	100
41	q	63/159 (40%)	55 (87%)	8 (13%)	0	100	100
42	r	8/131 (6%)	8 (100%)	0	0	100	100
44	v	28/113 (25%)	27 (96%)	1 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
45	x	209/256 (82%)	190 (91%)	19 (9%)	0	100	100
46	y	261/278 (94%)	239 (92%)	22 (8%)	0	100	100
47	z	230/275 (84%)	211 (92%)	19 (8%)	0	100	100
All	All	7578/9221 (82%)	7026 (93%)	550 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	201	ALA
16	P	329	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/106 (79%)	84 (100%)	0	100	100
2	B	132/184 (72%)	132 (100%)	0	100	100
3	C	175/179 (98%)	175 (100%)	0	100	100
4	D	331/340 (97%)	331 (100%)	0	100	100
5	E	166/220 (76%)	166 (100%)	0	100	100
6	F	353/396 (89%)	353 (100%)	0	100	100
7	G	571/625 (91%)	571 (100%)	0	100	100
8	H	271/272 (100%)	271 (100%)	0	100	100
9	I	151/195 (77%)	151 (100%)	0	100	100
10	J	123/186 (66%)	123 (100%)	0	100	100
11	K	78/86 (91%)	78 (100%)	0	100	100
12	L	518/568 (91%)	517 (100%)	1 (0%)	87	85
13	M	426/434 (98%)	426 (100%)	0	100	100
14	N	406/416 (98%)	406 (100%)	0	100	100
15	O	107/141 (76%)	107 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	P	273/334 (82%)	273 (100%)	0	100	100
17	Q	100/128 (78%)	100 (100%)	0	100	100
18	R	55/97 (57%)	55 (100%)	0	100	100
19	S	82/85 (96%)	82 (100%)	0	100	100
20	T	79/112 (70%)	79 (100%)	0	100	100
21	U	72/113 (64%)	72 (100%)	0	100	100
22	V	123/148 (83%)	123 (100%)	0	100	100
23	W	97/114 (85%)	97 (100%)	0	100	100
24	X	87/94 (93%)	87 (100%)	0	100	100
25	Z	99/115 (86%)	99 (100%)	0	100	100
26	a	48/53 (91%)	48 (100%)	0	100	100
27	b	32/53 (60%)	32 (100%)	0	100	100
28	c	64/71 (90%)	64 (100%)	0	100	100
29	d	58/66 (88%)	58 (100%)	0	100	100
30	e	59/73 (81%)	58 (98%)	1 (2%)	53	69
31	f	78/84 (93%)	78 (100%)	0	100	100
32	g	65/96 (68%)	65 (100%)	0	100	100
33	i	75/90 (83%)	75 (100%)	0	100	100
34	j	42/51 (82%)	42 (100%)	0	100	100
35	k	38/60 (63%)	38 (100%)	0	100	100
36	l	39/97 (40%)	39 (100%)	0	100	100
37	m	57/59 (97%)	57 (100%)	0	100	100
38	n	92/99 (93%)	92 (100%)	0	100	100
39	o	67/87 (77%)	67 (100%)	0	100	100
40	p	83/93 (89%)	83 (100%)	0	100	100
41	q	54/133 (41%)	54 (100%)	0	100	100
42	r	10/118 (8%)	10 (100%)	0	100	100
44	v	23/84 (27%)	23 (100%)	0	100	100
45	x	180/216 (83%)	180 (100%)	0	100	100
46	y	220/232 (95%)	220 (100%)	0	100	100
47	z	187/228 (82%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6530/7831 (83%)	6528 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
12	L	457	HIS
30	e	52	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	4	GLN
4	D	33	ASN
4	D	43	HIS
4	D	78	GLN
4	D	244	GLN
5	E	54	GLN
5	E	221	HIS
6	F	292	ASN
7	G	58	ASN
7	G	235	GLN
7	G	500	HIS
7	G	570	GLN
7	G	686	ASN
12	L	132	ASN
12	L	190	GLN
13	M	301	GLN
13	M	329	GLN
13	M	409	GLN
13	M	487	ASN
14	N	84	ASN
14	N	117	GLN
14	N	326	HIS
16	P	54	HIS
16	P	231	ASN
16	P	291	HIS
16	P	345	ASN
17	Q	143	ASN
18	R	92	ASN
18	R	109	HIS
19	S	35	ASN

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Mol	Chain	Res	Type
19	S	43	ASN
20	T	118	HIS
21	U	74	ASN
21	U	77	ASN
23	W	65	ASN
23	W	126	ASN
25	Z	41	ASN
26	a	24	ASN
26	a	30	HIS
27	b	13	GLN
28	c	36	ASN
29	d	21	ASN
30	e	47	HIS
32	g	47	ASN
32	g	95	GLN
35	k	26	ASN
38	n	76	ASN
45	x	225	ASN
46	y	42	HIS
46	y	125	ASN
46	y	160	HIS
46	y	184	ASN
47	z	47	ASN
47	z	107	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 3 are monoatomic - leaving 22 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	$\# Z > 2$
48	SF4	F	501	6	0,12,12	-	-	-		
48	SF4	G	802	7	0,12,12	-	-	-		
53	PC7	v	201	-	51,51,51	0.98	4 (7%)	57,59,59	1.06	2 (3%)
58	8Q1	W	200	-	32,34,34	1.62	6 (18%)	39,43,43	1.52	4 (10%)
52	PTY	H	402	-	49,49,49	0.89	4 (8%)	52,54,54	1.12	2 (3%)
60	PSF	z	301	-	28,29,29	1.20	4 (14%)	30,36,36	1.20	2 (6%)
48	SF4	G	803	7	0,12,12	-	-	-		
48	SF4	I	500	9	0,12,12	-	-	-		
51	UQ9	H	401	-	35,35,58	2.66	13 (37%)	43,45,73	1.61	9 (20%)
58	8Q1	n	200	-	32,34,34	1.62	6 (18%)	39,43,43	1.49	4 (10%)
54	PGT	N	501	-	40,40,50	1.18	4 (10%)	43,46,56	1.11	2 (4%)
48	SF4	B	500	2	0,12,12	-	-	-		
53	PC7	M	501	-	51,51,51	0.98	4 (7%)	57,59,59	1.10	2 (3%)
50	FMN	F	500	-	33,33,33	1.07	2 (6%)	48,50,50	1.23	7 (14%)
61	T7X	z	302	-	61,61,61	0.85	4 (6%)	70,73,73	1.07	2 (2%)
52	PTY	N	502	-	49,49,49	0.88	4 (8%)	52,54,54	1.08	2 (3%)
49	FES	G	801	7	0,4,4	-	-	-		
49	FES	E	500	5	0,4,4	-	-	-		
59	LMN	d	101	-	72,72,72	1.70	14 (19%)	92,98,98	1.17	6 (6%)
48	SF4	I	501	9	0,12,12	-	-	-		
52	PTY	M	502	-	49,49,49	0.89	4 (8%)	52,54,54	1.12	2 (3%)
56	NDP	P	500	-	51,52,52	2.33	8 (15%)	71,80,80	1.57	17 (23%)

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
48	SF4	F	501	6	-	-	0/6/5/5
48	SF4	G	802	7	-	-	0/6/5/5
53	PC7	v	201	-	-	28/55/55/55	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	8Q1	W	200	-	-	21/41/41/41	-
52	PTY	H	402	-	-	16/53/53/53	-
60	PSF	z	301	-	-	13/35/35/35	-
48	SF4	G	803	7	-	-	0/6/5/5
48	SF4	I	500	9	-	-	0/6/5/5
51	UQ9	H	401	-	-	9/30/54/81	0/1/1/1
58	8Q1	n	200	-	-	11/41/41/41	-
54	PGT	N	501	-	-	28/45/45/55	-
48	SF4	B	500	2	-	-	0/6/5/5
53	PC7	M	501	-	-	18/55/55/55	-
50	FMN	F	500	-	-	4/18/18/18	0/3/3/3
61	T7X	z	302	-	-	32/56/80/80	0/1/1/1
52	PTY	N	502	-	-	21/53/53/53	-
49	FES	G	801	7	-	-	0/1/1/1
49	FES	E	500	5	-	-	0/1/1/1
59	LMN	d	101	-	-	30/50/130/130	0/4/4/4
48	SF4	I	501	9	-	-	0/6/5/5
52	PTY	M	502	-	-	25/53/53/53	-
56	NDP	P	500	-	-	5/34/77/77	0/5/5/5

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	500	NDP	P2B-O2B	13.06	1.82	1.59
51	H	401	UQ9	C6-C1	10.74	1.54	1.35
58	W	200	8Q1	C39-N41	5.17	1.45	1.33
58	W	200	8Q1	C34-N36	5.12	1.45	1.33
58	n	200	8Q1	C34-N36	5.10	1.45	1.33
58	n	200	8Q1	C39-N41	5.08	1.45	1.33
51	H	401	UQ9	C4-C3	4.85	1.53	1.36
59	d	101	LMN	O5-C1	4.69	1.53	1.41
59	d	101	LMN	CBS-CCM	4.52	1.63	1.53
59	d	101	LMN	CBT-CCM	4.31	1.63	1.53
56	P	500	NDP	PA-O3	4.17	1.64	1.59
56	P	500	NDP	PN-O5D	4.11	1.75	1.59
51	H	401	UQ9	C7-C8	4.09	1.57	1.50
59	d	101	LMN	CBR-CCM	3.75	1.61	1.54
59	d	101	LMN	O1-C1	-3.55	1.34	1.40
50	F	500	FMN	C4A-N5	3.39	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	P	500	NDP	O2B-C2B	-3.27	1.32	1.44
54	N	501	PGT	O3-C11	3.03	1.42	1.33
54	N	501	PGT	O2-C31	2.97	1.42	1.34
59	d	101	LMN	OBY-CCR	2.86	1.49	1.41
59	d	101	LMN	OBZ-CCS	2.80	1.49	1.41
52	M	502	PTY	O7-C6	-2.77	1.40	1.46
52	H	402	PTY	O7-C6	-2.76	1.40	1.46
59	d	101	LMN	O4-C4	2.74	1.50	1.43
59	d	101	LMN	OBX-CCF	2.74	1.51	1.44
53	v	201	PC7	O2-C2	-2.71	1.40	1.46
60	z	301	PSF	O11-C3	-2.71	1.40	1.46
51	H	401	UQ9	C11-C9	2.67	1.56	1.51
53	M	501	PC7	O2-C2	-2.66	1.40	1.46
51	H	401	UQ9	C7-C6	2.54	1.56	1.51
51	H	401	UQ9	C26-C24	2.47	1.56	1.51
52	N	502	PTY	O7-C6	-2.47	1.40	1.46
50	F	500	FMN	C10-N1	2.46	1.38	1.33
56	P	500	NDP	C5A-C4A	2.45	1.43	1.39
51	H	401	UQ9	C16-C14	2.45	1.56	1.51
51	H	401	UQ9	C21-C19	2.44	1.56	1.51
59	d	101	LMN	OBX-CCJ	2.44	1.48	1.41
53	v	201	PC7	O3-C11	2.42	1.40	1.33
58	n	200	8Q1	C1-S44	2.42	1.82	1.76
58	W	200	8Q1	C1-S44	2.42	1.81	1.76
51	H	401	UQ9	O4-C4M	-2.38	1.40	1.45
60	z	301	PSF	O52-C5	2.38	1.40	1.33
56	P	500	NDP	C2B-C1B	2.37	1.59	1.53
61	z	302	T7X	O16-C8	-2.36	1.41	1.46
53	M	501	PC7	O3-C11	2.36	1.40	1.33
52	N	502	PTY	O4-C30	2.36	1.40	1.33
52	H	402	PTY	O4-C30	2.36	1.40	1.33
52	M	502	PTY	O4-C30	2.35	1.40	1.33
61	z	302	T7X	O18-C11	2.34	1.40	1.33
59	d	101	LMN	CBQ-CCM	2.33	1.58	1.54
52	M	502	PTY	O4-C1	-2.33	1.40	1.45
53	M	501	PC7	O3-C3	-2.32	1.40	1.45
61	z	302	T7X	O16-C10	2.32	1.40	1.34
61	z	302	T7X	O18-C9	-2.30	1.40	1.45
58	n	200	8Q1	O35-C34	-2.29	1.19	1.23
59	d	101	LMN	C3-C4	-2.29	1.46	1.52
58	W	200	8Q1	O35-C34	-2.28	1.19	1.23
53	v	201	PC7	O3-C3	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	H	402	PTY	O4-C1	-2.26	1.40	1.45
58	n	200	8Q1	C6-C1	2.24	1.53	1.50
54	N	501	PGT	P-O3P	2.24	1.68	1.59
56	P	500	NDP	C2A-N1A	2.24	1.37	1.33
52	N	502	PTY	O7-C8	2.22	1.40	1.34
52	N	502	PTY	O4-C1	-2.21	1.40	1.45
60	z	301	PSF	O52-C4	-2.20	1.40	1.45
58	n	200	8Q1	O40-C39	-2.20	1.18	1.23
51	H	401	UQ9	C6-C5	2.19	1.52	1.46
51	H	401	UQ9	C17-C18	2.19	1.57	1.50
58	W	200	8Q1	O40-C39	-2.19	1.18	1.23
53	M	501	PC7	O2-C31	2.13	1.40	1.34
53	v	201	PC7	O2-C31	2.13	1.40	1.34
52	H	402	PTY	O7-C8	2.13	1.40	1.34
60	z	301	PSF	O11-C1	2.13	1.40	1.34
51	H	401	UQ9	O3-C3M	-2.11	1.40	1.45
59	d	101	LMN	CBQ-CBK	2.10	1.59	1.52
56	P	500	NDP	C7N-N7N	2.09	1.39	1.33
58	W	200	8Q1	C6-C1	2.08	1.53	1.50
52	M	502	PTY	O7-C8	2.08	1.40	1.34
54	N	501	PGT	O2-C2	-2.07	1.41	1.46
59	d	101	LMN	O5-C5	2.07	1.49	1.44
51	H	401	UQ9	O5-C5	-2.02	1.18	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	n	200	8Q1	C6-C1-S44	5.31	119.73	113.40
58	W	200	8Q1	C6-C1-S44	5.22	119.63	113.40
56	P	500	NDP	P2B-O2B-C2B	-5.01	110.05	123.43
51	H	401	UQ9	C7-C8-C9	-4.50	119.07	126.83
61	z	302	T7X	O16-C10-C12	4.27	120.72	111.48
53	M	501	PC7	O2-C31-C32	4.21	120.58	111.48
59	d	101	LMN	CCR-O4-C4	-4.05	108.39	117.98
53	v	201	PC7	O2-C31-C32	4.03	120.20	111.48
52	H	402	PTY	O7-C8-C11	3.98	120.09	111.48
60	z	301	PSF	O11-C1-C13	3.89	119.90	111.48
52	M	502	PTY	O7-C8-C11	3.89	119.89	111.48
54	N	501	PGT	O2-C31-C32	3.88	119.88	111.48
52	N	502	PTY	O7-C8-C11	3.84	119.79	111.48
56	P	500	NDP	O2B-P2B-O1X	-3.65	96.31	109.33
51	H	401	UQ9	C12-C13-C14	-3.46	119.71	127.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	W	200	8Q1	O4-C1-C6	-3.41	120.04	123.98
56	P	500	NDP	O3-PA-O1A	-3.30	100.78	110.70
59	d	101	LMN	CCS-OCB-CCQ	-3.28	110.21	117.98
50	F	500	FMN	C4-N3-C2	-3.26	119.85	125.64
58	n	200	8Q1	O4-C1-C6	-3.21	120.27	123.98
56	P	500	NDP	PA-O5B-C5B	-3.18	103.13	121.35
51	H	401	UQ9	C17-C18-C19	-3.16	120.39	127.62
56	P	500	NDP	PN-O5D-C5D	-3.02	104.04	121.35
51	H	401	UQ9	C25-C24-C26	2.96	120.37	115.23
59	d	101	LMN	OBX-CCF-CCQ	2.90	115.72	109.72
52	M	502	PTY	O4-C30-C31	2.80	120.36	111.83
53	M	501	PC7	O3-C11-C12	2.76	120.24	111.83
51	H	401	UQ9	C22-C23-C24	-2.73	121.36	127.62
52	N	502	PTY	O4-C30-C31	2.72	120.12	111.83
58	W	200	8Q1	C43-S44-C1	2.69	109.80	101.84
52	H	402	PTY	O4-C30-C31	2.67	119.98	111.83
60	z	301	PSF	O52-C5-C6	2.67	119.97	111.83
50	F	500	FMN	C4A-C4-N3	2.67	120.04	113.25
56	P	500	NDP	O2N-PN-O3	2.65	114.45	107.27
61	z	302	T7X	O18-C11-C31	2.64	119.87	111.83
51	H	401	UQ9	C20-C19-C21	2.61	119.77	115.23
50	F	500	FMN	O4-C4-C4A	-2.58	119.73	126.53
56	P	500	NDP	O3X-P2B-O2X	2.56	117.42	107.80
59	d	101	LMN	CCJ-OBX-CCF	2.56	118.71	113.72
53	v	201	PC7	O3-C11-C12	2.55	119.61	111.83
51	H	401	UQ9	C15-C14-C16	2.51	119.58	115.23
50	F	500	FMN	C5A-C9A-N10	2.50	120.23	117.97
54	N	501	PGT	O3-C11-C12	2.47	119.37	111.83
56	P	500	NDP	C5B-C4B-C3B	-2.47	106.32	115.21
56	P	500	NDP	C2A-N1A-C6A	-2.43	114.73	118.73
56	P	500	NDP	O2N-PN-O1N	2.43	123.73	112.44
50	F	500	FMN	C4A-C10-N10	2.42	119.95	116.48
51	H	401	UQ9	C8-C7-C6	2.42	118.05	112.08
56	P	500	NDP	O5D-PN-O1N	-2.30	99.81	108.94
51	H	401	UQ9	C10-C9-C11	2.30	119.22	115.23
50	F	500	FMN	C9A-C5A-N5	-2.29	120.02	122.45
58	n	200	8Q1	C43-S44-C1	2.28	108.59	101.84
59	d	101	LMN	OBX-CCJ-CCL	2.26	115.02	110.37
56	P	500	NDP	N3A-C4A-N9A	2.25	130.99	127.17
56	P	500	NDP	O4B-C4B-C3B	2.23	109.57	105.15
50	F	500	FMN	C10-C4A-N5	-2.19	120.34	124.81
56	P	500	NDP	O3X-P2B-O2B	-2.16	97.43	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	W	200	8Q1	C38-C39-N41	2.12	120.20	116.34
58	n	200	8Q1	O4-C1-S44	-2.11	120.00	122.68
56	P	500	NDP	C5A-C4A-N3A	-2.11	123.81	126.72
56	P	500	NDP	C5D-C4D-C3D	-2.10	107.65	115.21
56	P	500	NDP	O2A-PA-O1A	2.08	122.14	112.44
59	d	101	LMN	CBL-CBR-CCM	-2.01	111.09	117.19

There are no chirality outliers.

All (261) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	F	500	FMN	N10-C1'-C2'-O2'
50	F	500	FMN	N10-C1'-C2'-C3'
50	F	500	FMN	C5'-O5'-P-O1P
52	H	402	PTY	C2-C3-O11-P1
52	H	402	PTY	C5-O14-P1-O11
52	H	402	PTY	C5-O14-P1-O12
52	M	502	PTY	N1-C2-C3-O11
52	M	502	PTY	C11-C8-O7-C6
52	M	502	PTY	C3-O11-P1-O12
52	M	502	PTY	C3-O11-P1-O13
52	M	502	PTY	C3-O11-P1-O14
52	M	502	PTY	C5-O14-P1-O11
52	M	502	PTY	C5-O14-P1-O13
52	N	502	PTY	O10-C8-O7-C6
52	N	502	PTY	C3-O11-P1-O12
52	N	502	PTY	C3-O11-P1-O14
53	v	201	PC7	C32-C31-O2-C2
53	v	201	PC7	C1-O3P-P-O1P
53	v	201	PC7	C1-O3P-P-O4P
53	v	201	PC7	C4-O4P-P-O3P
53	v	201	PC7	C4-O4P-P-O1P
53	v	201	PC7	C4-O4P-P-O2P
53	v	201	PC7	O4P-C4-C5-N
54	N	501	PGT	C32-C31-O2-C2
54	N	501	PGT	C1-O3P-P-O1P
54	N	501	PGT	C1-O3P-P-O2P
54	N	501	PGT	C1-O3P-P-O4P
54	N	501	PGT	C4-O4P-P-O3P
54	N	501	PGT	C4-O4P-P-O1P
56	P	500	NDP	C5D-O5D-PN-O1N
58	W	200	8Q1	O4-C1-C6-C7

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Mol	Chain	Res	Type	Atoms
58	W	200	8Q1	S44-C1-C6-C7
58	W	200	8Q1	O4-C1-S44-C43
58	W	200	8Q1	C6-C1-S44-C43
58	W	200	8Q1	O27-C28-C29-C30
58	W	200	8Q1	O27-C28-C29-C31
58	W	200	8Q1	O27-C28-C29-C32
58	W	200	8Q1	C28-C29-C32-C34
58	W	200	8Q1	C28-C29-C32-O33
58	W	200	8Q1	C30-C29-C32-C34
58	W	200	8Q1	C30-C29-C32-O33
58	W	200	8Q1	C31-C29-C32-C34
58	W	200	8Q1	C31-C29-C32-O33
58	W	200	8Q1	O33-C32-C34-N36
58	W	200	8Q1	N41-C42-C43-S44
58	n	200	8Q1	O4-C1-S44-C43
58	n	200	8Q1	C6-C1-S44-C43
58	n	200	8Q1	O27-C28-C29-C30
58	n	200	8Q1	O27-C28-C29-C31
58	n	200	8Q1	O27-C28-C29-C32
58	n	200	8Q1	C42-C43-S44-C1
58	n	200	8Q1	C28-O27-P24-O3
58	n	200	8Q1	C28-O27-P24-O2
58	n	200	8Q1	C28-O27-P24-O1
59	d	101	LMN	O5-C1-O1-CBS
59	d	101	LMN	CBK-CBQ-CCM-CBR
59	d	101	LMN	CBK-CBQ-CCM-CBS
59	d	101	LMN	CBK-CBQ-CCM-CBT
59	d	101	LMN	OBV-CBT-CCM-CBQ
59	d	101	LMN	OBV-CBT-CCM-CBR
59	d	101	LMN	OBX-CCJ-OBV-CBT
59	d	101	LMN	CCL-CCJ-OBV-CBT
60	z	301	PSF	CB-O1-P-O2
60	z	301	PSF	CB-O1-P-O4
60	z	301	PSF	CB-O1-P-O3
60	z	301	PSF	N-CA-CB-O1
60	z	301	PSF	C-CA-CB-O1
61	z	302	T7X	C12-C10-O16-C8
52	M	502	PTY	C31-C30-O4-C1
53	M	501	PC7	C12-C11-O3-C3
52	M	502	PTY	O30-C30-O4-C1
53	M	501	PC7	O11-C11-O3-C3
59	d	101	LMN	OBZ-CCS-OCB-CCQ

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Mol	Chain	Res	Type	Atoms
59	d	101	LMN	CCW-CCS-OCB-CCQ
52	M	502	PTY	O10-C8-O7-C6
53	v	201	PC7	O31-C31-O2-C2
54	N	501	PGT	O31-C31-O2-C2
61	z	302	T7X	O17-C10-O16-C8
52	N	502	PTY	C11-C8-O7-C6
51	H	401	UQ9	C25-C24-C26-C27
51	H	401	UQ9	C12-C11-C9-C10
51	H	401	UQ9	C23-C24-C26-C27
51	H	401	UQ9	C12-C11-C9-C8
56	P	500	NDP	O4D-C1D-N1N-C6N
59	d	101	LMN	OAJ-CBN-CCD-OBZ
51	H	401	UQ9	C9-C11-C12-C13
59	d	101	LMN	OAJ-CBN-CCD-CCO
59	d	101	LMN	C2-C1-O1-CBS
60	z	301	PSF	C13-C1-O11-C3
59	d	101	LMN	CBI-CBK-CBQ-CCM
56	P	500	NDP	O4B-C4B-C5B-O5B
51	H	401	UQ9	C19-C21-C22-C23
59	d	101	LMN	OBV-CBT-CCM-CBS
59	d	101	LMN	O5-C5-C6-O6
61	z	302	T7X	C11-C31-C32-C33
53	v	201	PC7	C11-C12-C13-C14
60	z	301	PSF	O12-C1-O11-C3
51	H	401	UQ9	C24-C26-C27-C28
61	z	302	T7X	C31-C11-O18-C9
54	N	501	PGT	C31-C32-C33-C34
53	v	201	PC7	C18-C19-C20-C21
52	H	402	PTY	C33-C34-C35-C36
53	v	201	PC7	C20-C21-C22-C23
54	N	501	PGT	C17-C18-C19-C20
53	M	501	PC7	C43-C44-C45-C46
59	d	101	LMN	CBJ-CBL-CBR-CCM
52	M	502	PTY	C22-C23-C24-C25
61	z	302	T7X	O13-C7-C8-C9
53	M	501	PC7	C13-C14-C15-C16
52	M	502	PTY	C19-C20-C21-C22
53	v	201	PC7	C33-C34-C35-C36
59	d	101	LMN	CBG-CBI-CBK-CBQ
52	N	502	PTY	C25-C26-C27-C28
61	z	302	T7X	O19-C11-O18-C9
53	M	501	PC7	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
53	v	201	PC7	C34-C35-C36-C37
52	M	502	PTY	C24-C25-C26-C27
58	W	200	8Q1	N36-C37-C38-C39
53	v	201	PC7	C19-C20-C21-C22
52	M	502	PTY	O14-C5-C6-O7
54	N	501	PGT	C15-C16-C17-C18
58	W	200	8Q1	C6-C7-C8-C9
52	H	402	PTY	C11-C8-O7-C6
61	z	302	T7X	C36-C37-C38-C39
53	v	201	PC7	O2-C2-C3-O3
61	z	302	T7X	C12-C13-C14-C15
52	H	402	PTY	C23-C24-C25-C26
59	d	101	LMN	CBD-CBF-CBH-CBJ
52	N	502	PTY	C32-C33-C34-C35
54	N	501	PGT	C13-C14-C15-C16
59	d	101	LMN	CBC-CBE-CBG-CBI
58	W	200	8Q1	O33-C32-C34-O35
52	H	402	PTY	C11-C12-C13-C14
52	M	502	PTY	O14-C5-C6-C1
59	d	101	LMN	OAI-CBM-CCC-OBY
58	W	200	8Q1	C11-C10-C9-C8
61	z	302	T7X	C32-C33-C34-C35
56	P	500	NDP	C3B-C4B-C5B-O5B
58	n	200	8Q1	C12-C13-C14-C15
52	N	502	PTY	O4-C1-C6-C5
54	N	501	PGT	C1-C2-C3-O3
60	z	301	PSF	C2-C3-C4-O52
53	M	501	PC7	C41-C42-C43-C44
53	v	201	PC7	C17-C18-C19-C20
61	z	302	T7X	C39-C40-C41-C42
61	z	302	T7X	C33-C34-C35-C36
52	N	502	PTY	C1-C6-O7-C8
54	N	501	PGT	O4P-C4-C5-C6
53	M	501	PC7	O3P-C1-C2-O2
53	v	201	PC7	O3P-C1-C2-O2
52	N	502	PTY	C37-C38-C39-C40
53	v	201	PC7	C14-C15-C16-C17
60	z	301	PSF	O11-C3-C4-O52
53	v	201	PC7	C12-C13-C14-C15
53	M	501	PC7	C42-C43-C44-C45
53	M	501	PC7	C35-C36-C37-C38
53	M	501	PC7	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
54	N	501	PGT	O4P-C4-C5-O5
61	z	302	T7X	C41-C42-C43-C44
53	v	201	PC7	C1-C2-C3-O3
52	H	402	PTY	O10-C8-O7-C6
61	z	302	T7X	C15-C16-C17-C18
61	z	302	T7X	C19-C20-C21-C22
61	z	302	T7X	C22-C23-C24-C25
52	N	502	PTY	C11-C12-C13-C14
53	M	501	PC7	C16-C17-C18-C19
53	M	501	PC7	C32-C33-C34-C35
54	N	501	PGT	O3P-C1-C2-C3
60	z	301	PSF	O2-C2-C3-C4
52	N	502	PTY	C33-C34-C35-C36
53	M	501	PC7	C20-C21-C22-C23
51	H	401	UQ9	C1-C6-C7-C8
54	N	501	PGT	C16-C17-C18-C19
61	z	302	T7X	C9-C8-O16-C10
52	H	402	PTY	C14-C15-C16-C17
61	z	302	T7X	C40-C41-C42-C43
52	N	502	PTY	O14-C5-C6-O7
60	z	301	PSF	O2-C2-C3-O11
61	z	302	T7X	O13-C7-C8-O16
51	H	401	UQ9	C5-C6-C7-C8
52	N	502	PTY	C2-C3-O11-P1
53	v	201	PC7	C5-C4-O4P-P
54	N	501	PGT	O2-C2-C3-O3
53	M	501	PC7	O4P-C4-C5-N
54	N	501	PGT	C12-C13-C14-C15
59	d	101	LMN	O1-CBS-CCM-CBQ
59	d	101	LMN	O1-CBS-CCM-CBR
53	v	201	PC7	C38-C39-C40-C41
53	v	201	PC7	O3P-C1-C2-C3
52	M	502	PTY	C11-C12-C13-C14
52	H	402	PTY	C35-C36-C37-C38
54	N	501	PGT	C5-C4-O4P-P
52	H	402	PTY	C12-C13-C14-C15
59	d	101	LMN	CCM-CBT-OBV-CCJ
52	N	502	PTY	O4-C1-C6-O7
52	H	402	PTY	C13-C14-C15-C16
52	M	502	PTY	C33-C34-C35-C36
52	H	402	PTY	N1-C2-C3-O11
54	N	501	PGT	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
53	v	201	PC7	C15-C16-C17-C18
52	N	502	PTY	O14-C5-C6-C1
53	M	501	PC7	O3P-C1-C2-C3
54	N	501	PGT	O3P-C1-C2-O2
61	z	302	T7X	C38-C39-C40-C41
53	v	201	PC7	O3-C11-C12-C13
61	z	302	T7X	C25-C26-C27-C28
53	M	501	PC7	C19-C20-C21-C22
61	z	302	T7X	O18-C11-C31-C32
52	N	502	PTY	C39-C40-C41-C42
54	N	501	PGT	O3-C11-C12-C13
53	v	201	PC7	C41-C42-C43-C44
52	M	502	PTY	C37-C38-C39-C40
59	d	101	LMN	CAW-CAY-CBA-CBC
53	v	201	PC7	C39-C40-C41-C42
52	H	402	PTY	C37-C38-C39-C40
53	M	501	PC7	C21-C22-C23-C24
61	z	302	T7X	C31-C32-C33-C34
61	z	302	T7X	C7-C8-C9-O18
52	M	502	PTY	C15-C16-C17-C18
52	M	502	PTY	C8-C11-C12-C13
52	M	502	PTY	C25-C26-C27-C28
52	N	502	PTY	C31-C30-O4-C1
52	N	502	PTY	O30-C30-O4-C1
53	M	501	PC7	C14-C15-C16-C17
61	z	302	T7X	C13-C14-C15-C16
59	d	101	LMN	CAZ-CBB-CBD-CBF
52	H	402	PTY	C18-C19-C20-C21
61	z	302	T7X	C16-C17-C18-C19
61	z	302	T7X	C18-C19-C20-C21
61	z	302	T7X	C21-C22-C23-C24
54	N	501	PGT	C37-C38-C39-C40
59	d	101	LMN	CBB-CBD-CBF-CBH
56	P	500	NDP	C4B-C5B-O5B-PA
54	N	501	PGT	O11-C11-O3-C3
54	N	501	PGT	O5-C5-C6-O6
61	z	302	T7X	C24-C25-C26-C27
58	n	200	8Q1	C13-C14-C15-C16
54	N	501	PGT	C12-C11-O3-C3
50	F	500	FMN	C5'-O5'-P-O2P
52	N	502	PTY	C14-C15-C16-C17
52	M	502	PTY	C35-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
61	z	302	T7X	O16-C10-C12-C13
61	z	302	T7X	C1-O1-P1-O11
58	W	200	8Q1	C29-C32-C34-O35
52	N	502	PTY	C30-C31-C32-C33
53	v	201	PC7	C16-C17-C18-C19
59	d	101	LMN	CAY-CBA-CBC-CBE
52	M	502	PTY	C12-C11-C8-O7
54	N	501	PGT	O2-C31-C32-C33
52	N	502	PTY	C36-C37-C38-C39
60	z	301	PSF	O11-C1-C13-C14
61	z	302	T7X	C34-C35-C36-C37
52	H	402	PTY	C15-C16-C17-C18
58	W	200	8Q1	C29-C32-C34-N36
61	z	302	T7X	O17-C10-C12-C13
52	M	502	PTY	C12-C11-C8-O10
54	N	501	PGT	O31-C31-C32-C33
59	d	101	LMN	CCF-CCQ-OCB-CCS
60	z	301	PSF	O12-C1-C13-C14
52	M	502	PTY	C21-C22-C23-C24
59	d	101	LMN	OBY-CCR-O4-C4

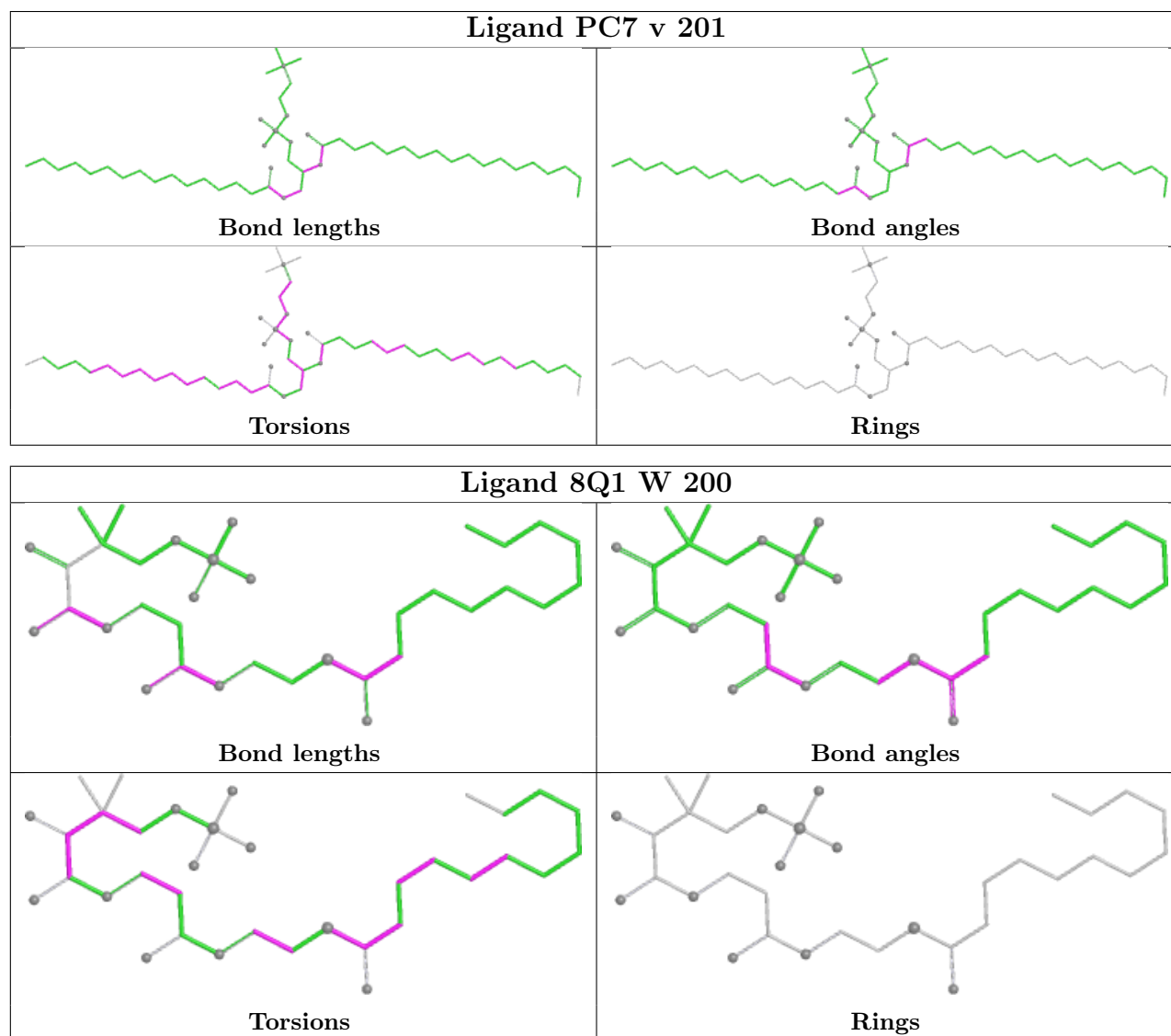
There are no ring outliers.

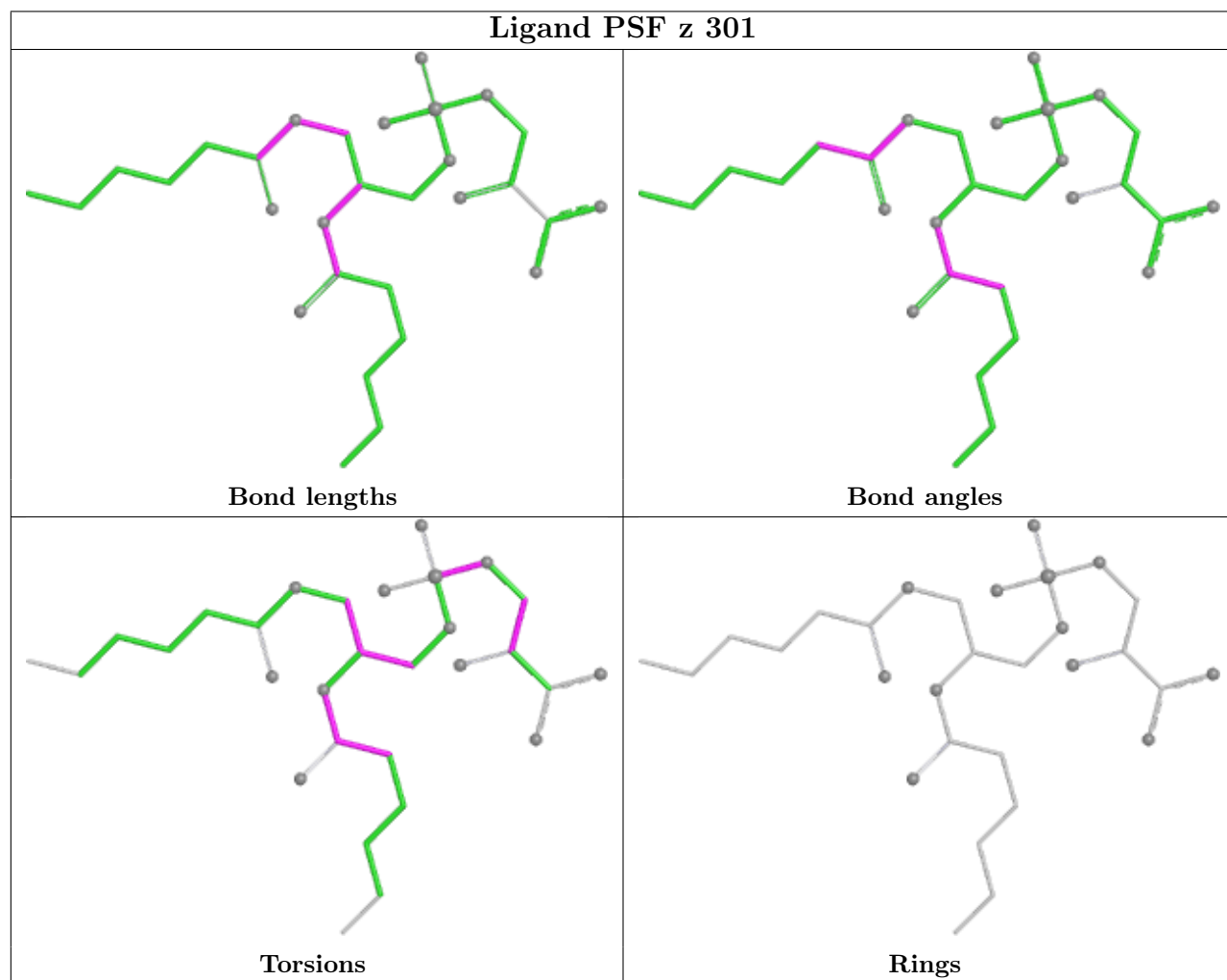
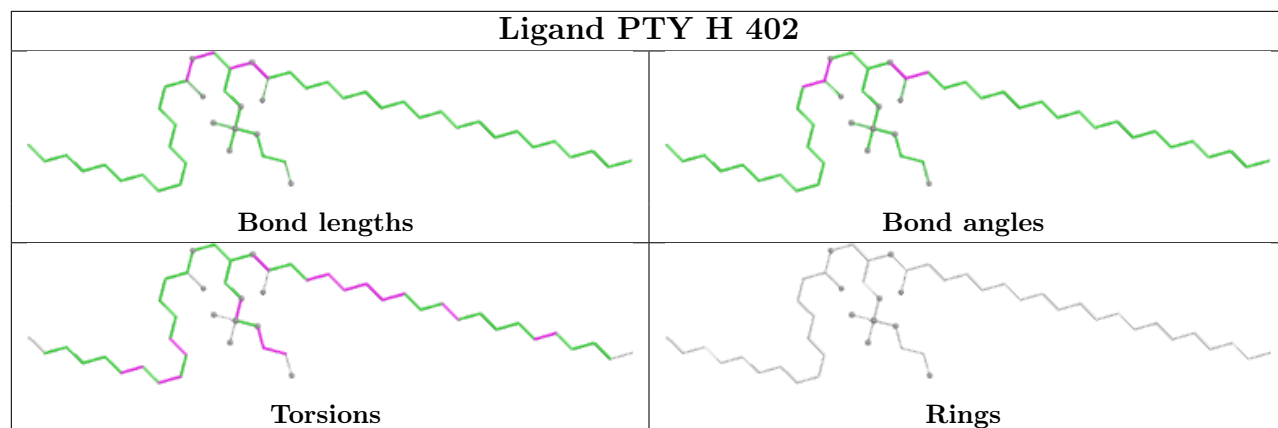
13 monomers are involved in 38 short contacts:

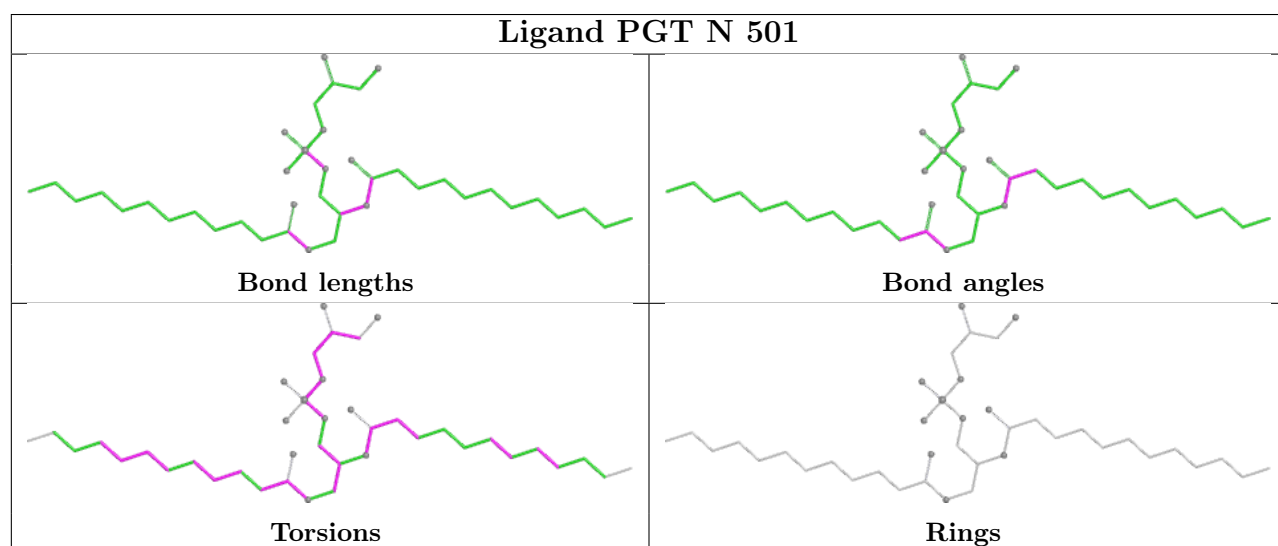
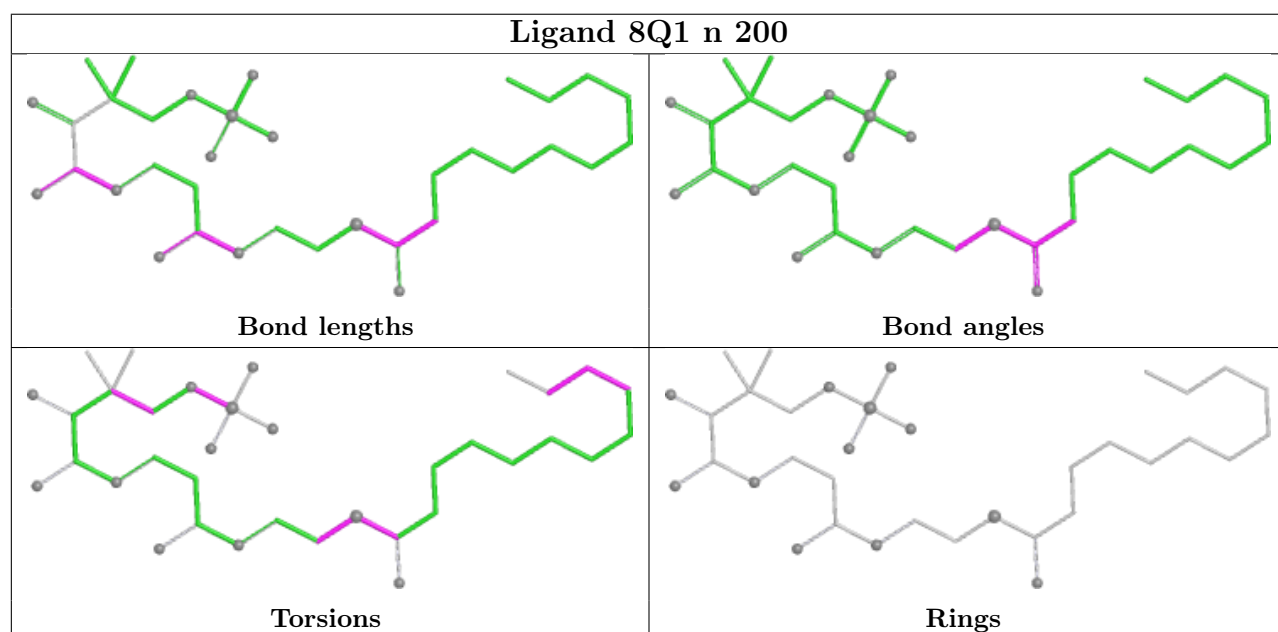
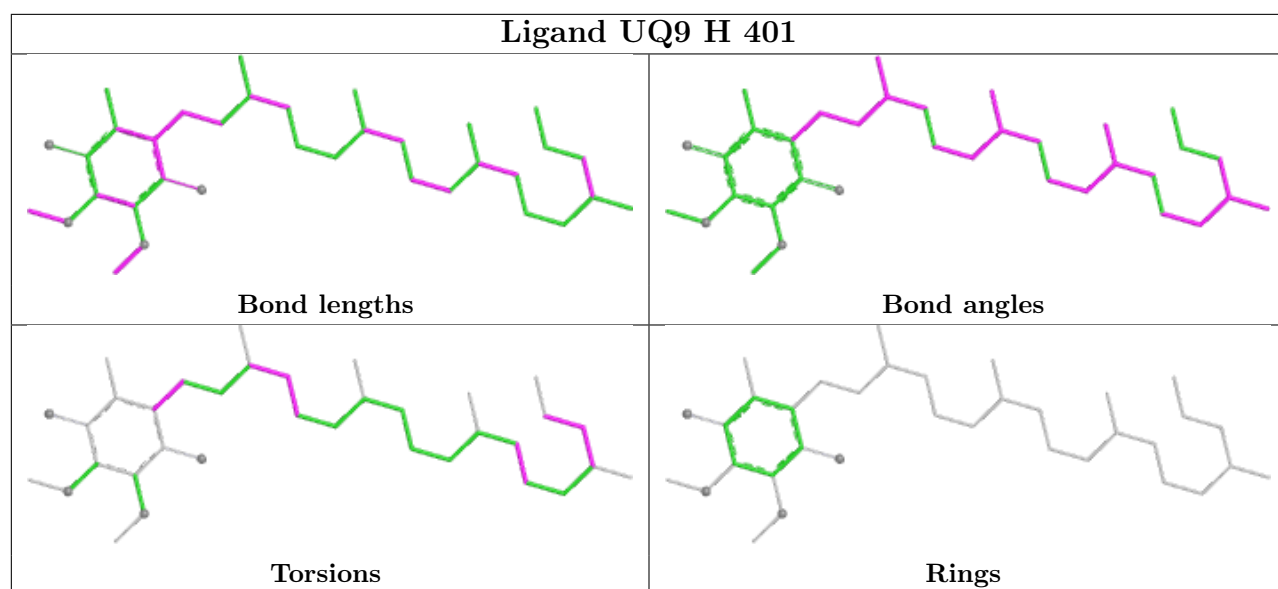
Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	F	501	SF4	2	0
48	G	802	SF4	1	0
53	v	201	PC7	4	0
58	W	200	8Q1	2	0
52	H	402	PTY	3	0
51	H	401	UQ9	2	0
54	N	501	PGT	1	0
53	M	501	PC7	6	0
50	F	500	FMN	3	0
52	N	502	PTY	1	0
49	E	500	FES	2	0
59	d	101	LMN	7	0
56	P	500	NDP	4	0

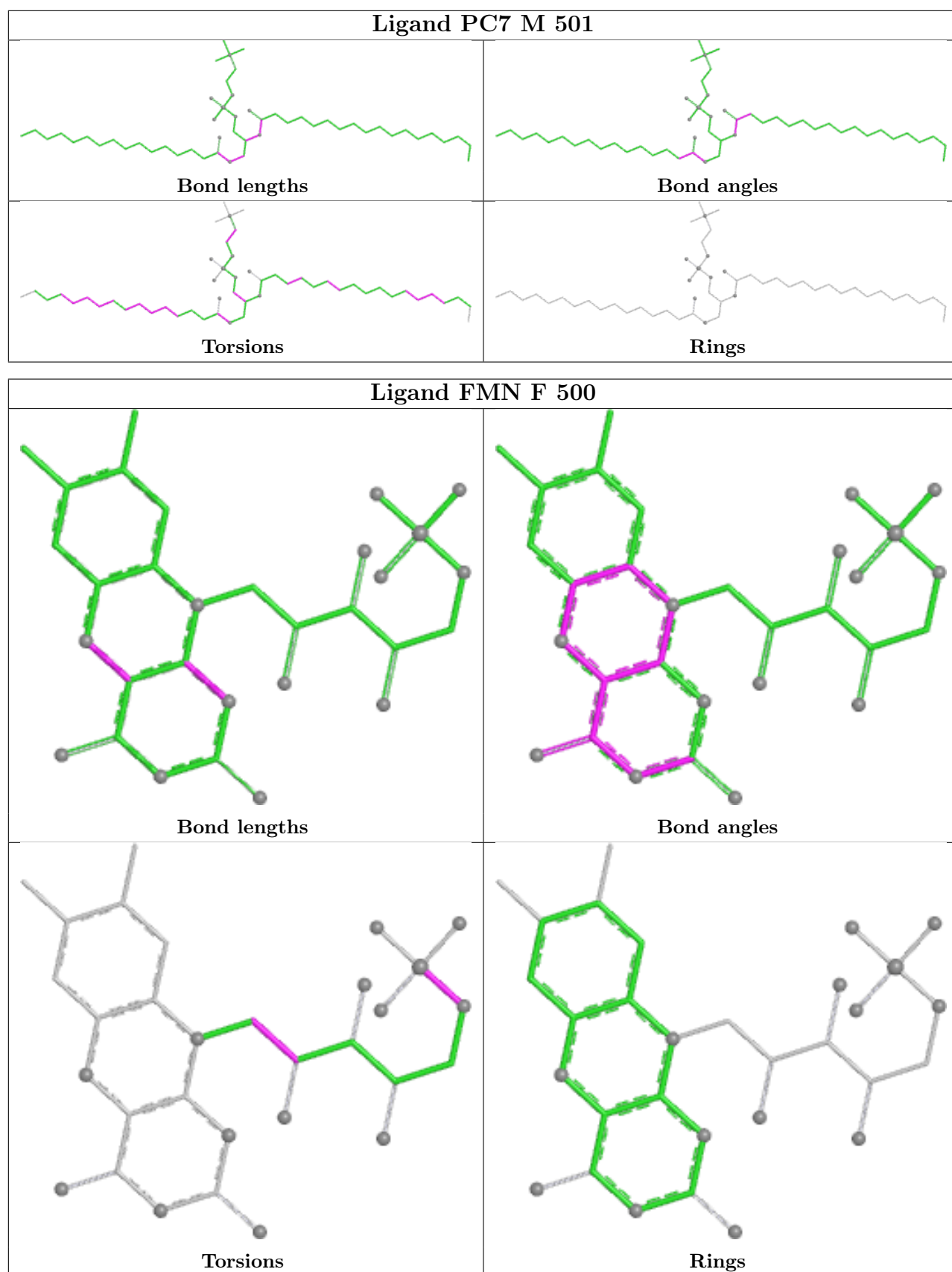
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

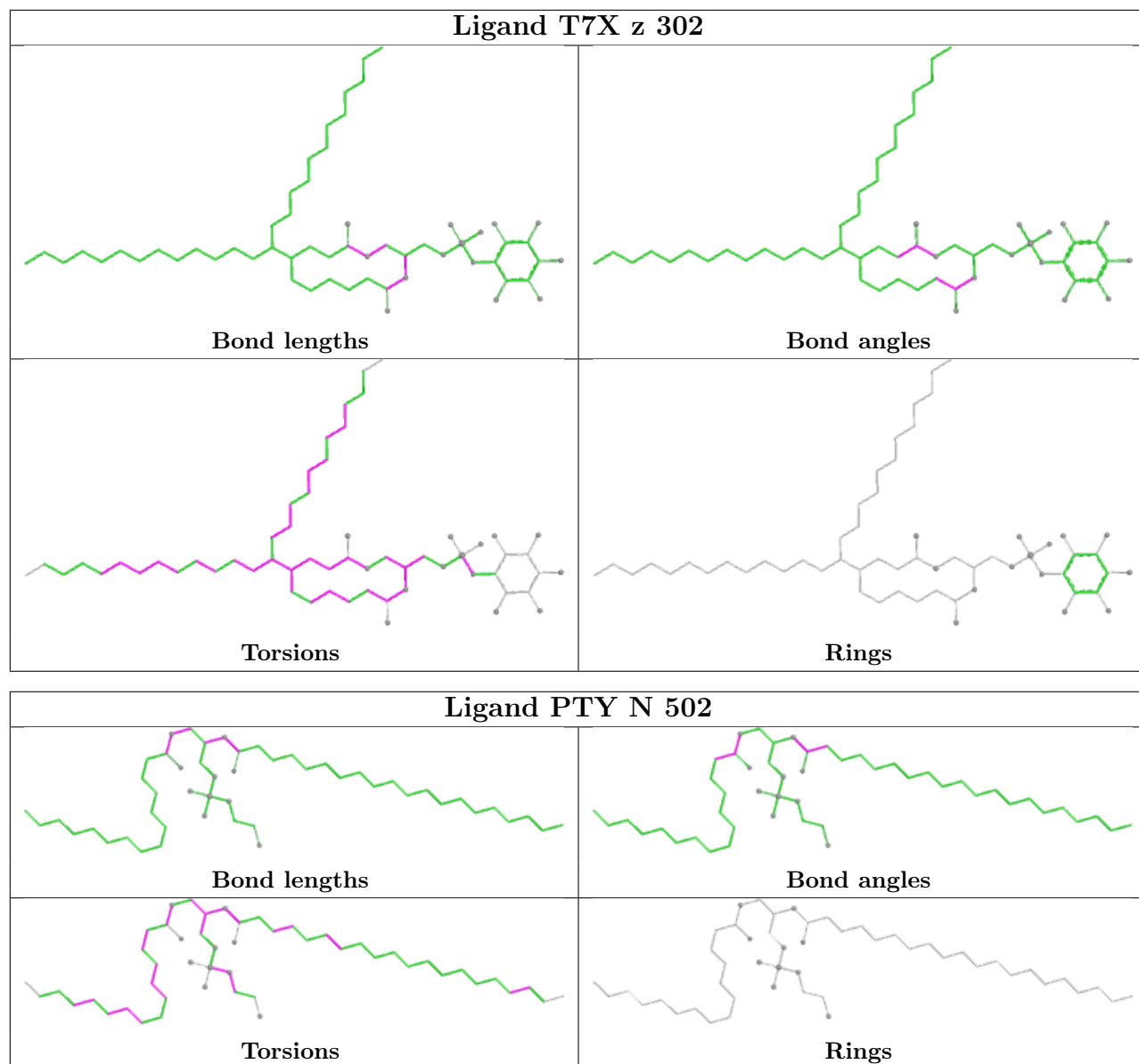
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

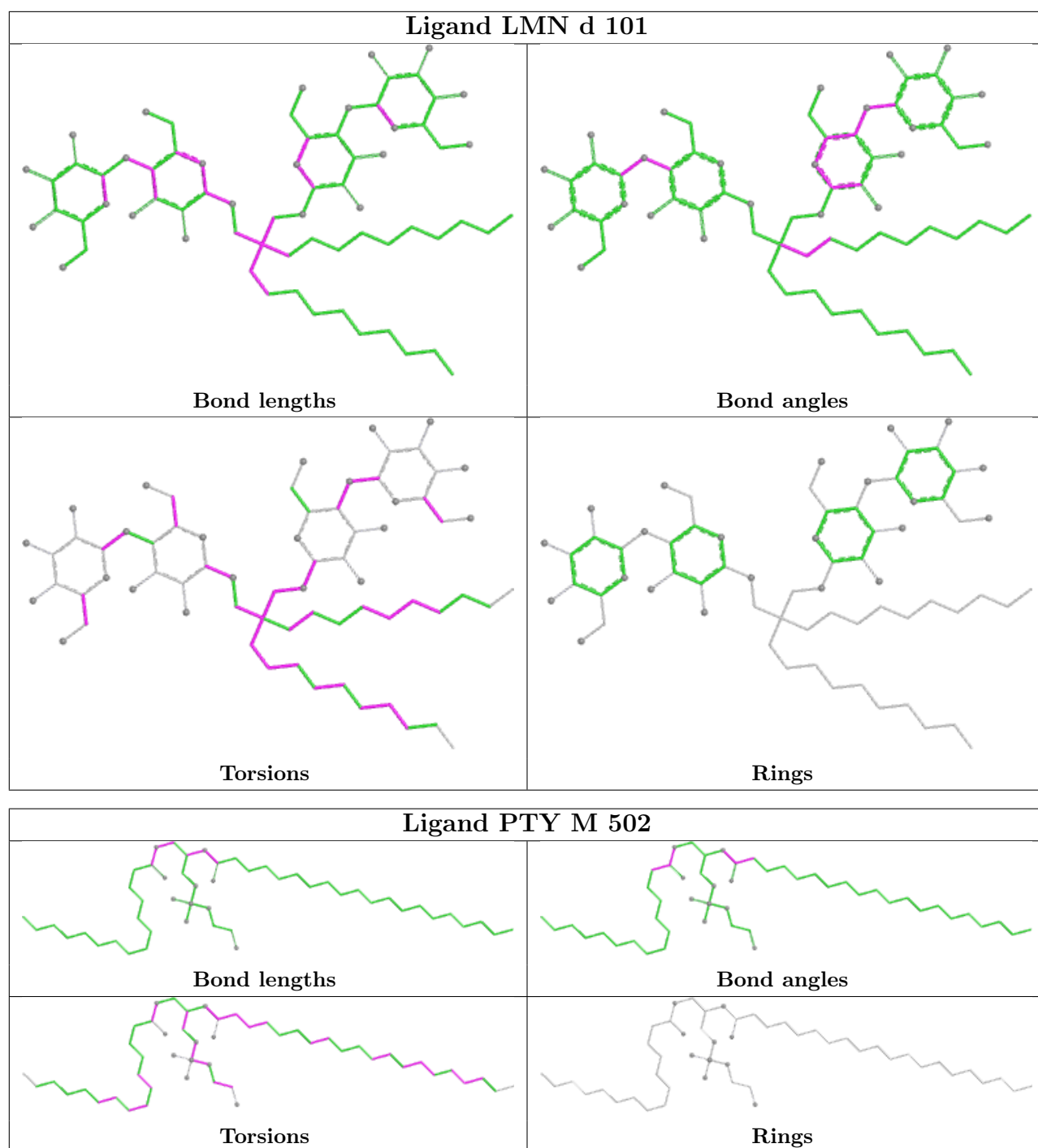


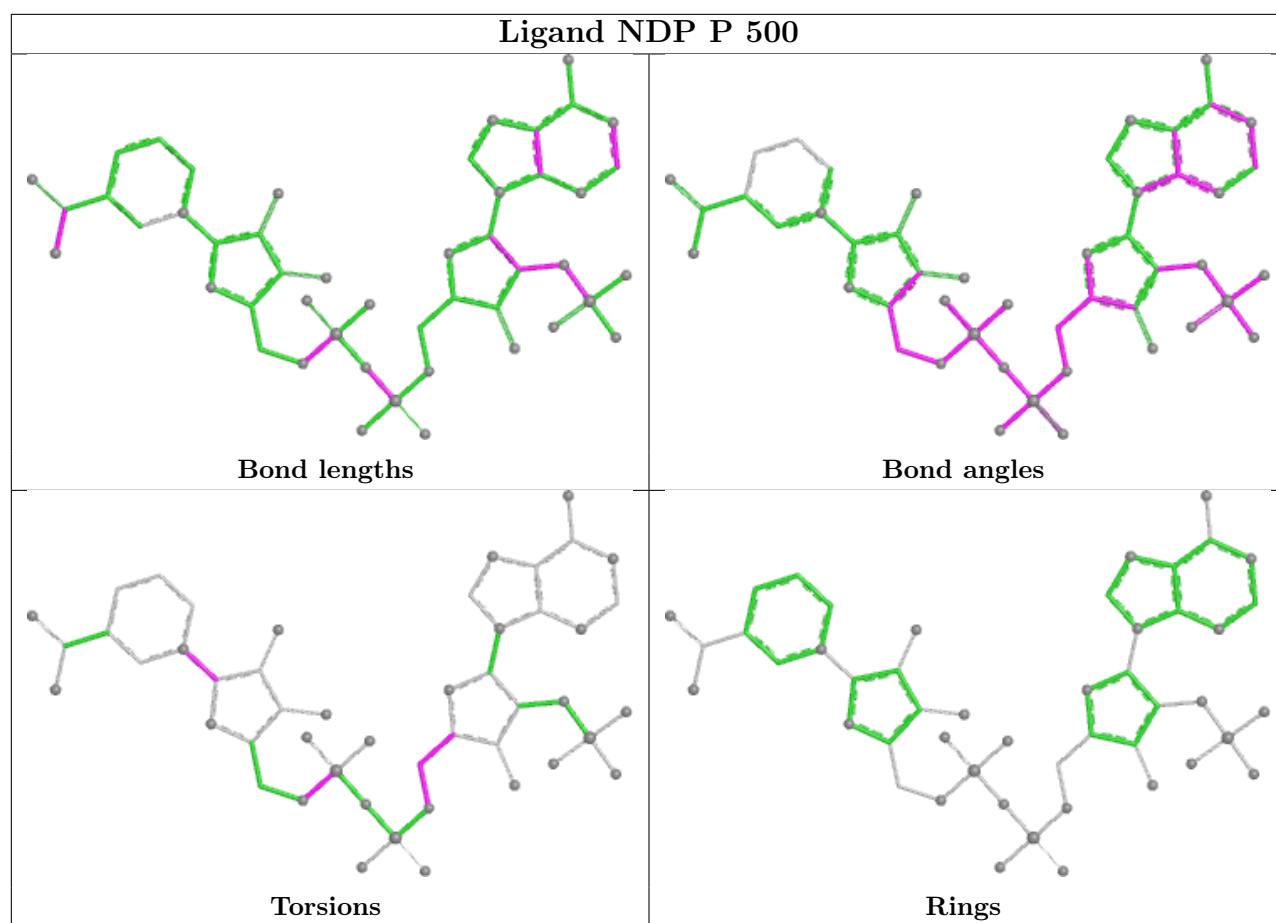












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

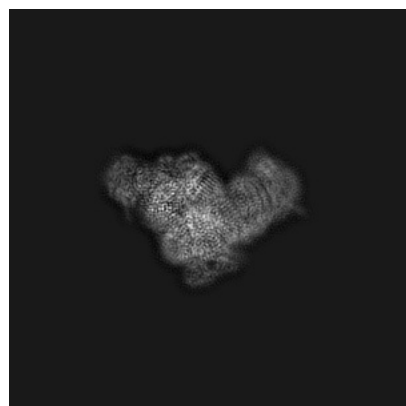
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11876. These allow visual inspection of the internal detail of the map and identification of artifacts.

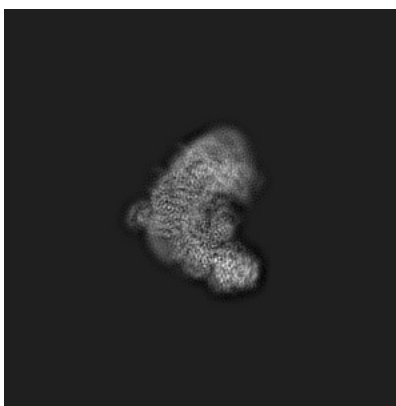
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

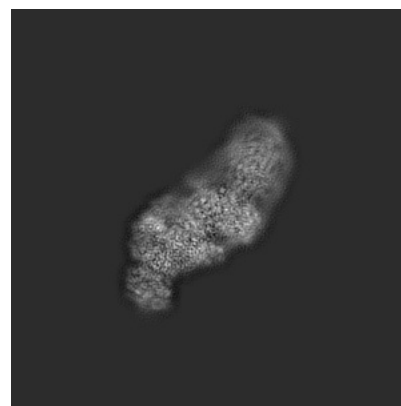
6.1.1 Primary map



X

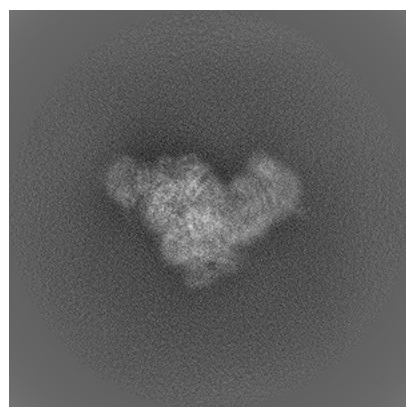


Y

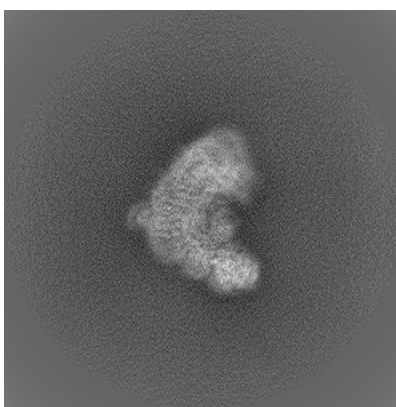


Z

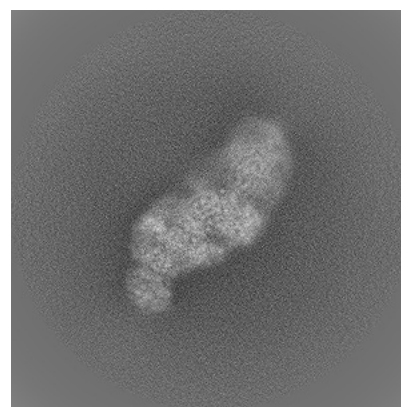
6.1.2 Raw map



X



Y

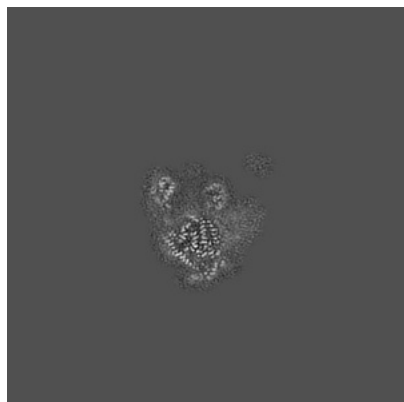


Z

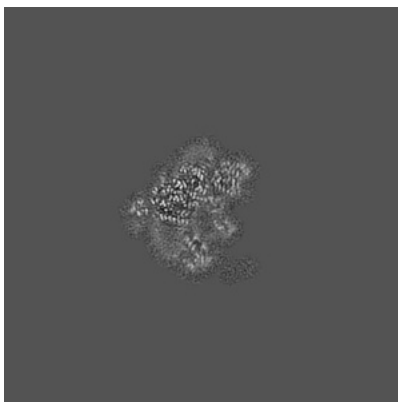
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

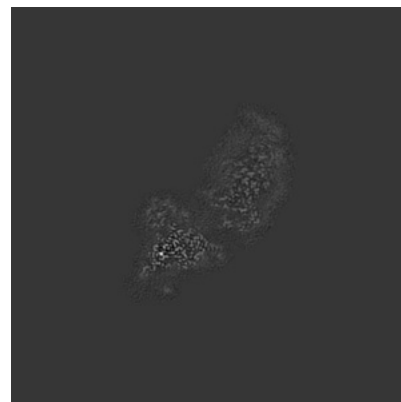
6.2.1 Primary map



X Index: 300

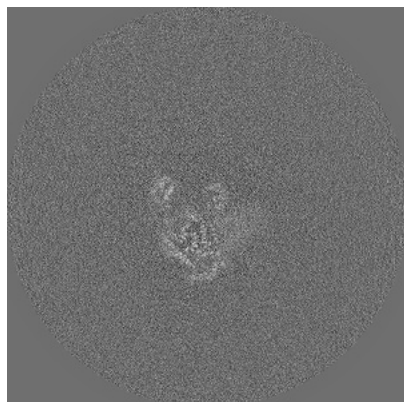


Y Index: 300

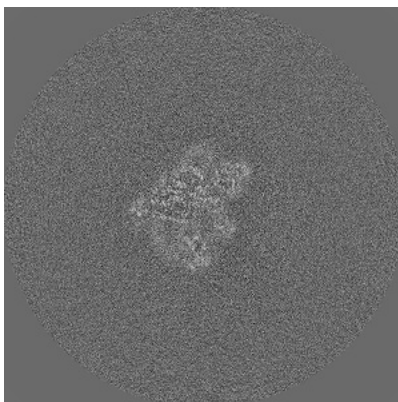


Z Index: 300

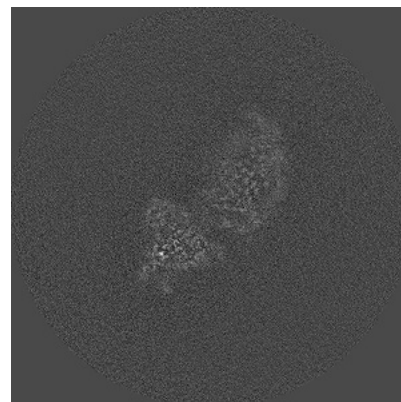
6.2.2 Raw map



X Index: 300



Y Index: 300



Z Index: 300

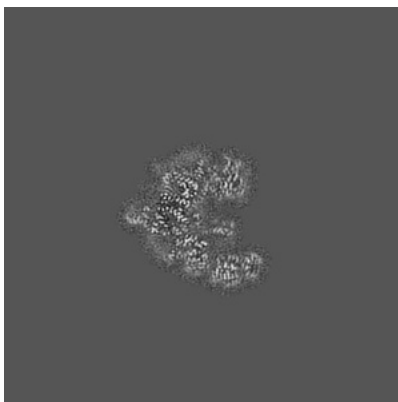
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

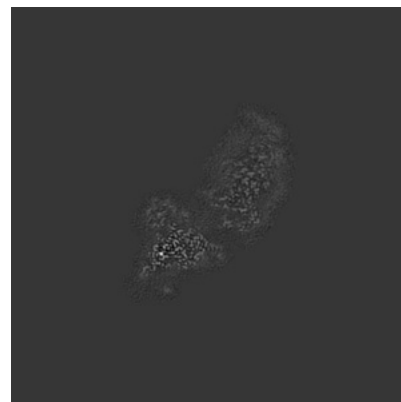
6.3.1 Primary map



X Index: 222

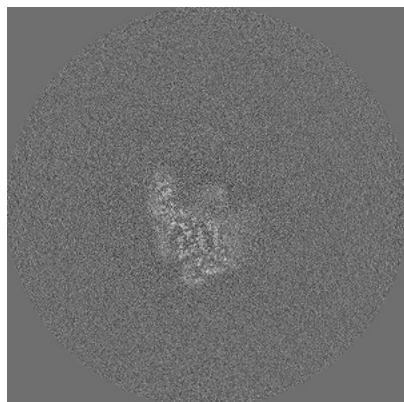


Y Index: 273

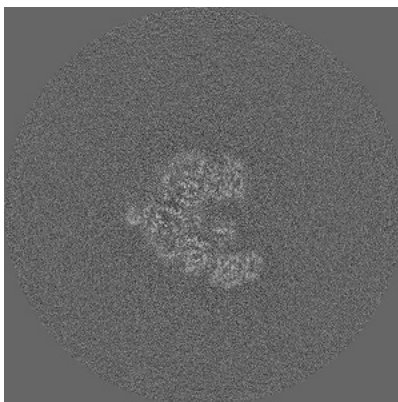


Z Index: 300

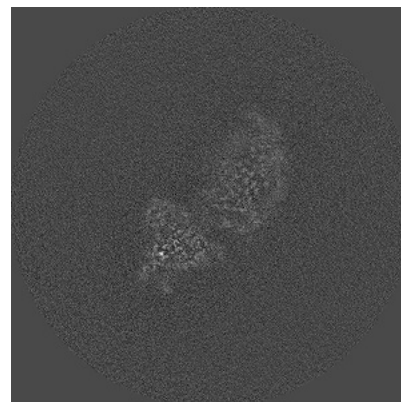
6.3.2 Raw map



X Index: 289



Y Index: 272

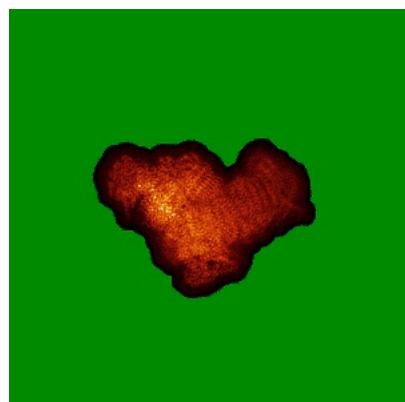


Z Index: 300

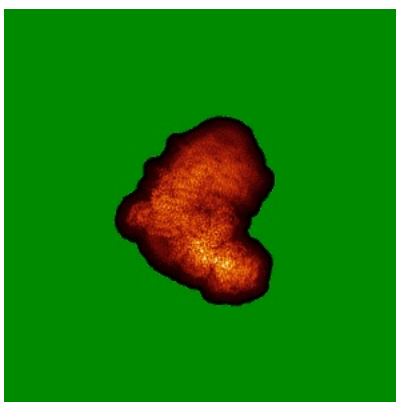
The images above show the largest variance slices of the map in three orthogonal directions.

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

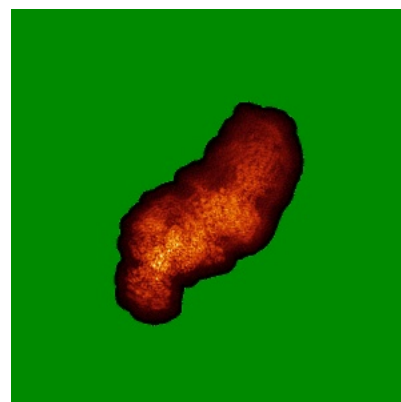
6.4.1 Primary map



X

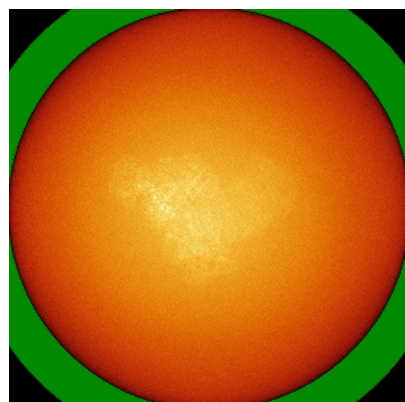


Y

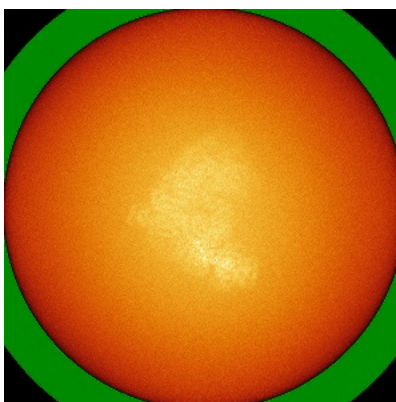


Z

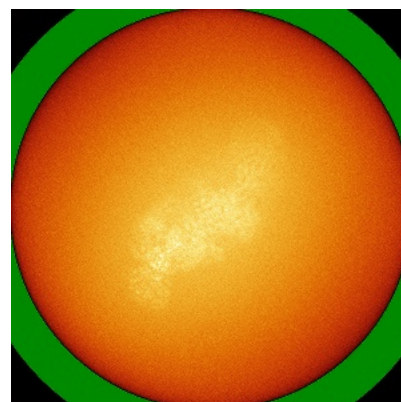
6.4.2 Raw map



X



Y

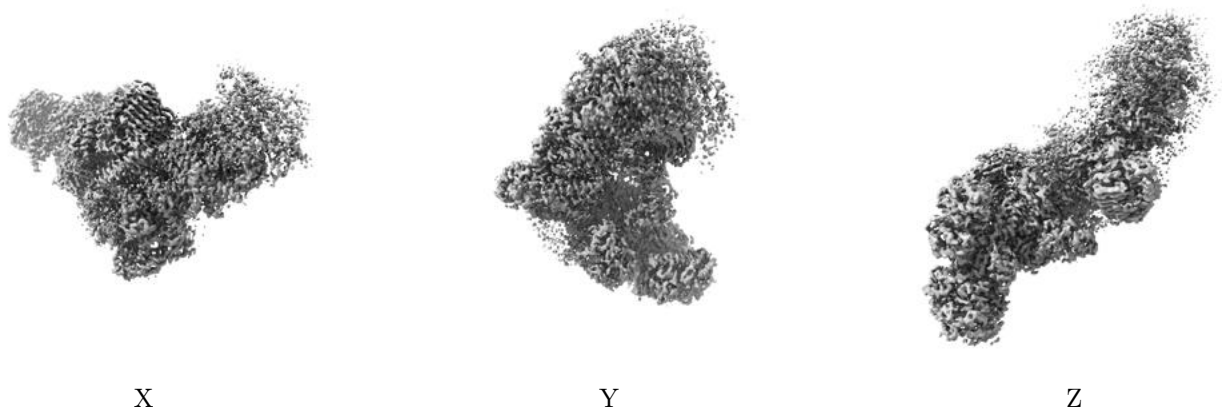


Z

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.

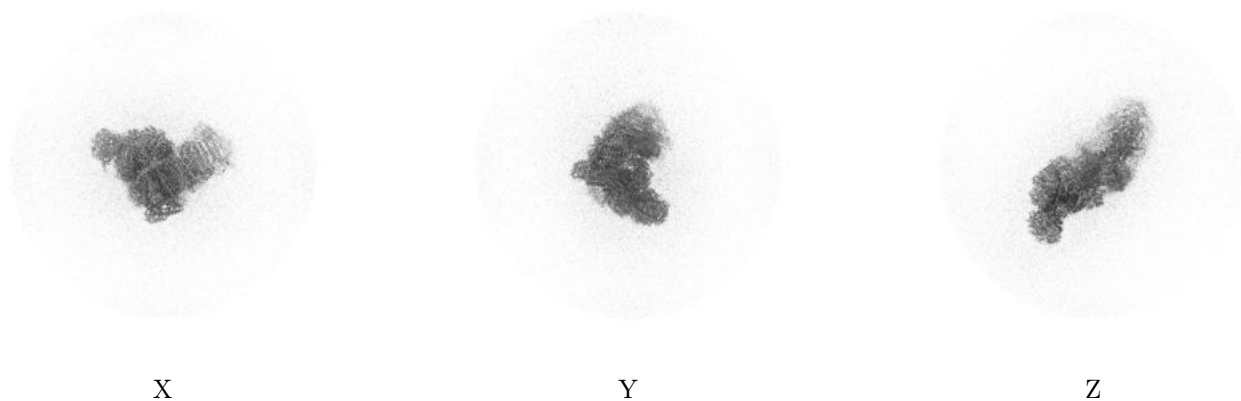
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.011. 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.

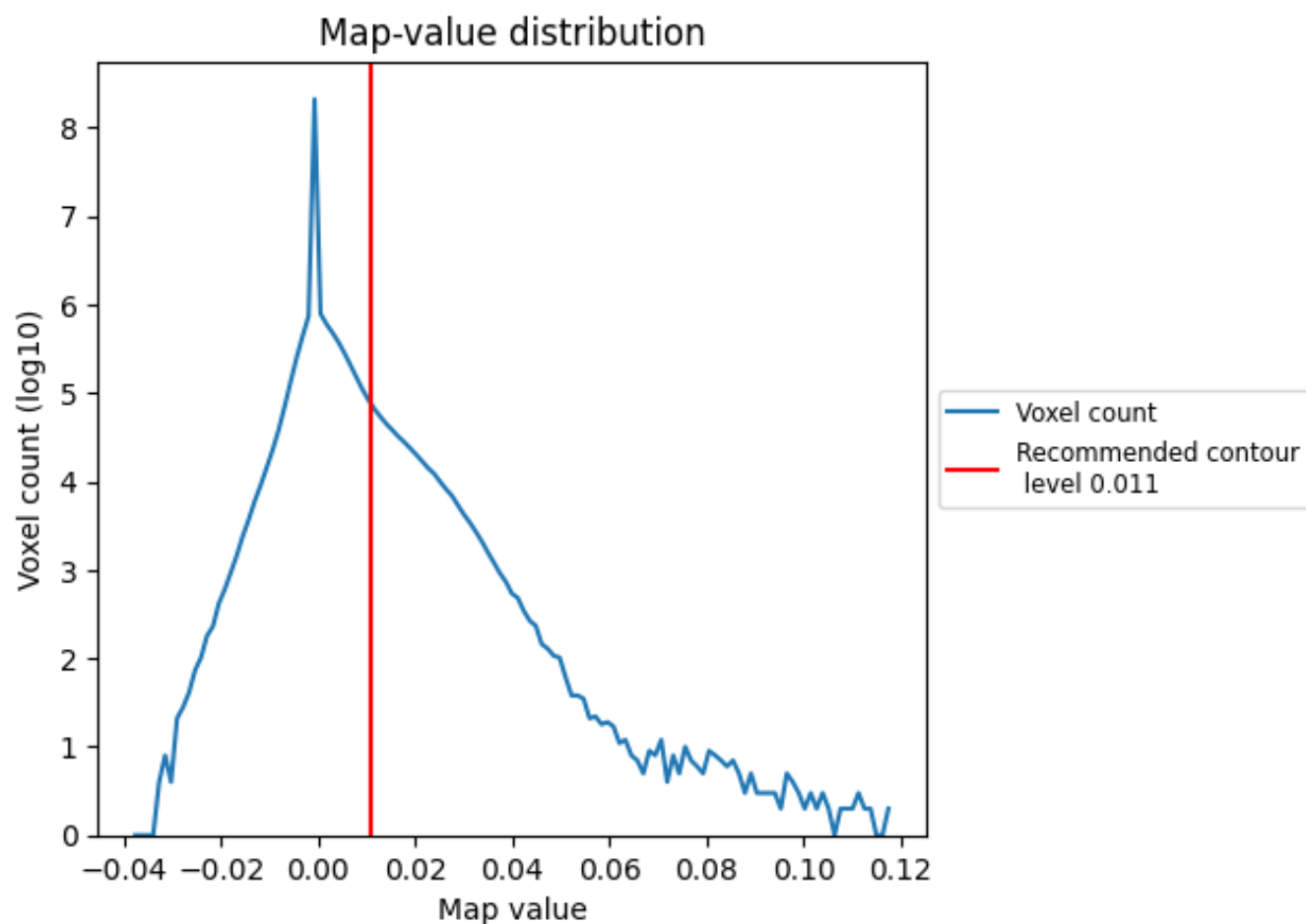
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

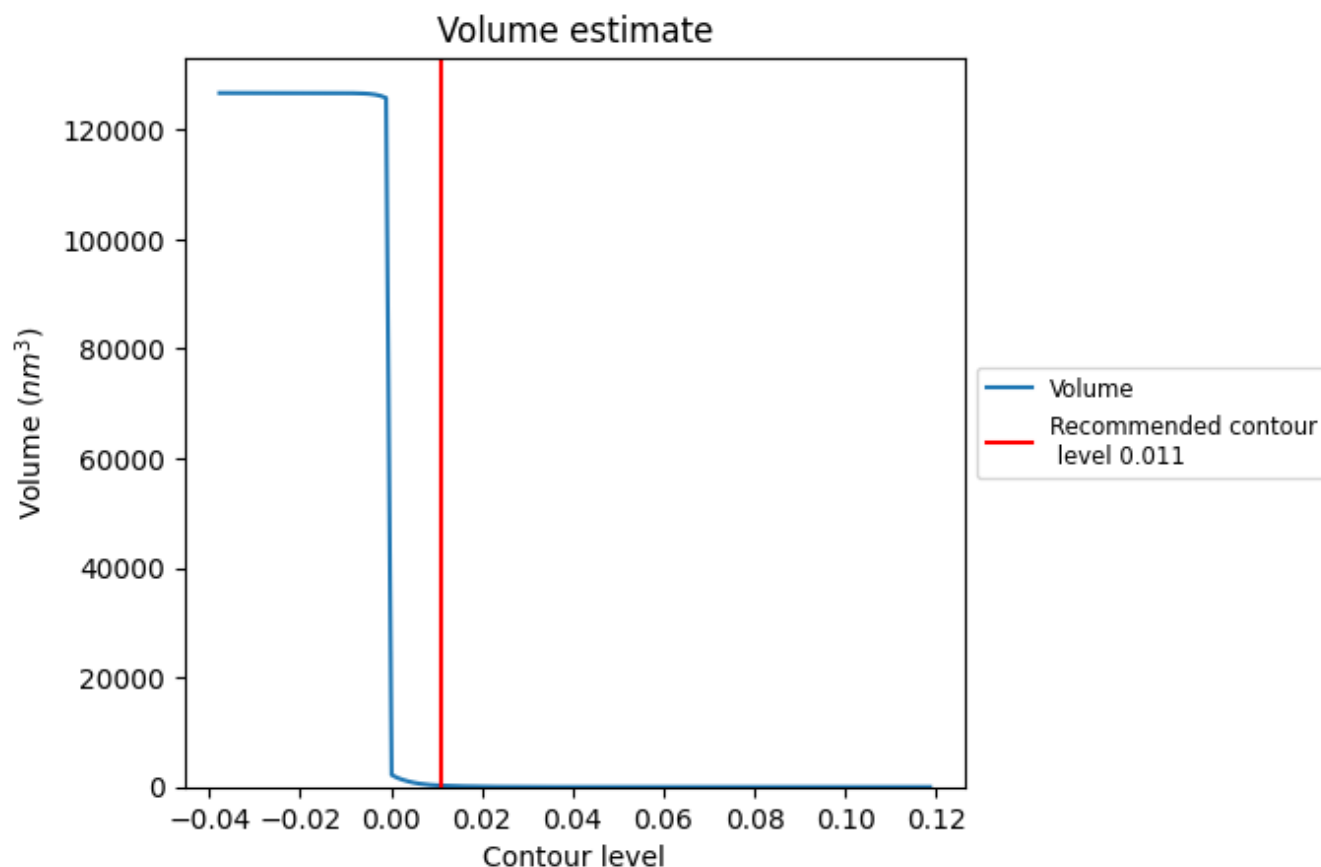
This section contains the results of statistical analysis of the map.

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.

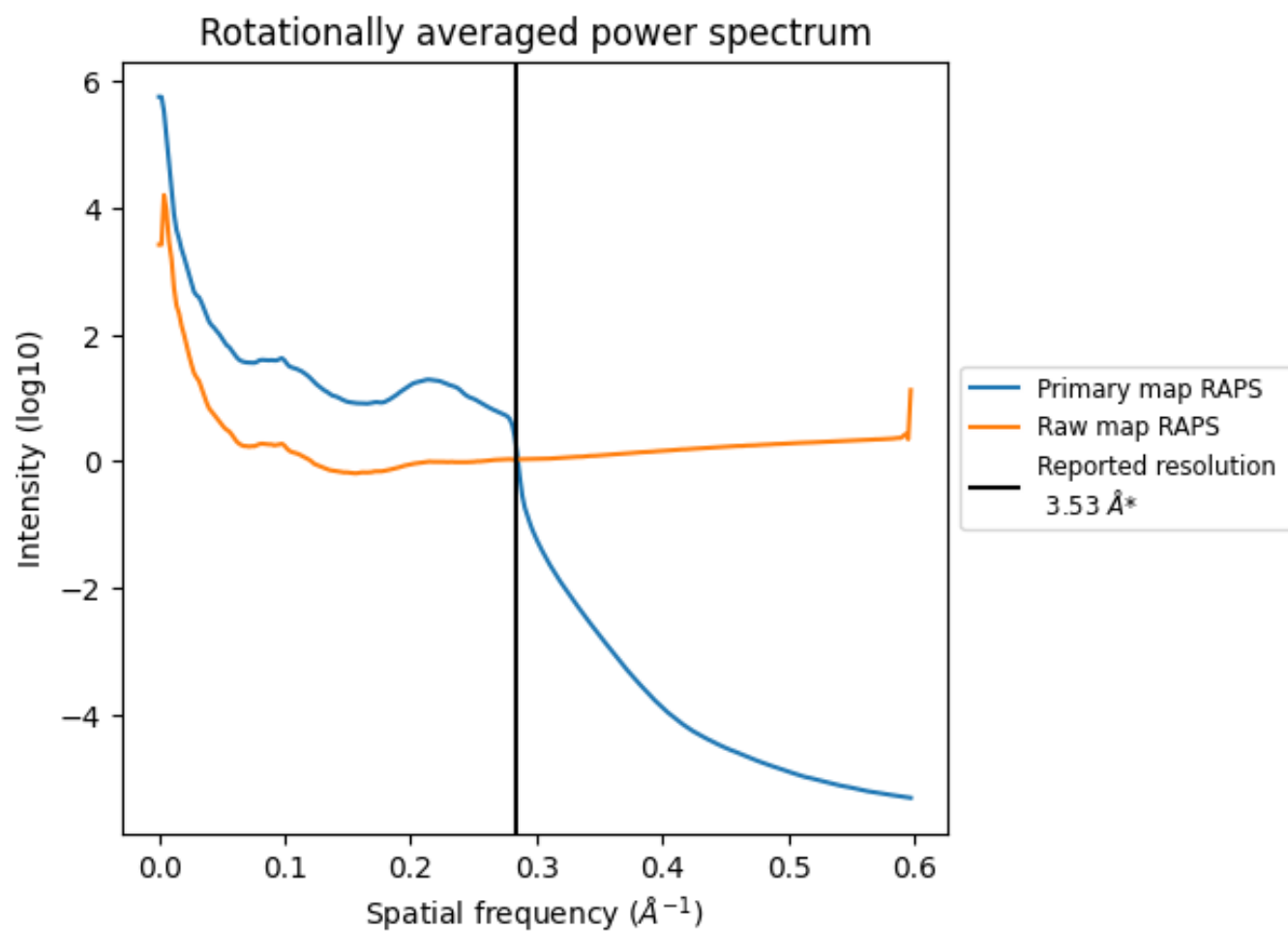
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 255 nm^3 ; this corresponds to an approximate mass of 230 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

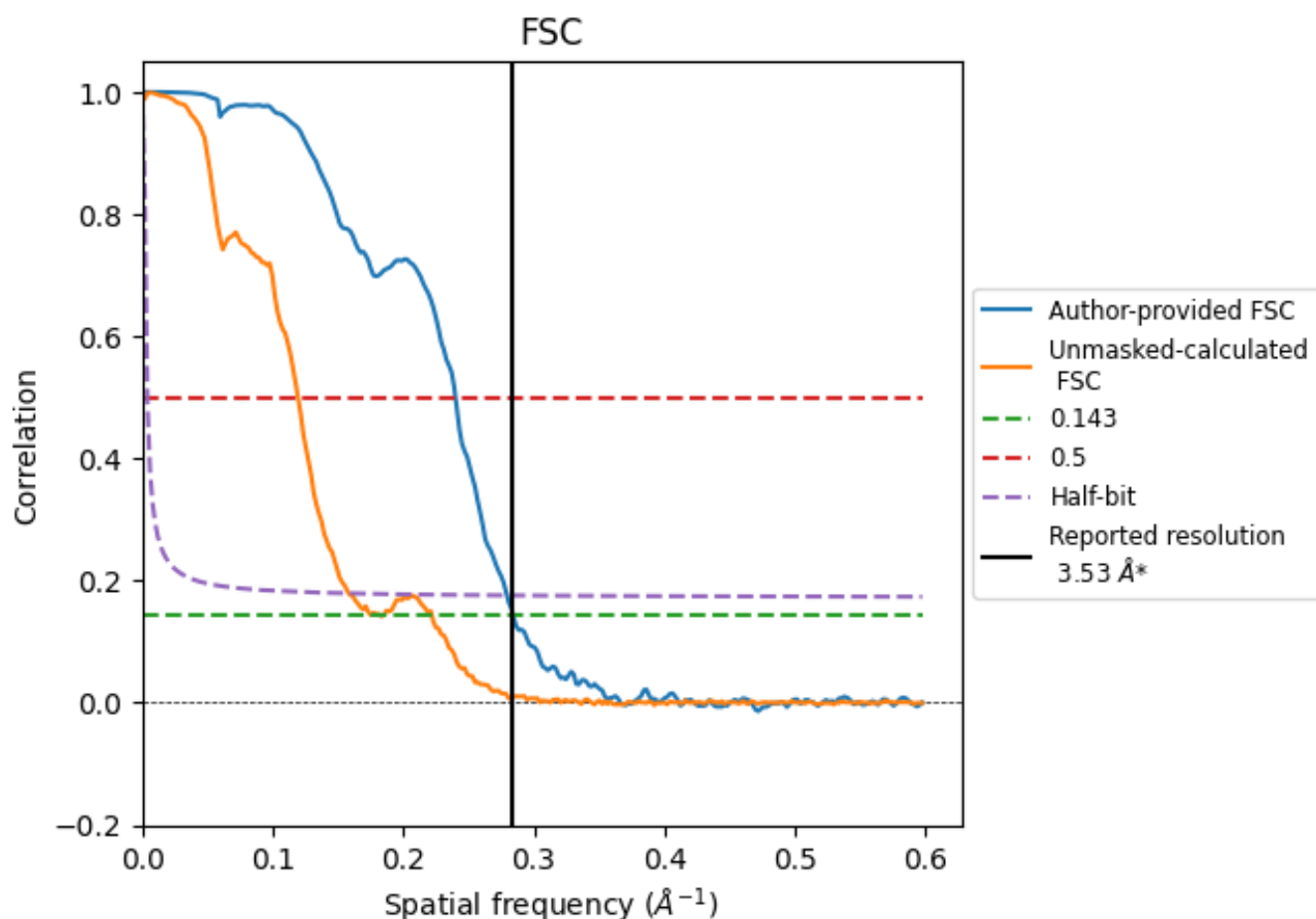


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

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 0.283 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

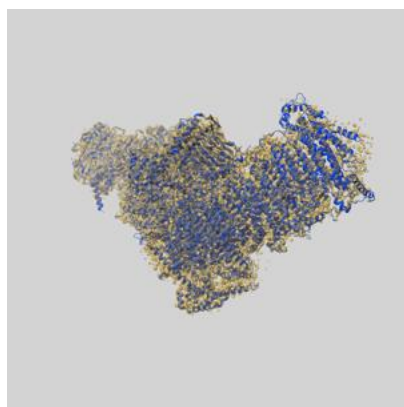
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.52	4.17	3.58
Unmasked-calculated*	5.48	8.38	6.31

*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 5.48 differs from the reported value 3.53 by more than 10 %

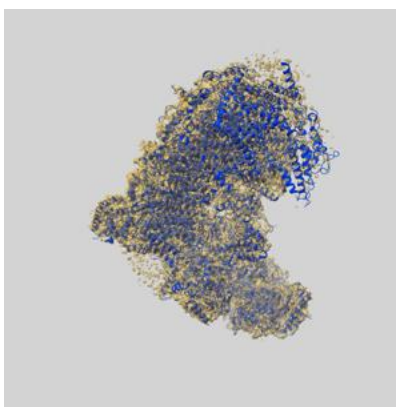
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11876 and PDB model 7AR8. Per-residue inclusion information can be found in [section 3](#) on [page 20](#).

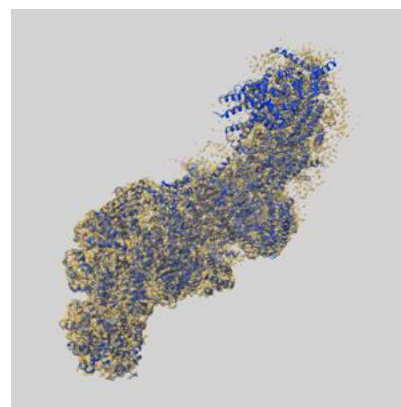
9.1 Map-model overlay [i](#)



X



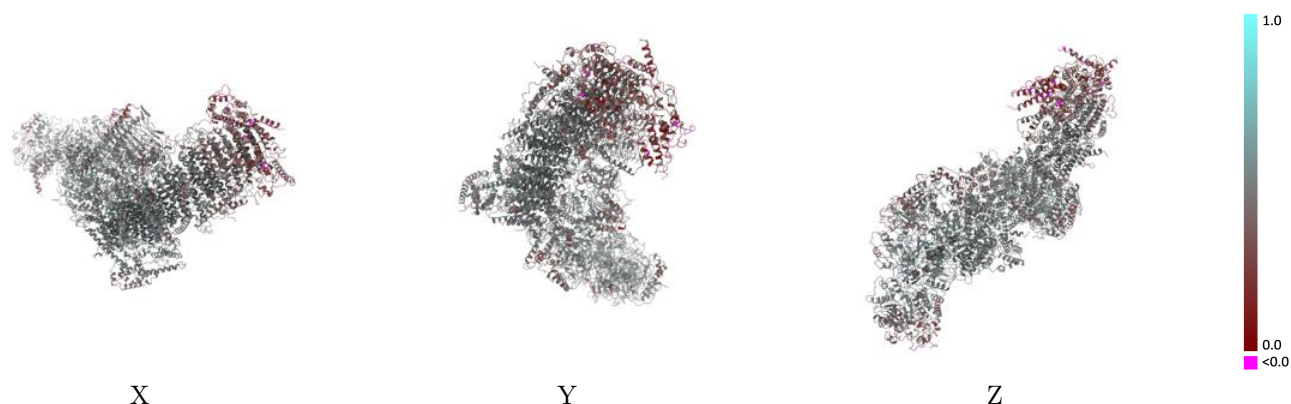
Y



Z

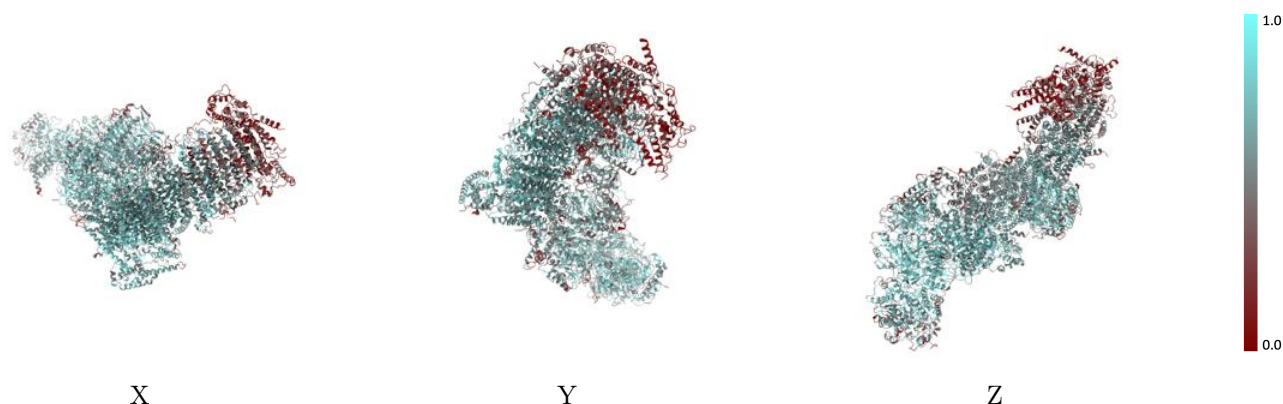
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



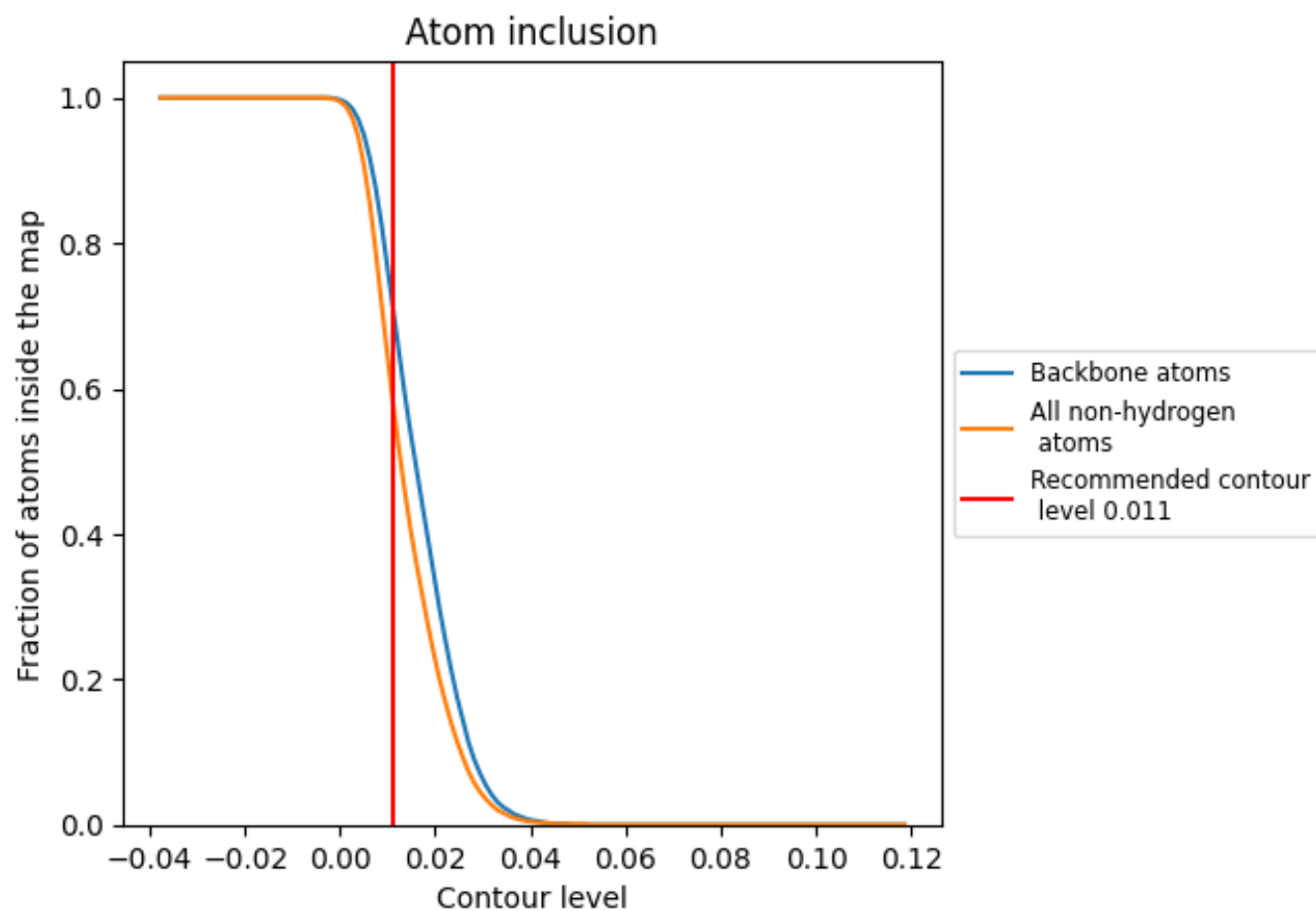
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.011).

9.4 Atom inclusion [i](#)



At the recommended contour level, 72% of all backbone atoms, 59% 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 (0.011) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5870	 0.4640
A	 0.6700	 0.5110
B	 0.7650	 0.5270
C	 0.7620	 0.5250
D	 0.7500	 0.5250
E	 0.5860	 0.4300
F	 0.5990	 0.4480
G	 0.7110	 0.5020
H	 0.6770	 0.5050
I	 0.7680	 0.5280
J	 0.6760	 0.5080
K	 0.6240	 0.4950
L	 0.3420	 0.3860
M	 0.6240	 0.4920
N	 0.6950	 0.5120
O	 0.4660	 0.4690
P	 0.5330	 0.4380
Q	 0.6830	 0.5180
R	 0.6970	 0.5130
S	 0.6250	 0.4400
T	 0.0590	 0.2200
U	 0.3630	 0.3910
V	 0.6280	 0.4660
W	 0.5370	 0.4540
X	 0.6330	 0.4640
Z	 0.6400	 0.4780
a	 0.6570	 0.4830
b	 0.6300	 0.4860
c	 0.4270	 0.4000
d	 0.6560	 0.4880
e	 0.7320	 0.4950
f	 0.7370	 0.5050
g	 0.4710	 0.4420
i	 0.6290	 0.4670
j	 0.1910	 0.3270



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Chain	Atom inclusion	Q-score
k	 0.1020	 0.2430
l	 0.1520	 0.2900
m	 0.3430	 0.4120
n	 0.1850	 0.2900
o	 0.2330	 0.3210
p	 0.4750	 0.4170
q	 0.1940	 0.4040
r	 0.1930	 0.3340
u	 0.6670	 0.4100
v	 0.5640	 0.4920
x	 0.6510	 0.4940
y	 0.6020	 0.4610
z	 0.6100	 0.4680