



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 08:42 AM UTC

PDB ID : 7AR7 / pdb_00007ar7
EMDB ID : EMD-11875
Title : Cryo-EM structure of Arabidopsis thaliana complex-I (open conformation)
Authors : Klusch, N.; Kuelbrandt, W.
Deposited on : 2020-10-23
Resolution : 3.72 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

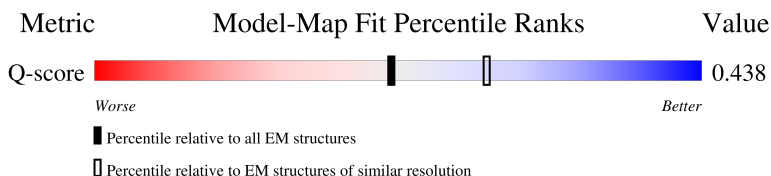
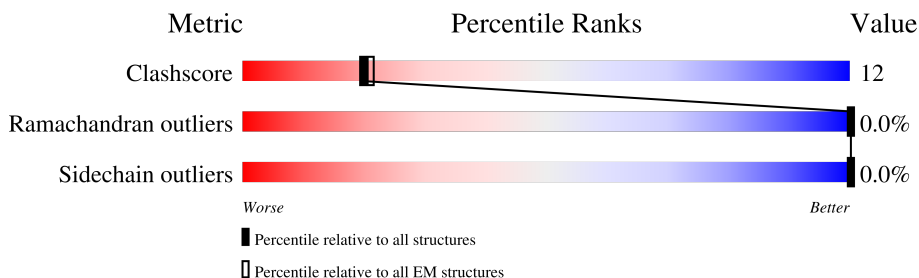
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.72 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	10474 (3.22 - 4.22)

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	16% 55% 23% 23%
2	B	157	76% 24%
3	C	185	74% 26%
4	D	385	68% 32%

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Mol	Chain	Length	Quality of chain
5	E	192	
6	F	434	
7	G	688	
8	H	324	
9	I	169	
10	J	205	
11	K	88	
12	L	615	
13	M	487	
14	N	488	
15	P	331	
16	Q	119	
17	R	62	
18	S	93	
19	T	84	
20	U	83	
21	V	140	
22	W	133	
23	X	96	
24	Z	125	
25	a	58	
26	b	40	
27	c	76	
28	d	75	
29	e	64	

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Mol	Chain	Length	Quality of chain
30	f	100	
31	g	72	
32	i	85	
33	j	51	
34	k	47	
35	l	46	
36	m	67	
37	n	109	
38	o	80	
39	p	93	
40	q	63	
41	r	10	
42	u	30	
43	v	30	
44	x	214	
45	y	268	
46	z	233	

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
47	SF4	B	500	-	-	X	-
47	SF4	F	501	-	-	X	-
48	FES	E	500	-	-	X	-

2 Entry composition

There are 59 unique types of molecules in this entry. The entry contains 60606 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 [ubiquinone] iron-sulfur protein 2.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	70	LEU	SER	conflict	UNP P93306
D	227	SER	PRO	conflict	UNP P93306
D	309	LEU	SER	conflict	UNP P93306
D	363	SER	LEU	conflict	UNP P93306

- 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		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	126	ARG	TRP	conflict	UNP P92558

- 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-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	88	Total	C	N	O	S	0	0
			692	466	107	112	7		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	44	LEU	SER	conflict	UNP Q04614

- 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 are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	91	PHE	SER	conflict	UNP P29388
L	288	PHE	SER	conflict	UNP P29388
L	537	LEU	PRO	conflict	UNP P29388

- 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 are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	146	PHE	PRO	conflict	UNP P93313
M	326	LEU	PRO	conflict	UNP P93313
M	383	PHE	SER	conflict	UNP P93313

- 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 NADH dehydrogenase [ubiquinone] 1 alpha subcomplex sub-unit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	331	Total	C	N	O	S	0	0
			2556	1641	438	462	15		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

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

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

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

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	93	Total	C	N	O	S	0	0
			728	459	129	134	6		

- Molecule 19 is a protein called Acyl carrier protein 1, mitochondrial.

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

- Molecule 20 is a protein called Acyl carrier protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	U	83	Total	C	N	O	S	0	0
			650	411	103	135	1		

- Molecule 21 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	W	108	Total	C	N	O	S	0	0
			880	563	156	158	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	X	96	Total	C	N	O	S	0	0
			763	478	131	142	12		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	125	Total	C	N	O	S	0	0
			997	640	175	177	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	58	Total	C	N	O	S	0	0
			470	302	84	79	5		

- Molecule 26 is a protein called At2g46540/F11C10.23.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	40	Total	C	N	O	S	0	0
			295	195	48	49	3		

- Molecule 27 is a protein called Transmembrane protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	76	Total	C	N	O	S	0	0
			617	396	115	100	6		

- Molecule 28 is a protein called Excitatory amino acid transporter.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	75	Total	C	N	O	S	0	0
			592	382	106	99	5		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-A.

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

- Molecule 30 is a protein called At4g16450.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	100	Total	C	N	O	S	0	0
			752	484	122	141	5		

- Molecule 31 is a protein called ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	72	Total	C	N	O	S	0	0
			586	379	100	104	3		

- Molecule 32 is a protein called At1g67350.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	85	Total	C	N	O	S	0	0
			737	466	135	131	5		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2.

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

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A.

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

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

8, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	l	46	Total	C	N	O	0	0
			360	241	57	62		

- Molecule 36 is a protein called AT2G31490 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	67	Total	C	N	O	S	0	0
			565	364	104	95	2		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

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

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	80	Total	C	N	O	S	0	0
			657	413	115	119	10		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B.

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

- Molecule 40 is a protein called Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	63	Total	C	N	O	0	0
			520	332	92	96		

- Molecule 41 is a protein called B14.5a.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	r	10	Total	C	N	O	0	0
			87	58	17	12		

- Molecule 42 is a protein called unknown.

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

- Molecule 43 is a protein called Uncharacterized protein At2g27730, mitochondrial.

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

- Molecule 44 is a protein called Gamma carbonic anhydrase-like 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	x	214	Total	C	N	O	S	0	0
			1659	1063	285	306	5		

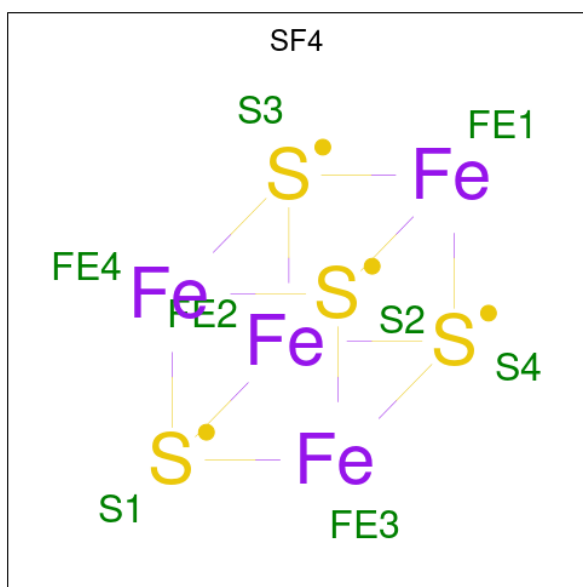
- Molecule 45 is a protein called Gamma carbonic anhydrase 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	y	268	Total	C	N	O	S	0	0
			2032	1271	363	391	7		

- Molecule 46 is a protein called Gamma carbonic anhydrase 1, mitochondrial.

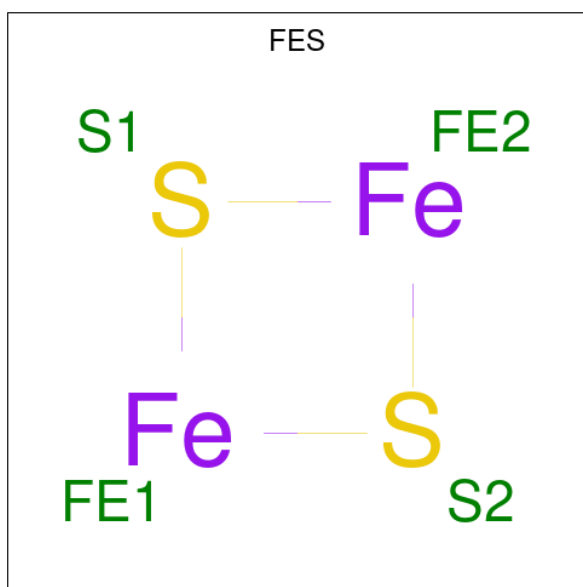
Mol	Chain	Residues	Atoms					AltConf	Trace
46	z	233	Total	C	N	O	S	0	0
			1772	1111	325	330	6		

- Molecule 47 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



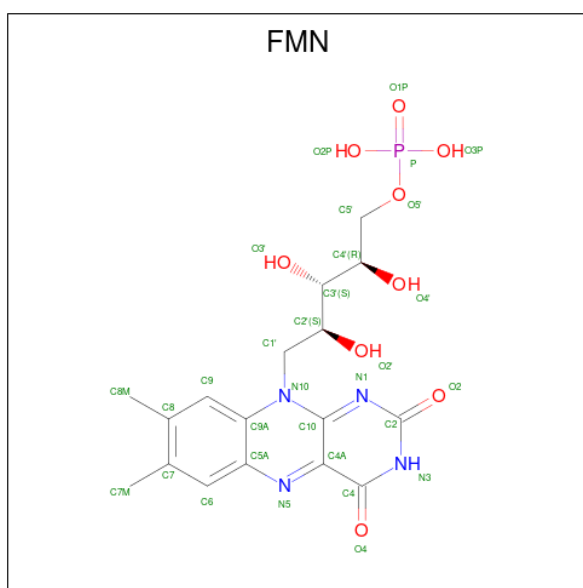
Mol	Chain	Residues	Atoms			AltConf
47	B	1	Total	Fe	S	0
			8	4	4	
47	F	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	G	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	
47	I	1	Total	Fe	S	0
			8	4	4	

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



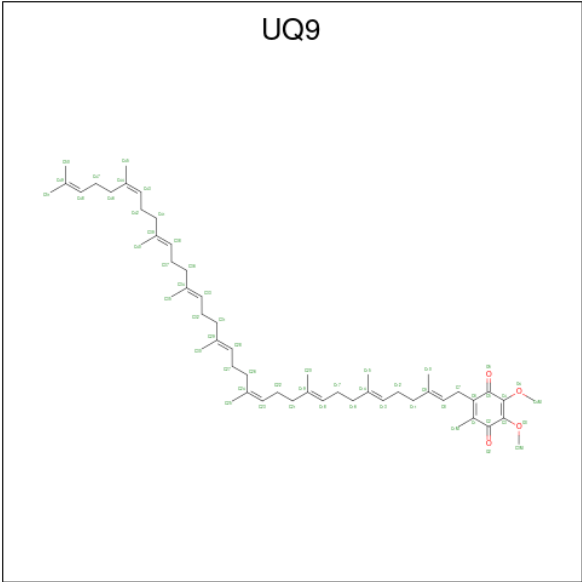
Mol	Chain	Residues	Atoms			AltConf
48	E	1	Total	Fe	S	0
			4	2	2	
48	G	1	Total	Fe	S	0
			4	2	2	

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



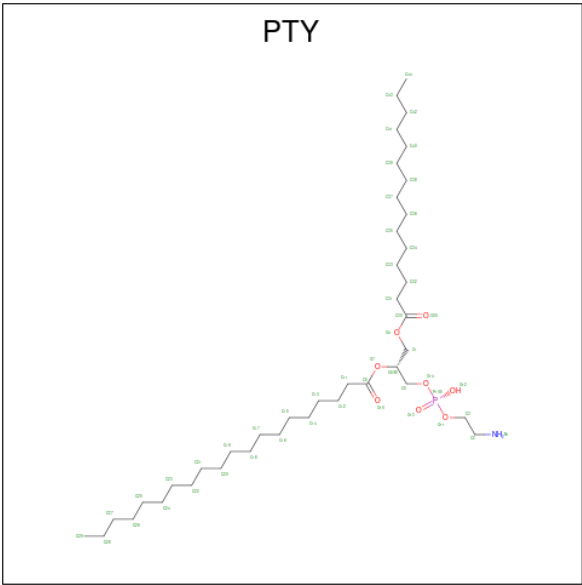
Mol	Chain	Residues	Atoms					AltConf
49	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 50 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$).



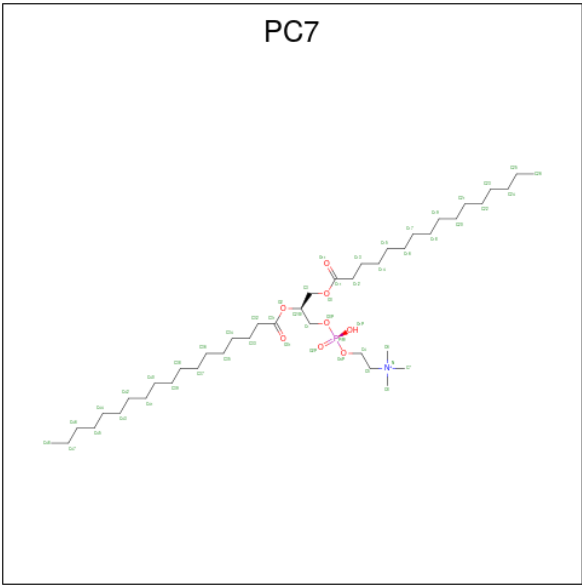
Mol	Chain	Residues	Atoms			AltConf
50	H	1	Total	C	O	0
			35	31	4	

- Molecule 51 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: C₄₀H₈₀NO₈P).



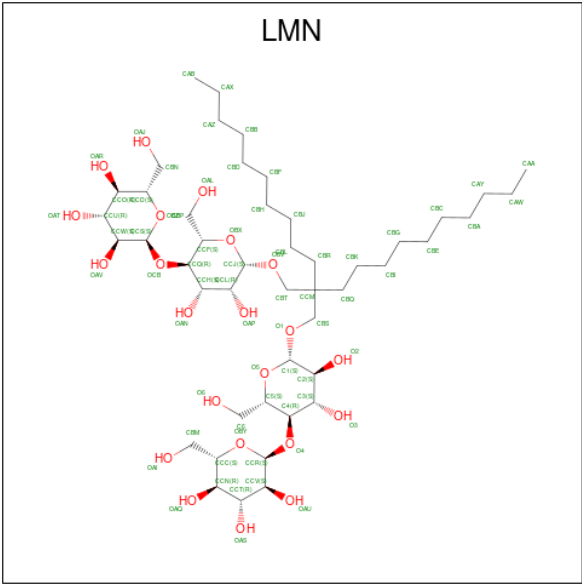
Mol	Chain	Residues	Atoms					AltConf
51	I	1	Total	C	N	O	P	0
			50	40	1	8	1	
51	M	1	Total	C	N	O	P	0
			50	40	1	8	1	
51	N	1	Total	C	N	O	P	0
			50	40	1	8	1	

- Molecule 52 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).



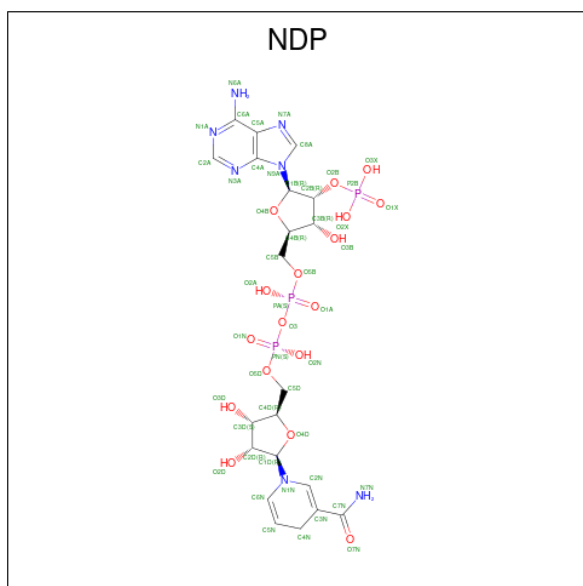
Mol	Chain	Residues	Atoms					AltConf
52	M	1	Total	C	N	O	P	0
			52	42	1	8	1	
52	f	1	Total	C	N	O	P	0
			52	42	1	8	1	

- Molecule 53 is Lauryl Maltose Neopentyl Glycol (CCD ID: LMN) (formula: C₄₇H₈₈O₂₂).



Mol	Chain	Residues	Atoms			AltConf
53	M	1	Total	C	O	0
			69	47	22	

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

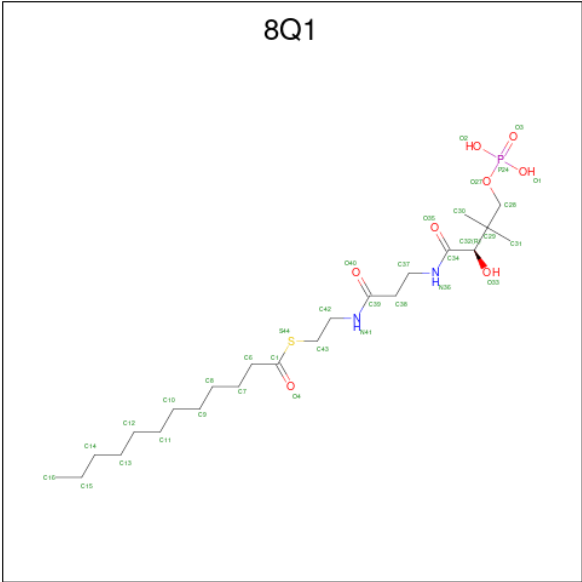


Mol	Chain	Residues	Atoms					AltConf
54	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

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

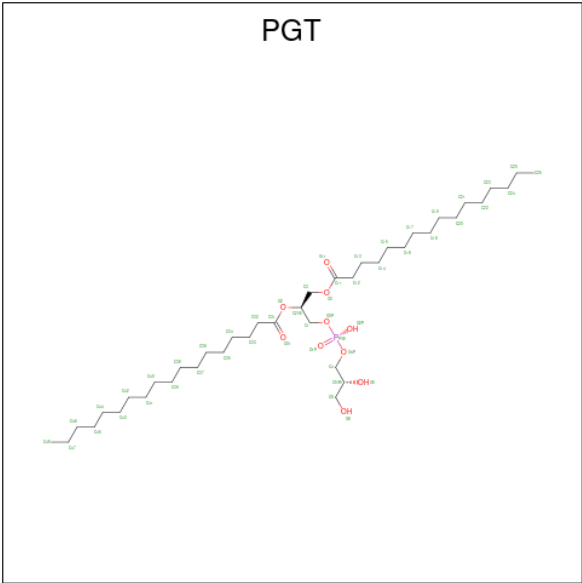
Mol	Chain	Residues	Atoms		AltConf
55	R	1	Total	Zn	0
			1	1	
55	y	1	Total	Zn	0
			1	1	

- Molecule 56 is S-[2-({N-[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alanyl}amino)ethyl] dodecanethioate (CCD ID: 8Q1) (formula: $C_{23}H_{45}N_2O_8PS$).



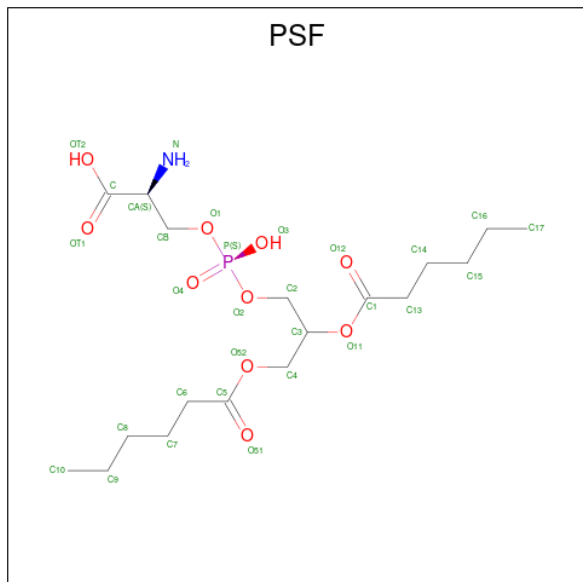
Mol	Chain	Residues	Atoms						AltConf
56	W	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	
56	n	1	Total	C	N	O	P	S	0
			35	23	2	8	1	1	

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



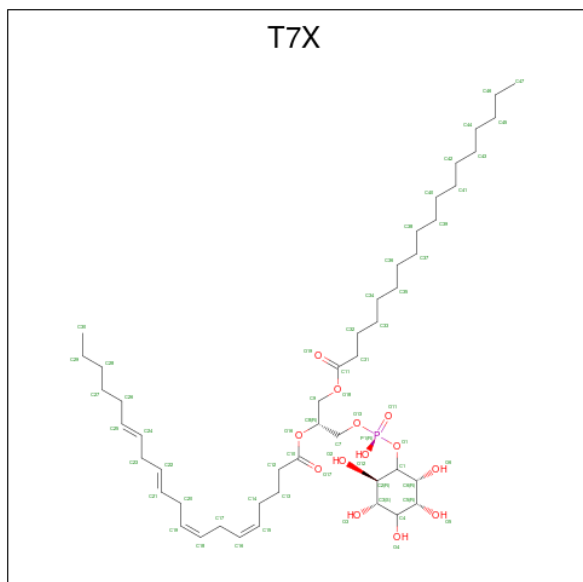
Mol	Chain	Residues	Atoms				AltConf
57	y	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 58 is 1,2-DICAPROYL-SN-PHOSPHATIDYL-L-SERINE (CCD ID: PSF) (formula: $C_{18}H_{34}NO_{10}P$).



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

- Molecule 59 is Phosphatidylinositol (CCD ID: T7X) (formula: $C_{47}H_{83}O_{13}P$).

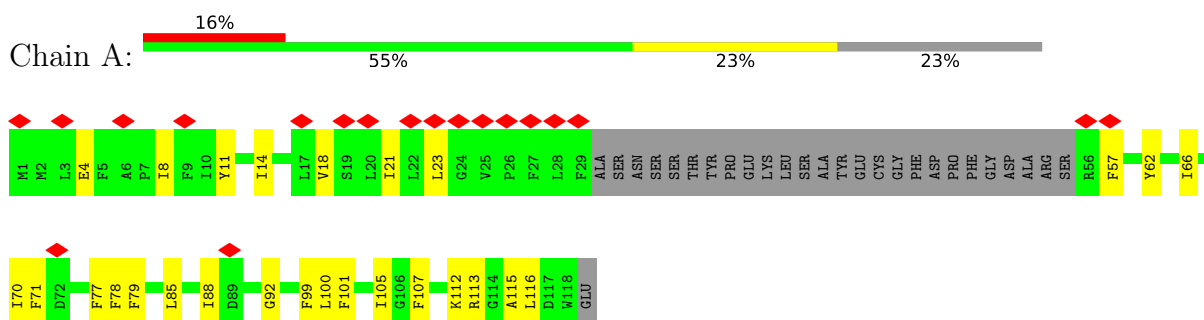


Mol	Chain	Residues	Atoms				AltConf
59	z	1	Total	C	O	P	0
			61	47	13	1	

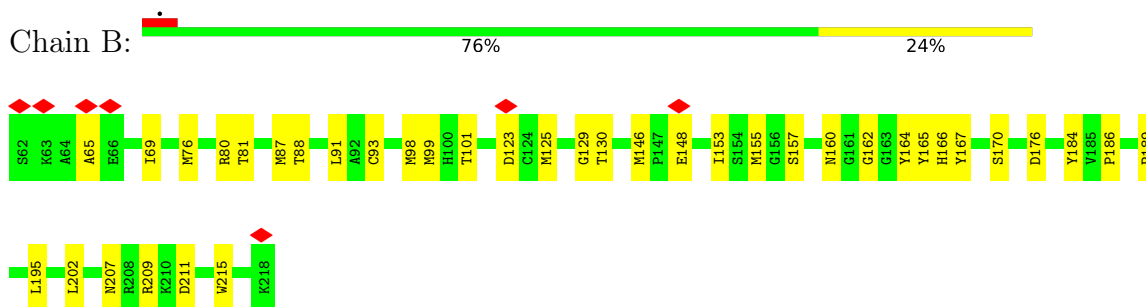
3 Residue-property plots [i](#)

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

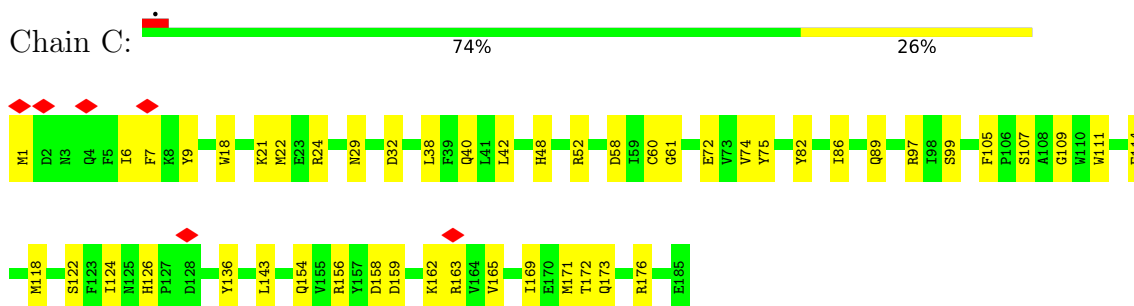
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



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

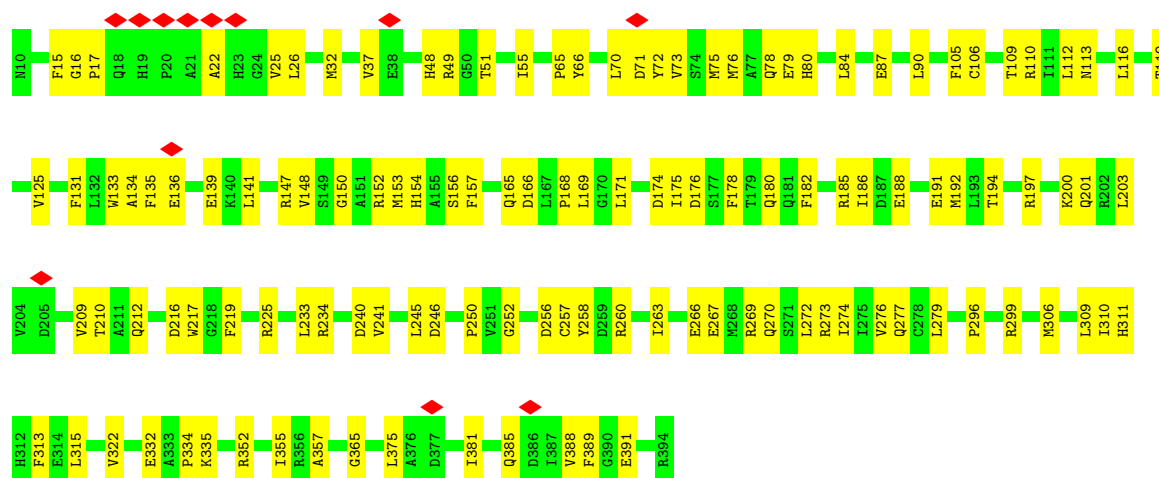


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3

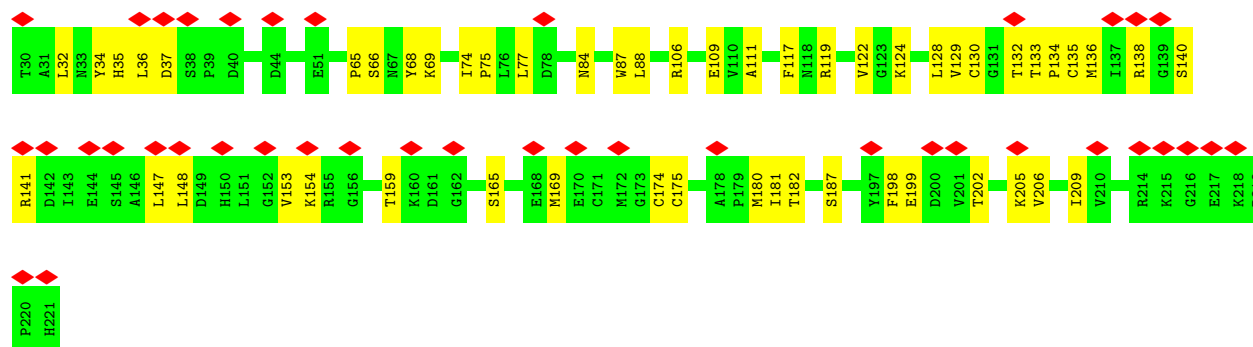
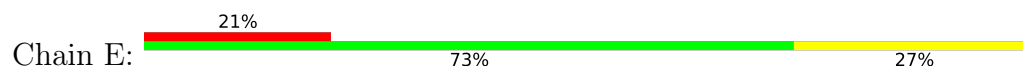


- Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2

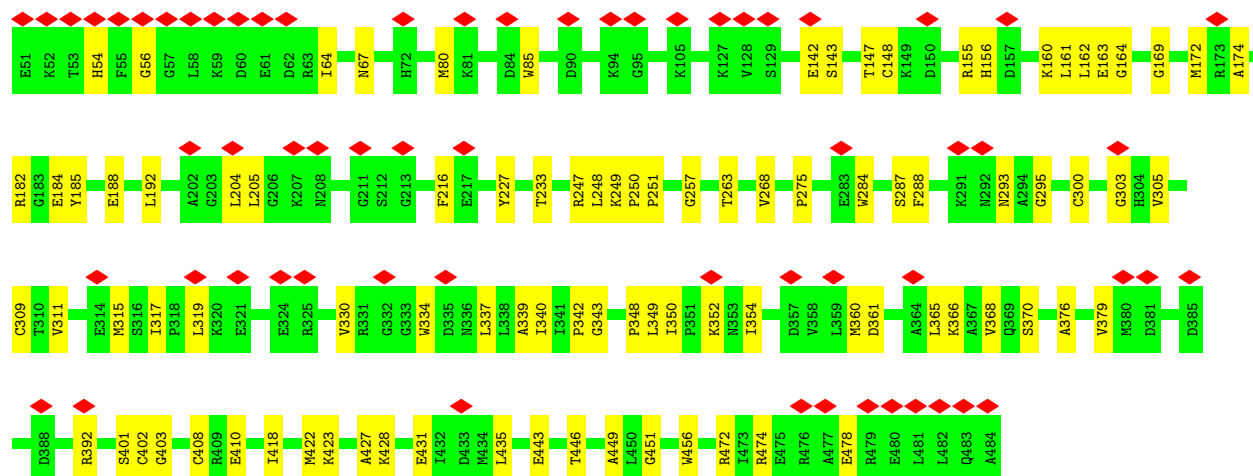
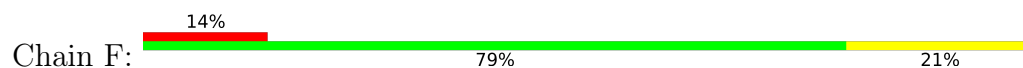




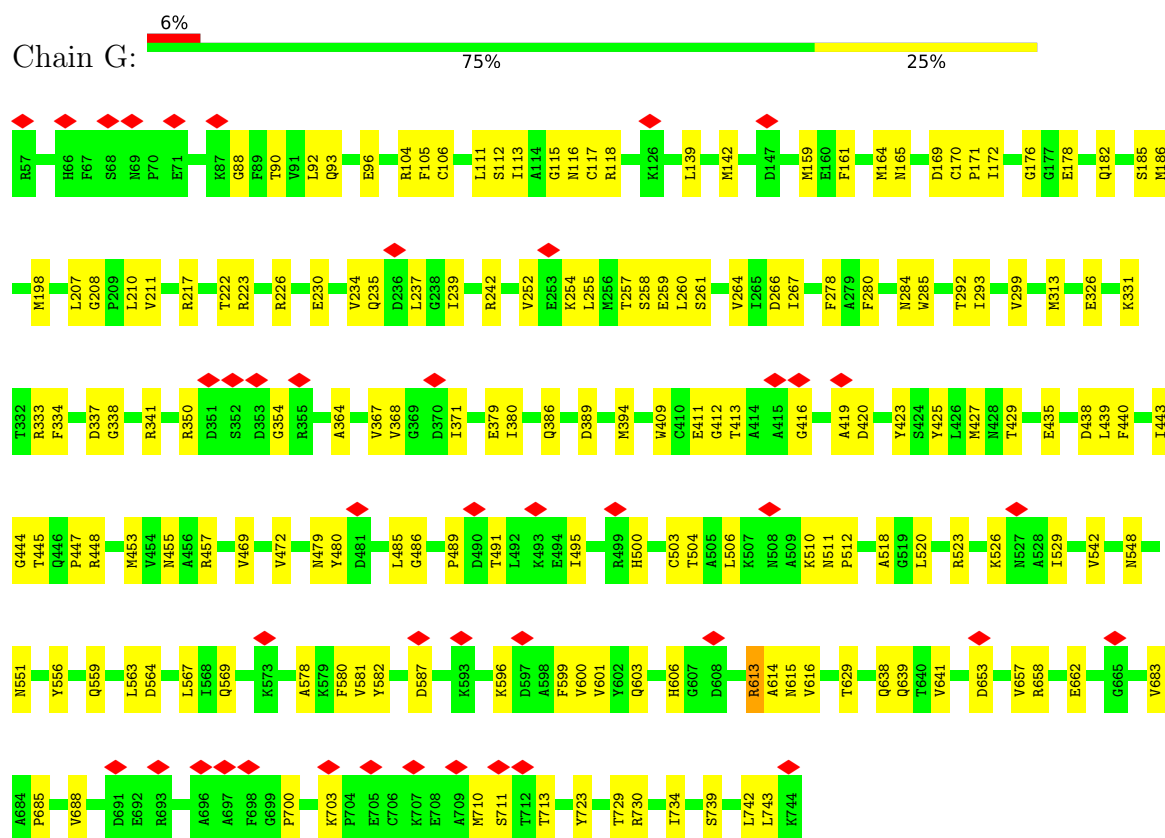
- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



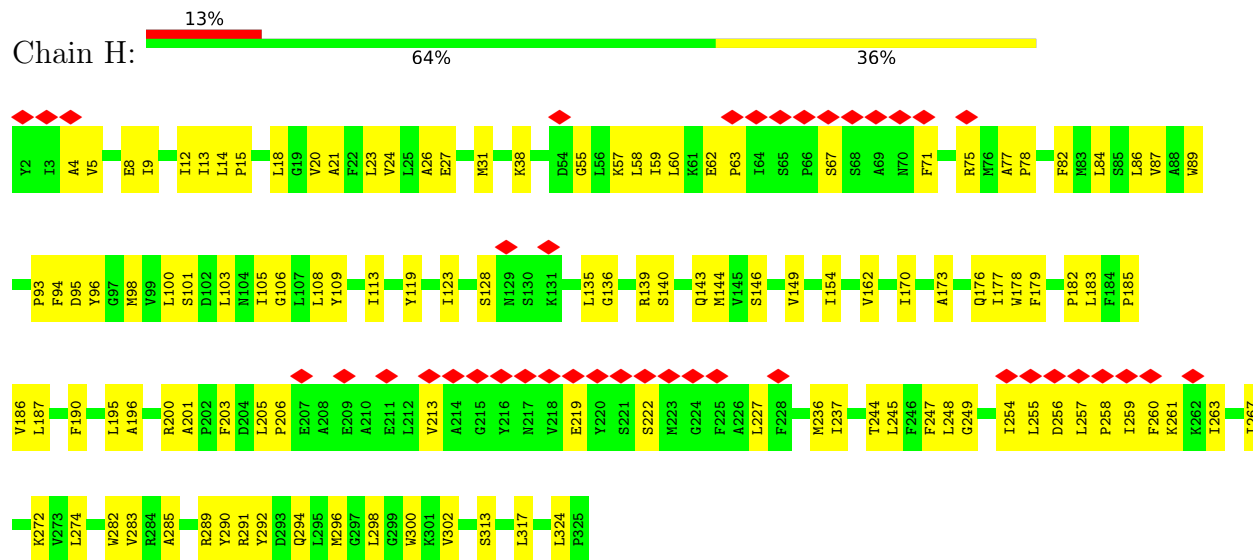
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial



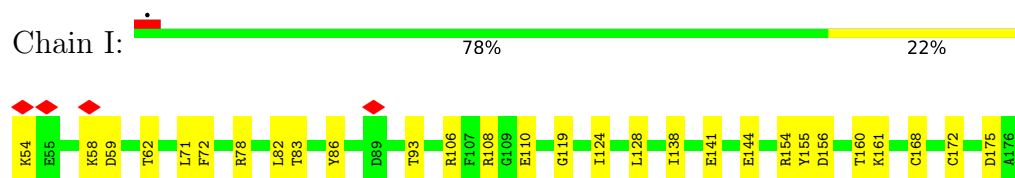
- Molecule 7: NADH dehydrogenase [ubiquinone] iron-sulfur protein 1, mitochondrial



• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

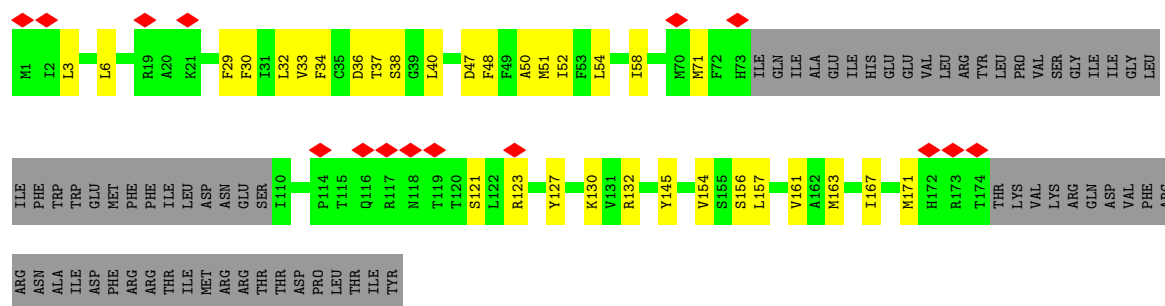


• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8-A, mitochondrial

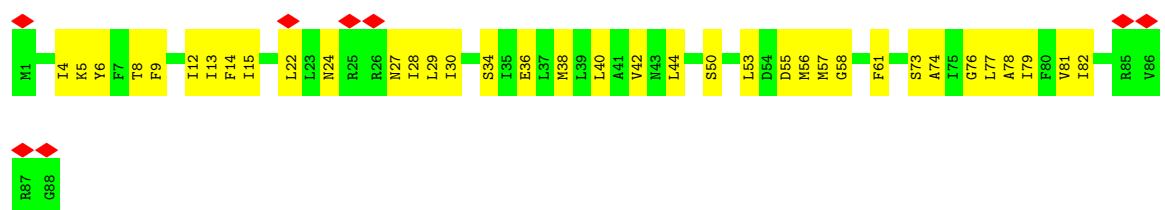




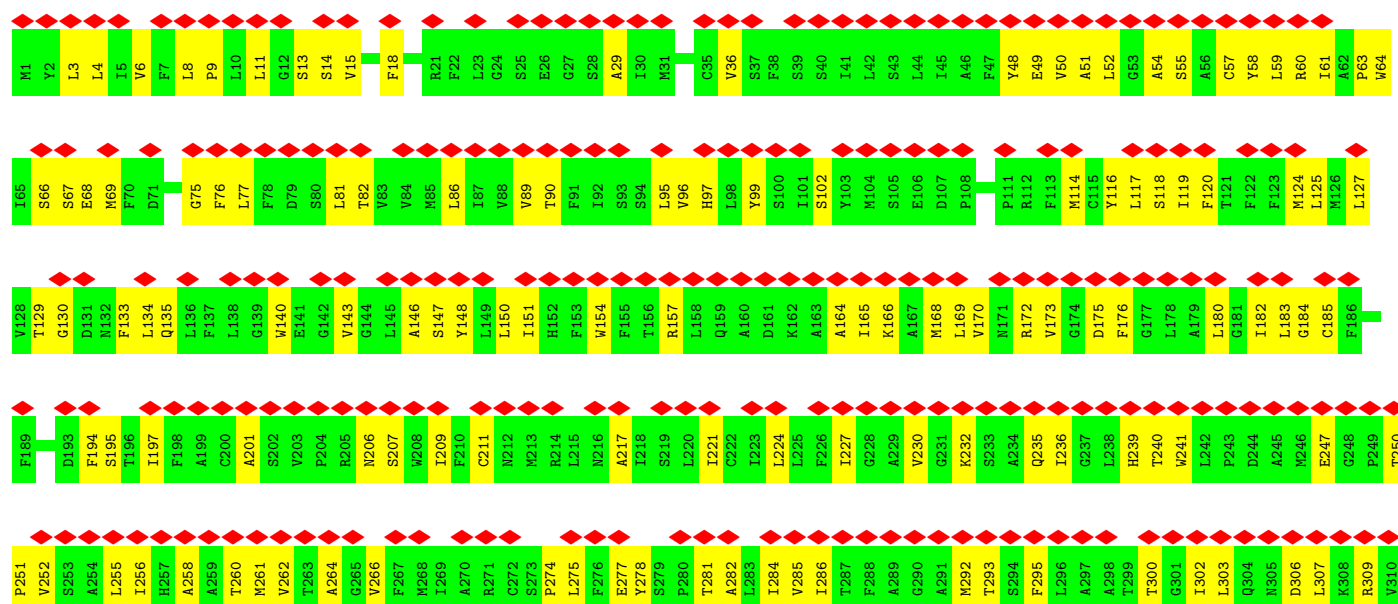
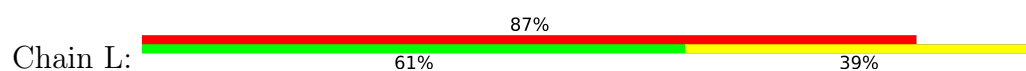
- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

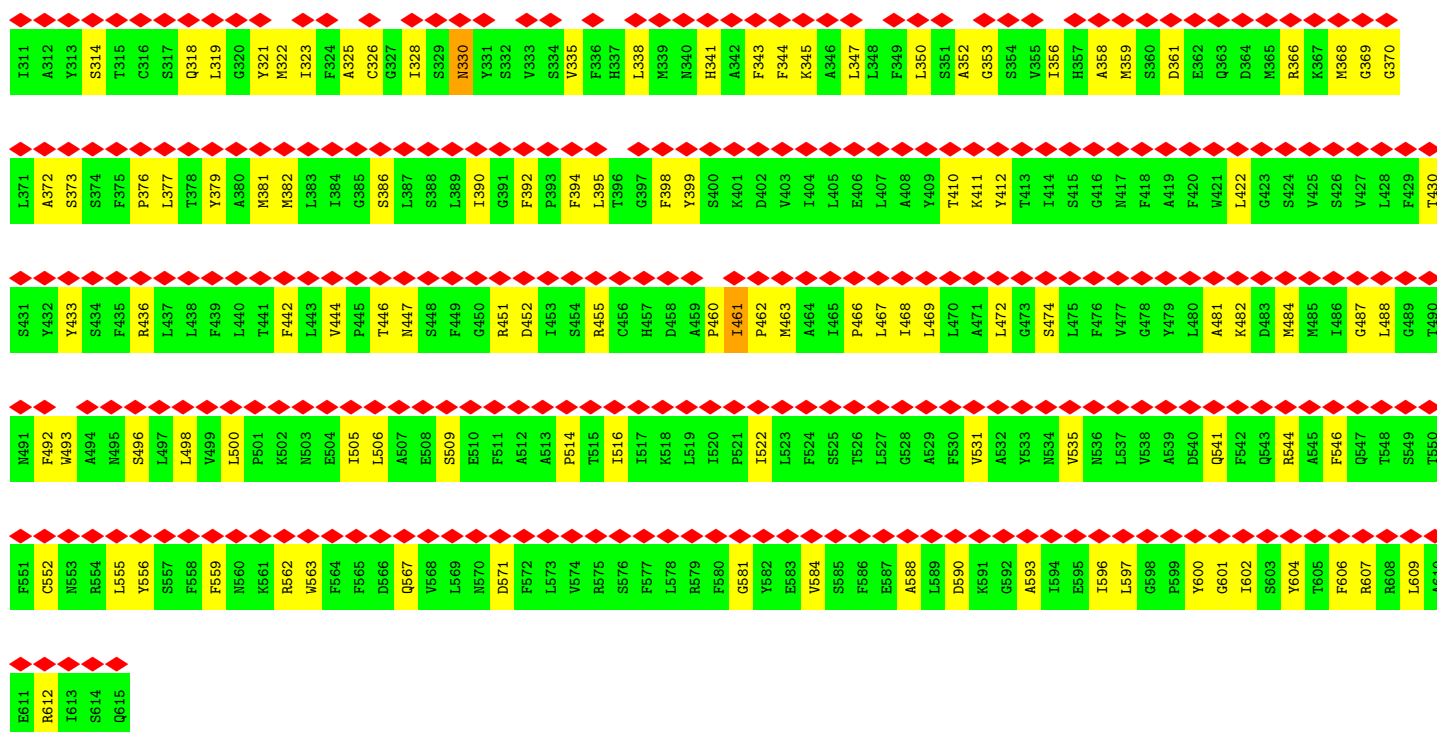


- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

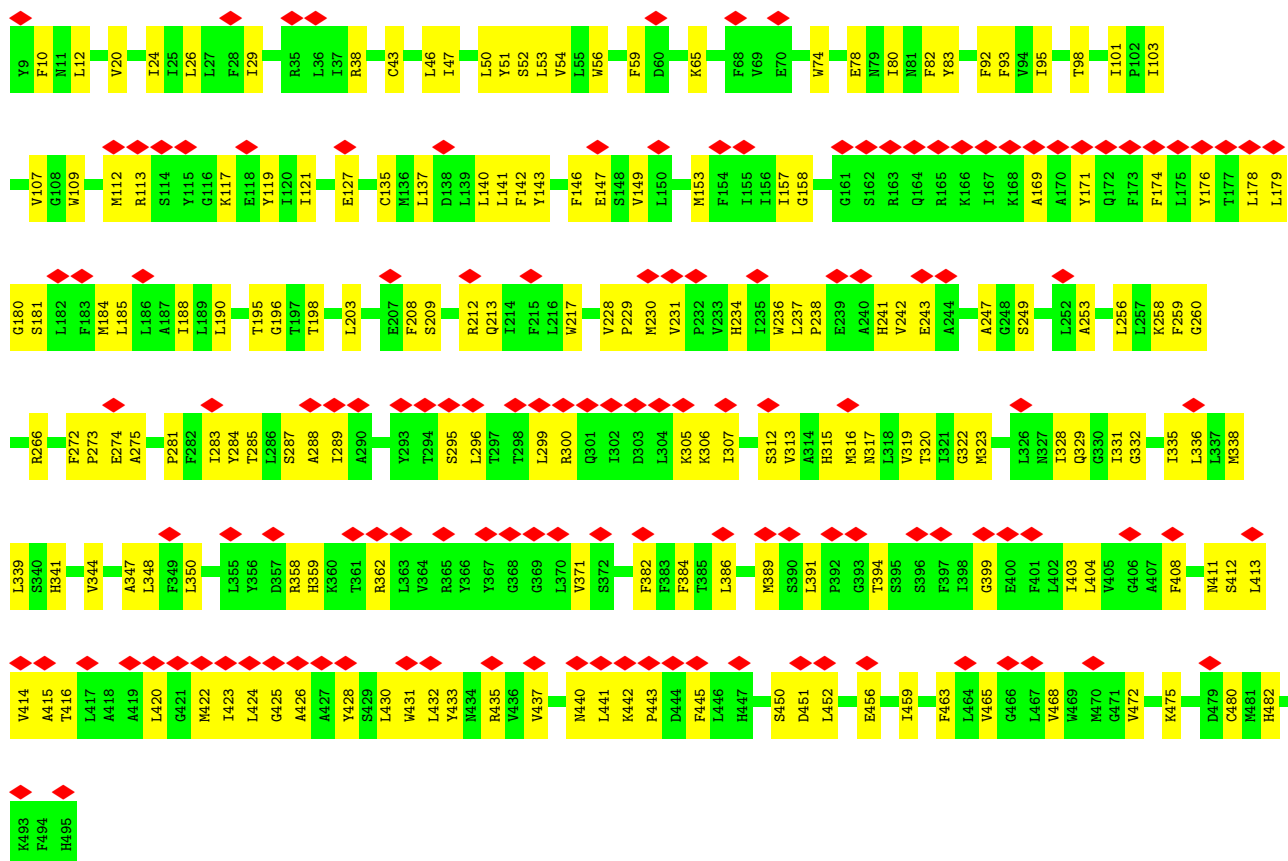


- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

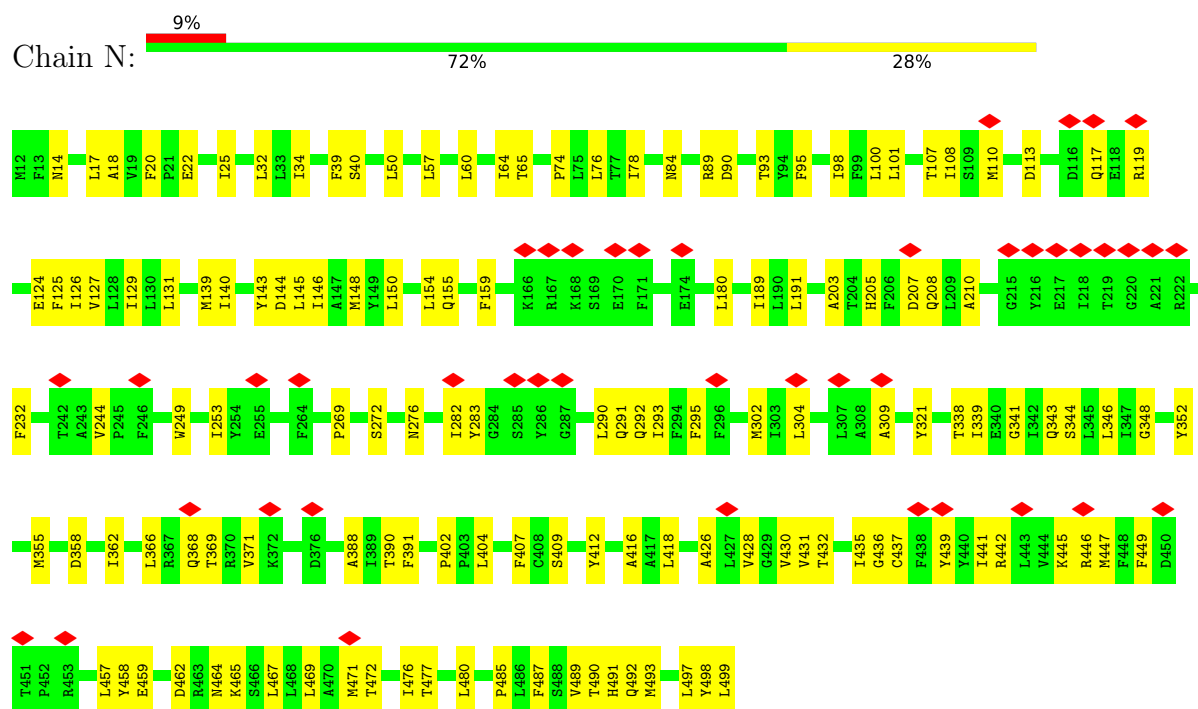




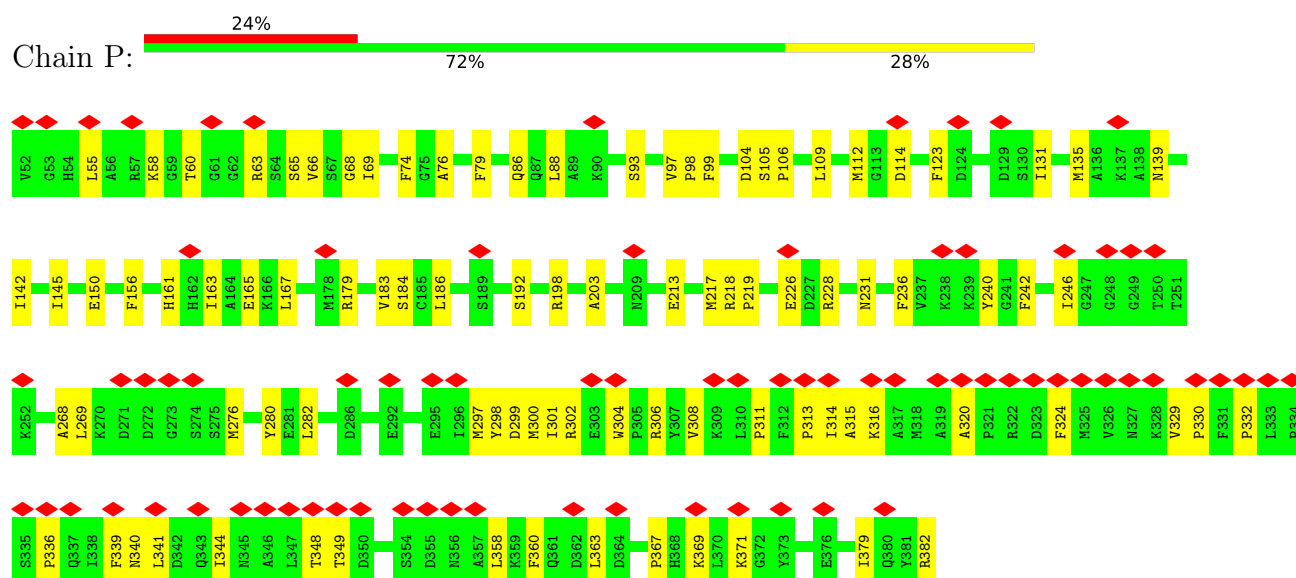
• Molecule 13: NADH-ubiquinone oxidoreductase chain 4



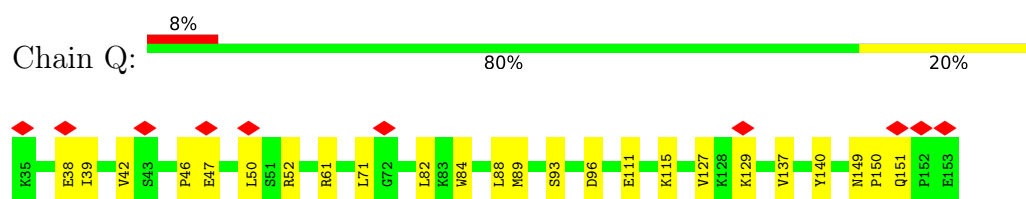
- Molecule 14: NADH-ubiquinone oxidoreductase chain 2



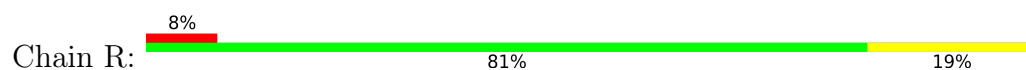
- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



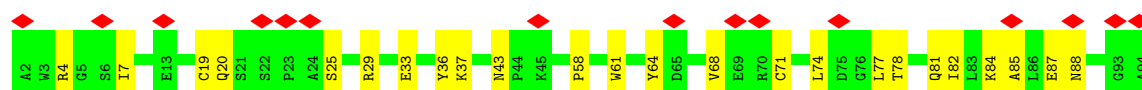
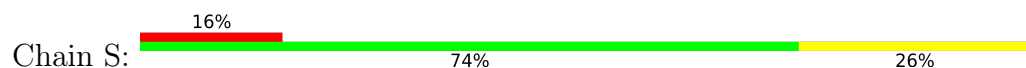
- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



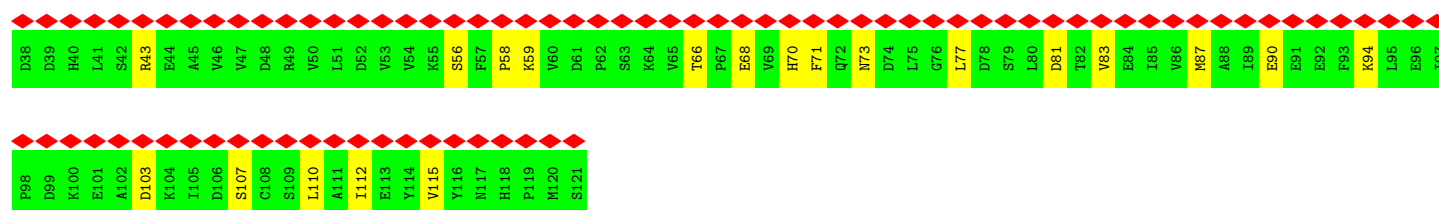
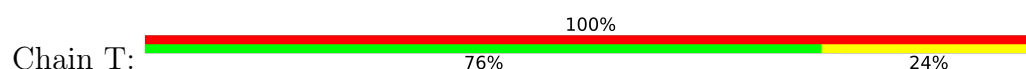
- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



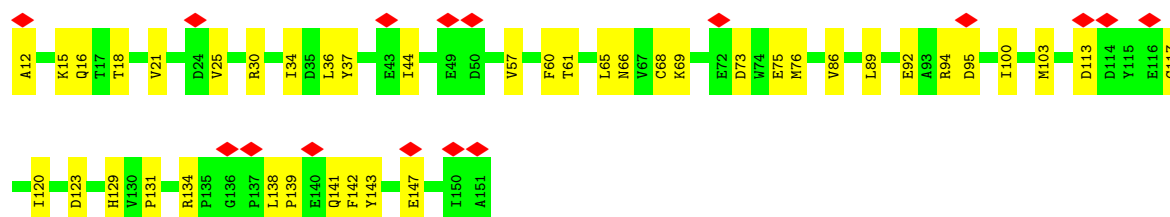
- Molecule 19: Acyl carrier protein 1, mitochondrial



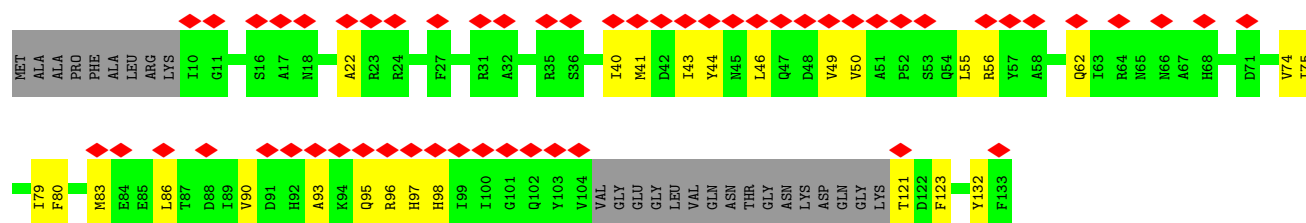
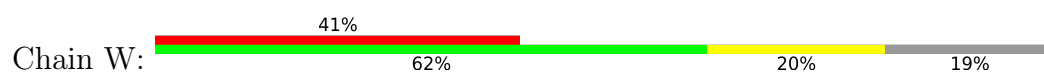
- Molecule 20: Acyl carrier protein 2, mitochondrial



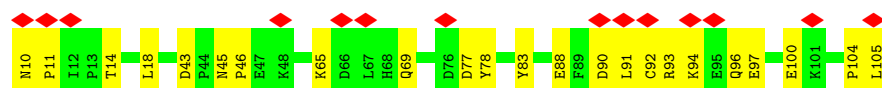
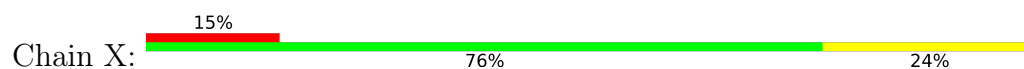
- Molecule 21: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5, mitochondrial



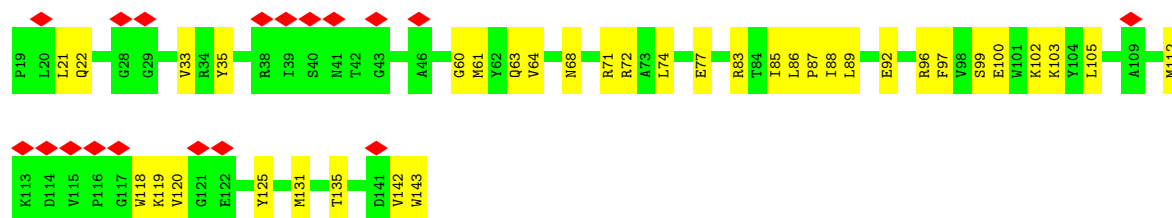
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



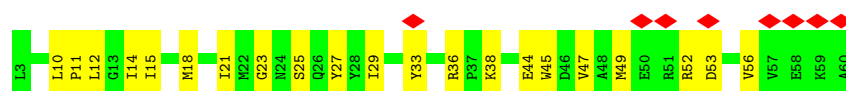
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8-B



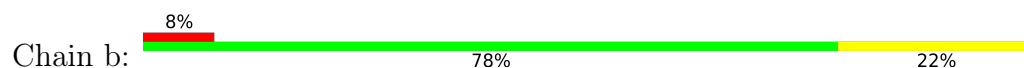
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13-A



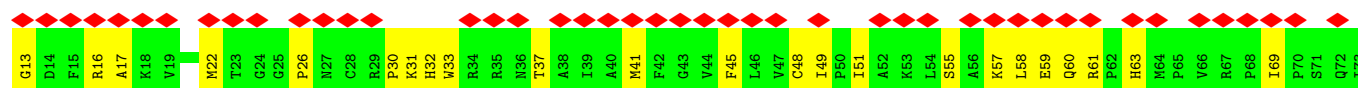
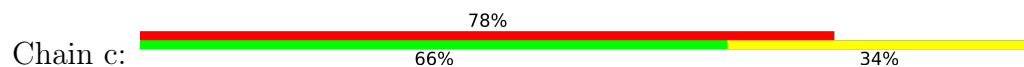
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

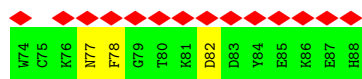


- Molecule 26: At2g46540/F11C10.23

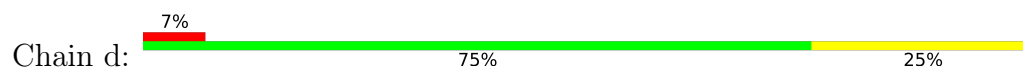


- Molecule 27: Transmembrane protein

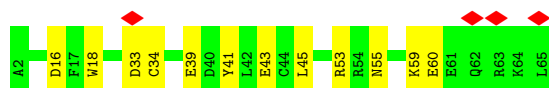
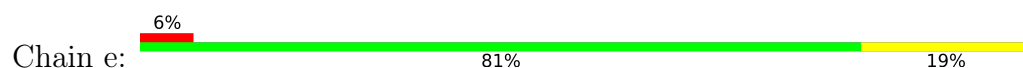




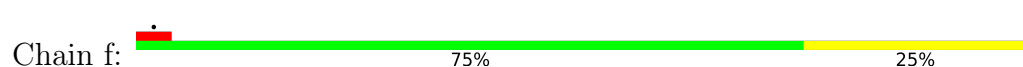
- Molecule 28: Excitatory amino acid transporter



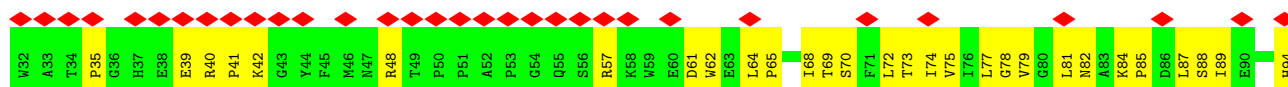
- Molecule 29: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5-A



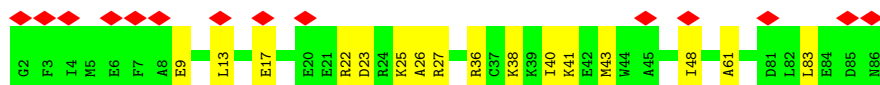
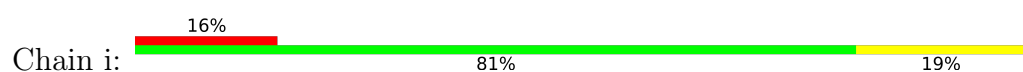
- Molecule 30: At4g16450



- Molecule 31: ESSS subunit of NADH:ubiquinone oxidoreductase (Complex I) protein



- Molecule 32: At1g67350

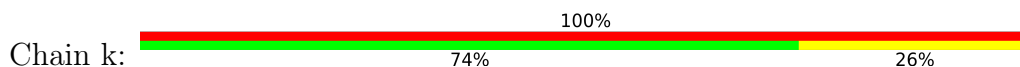


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2

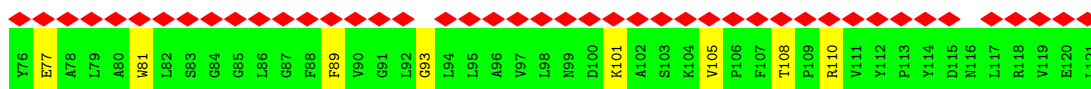
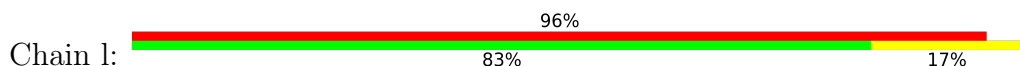




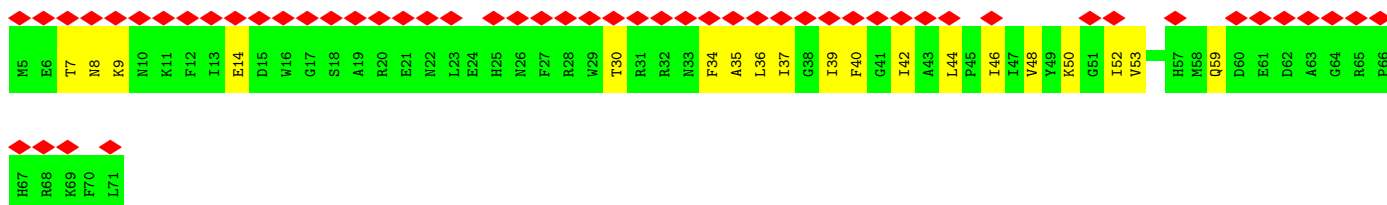
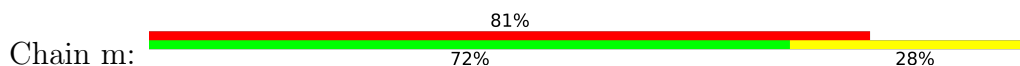
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3-A



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



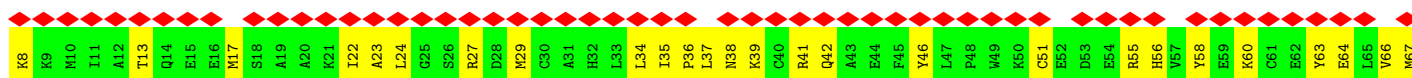
- Molecule 36: AT2G31490 protein



- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

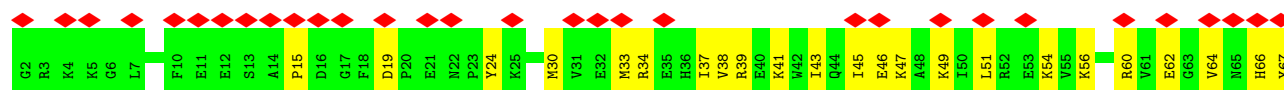


- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

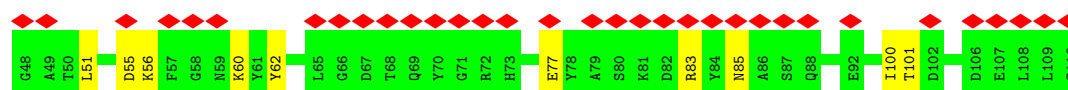
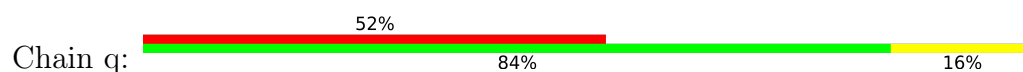




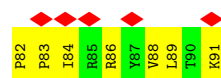
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10-B



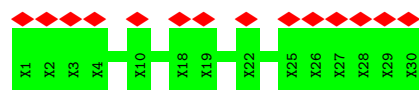
- Molecule 40: Probable NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 41: B14.5a



- Molecule 42: unknown

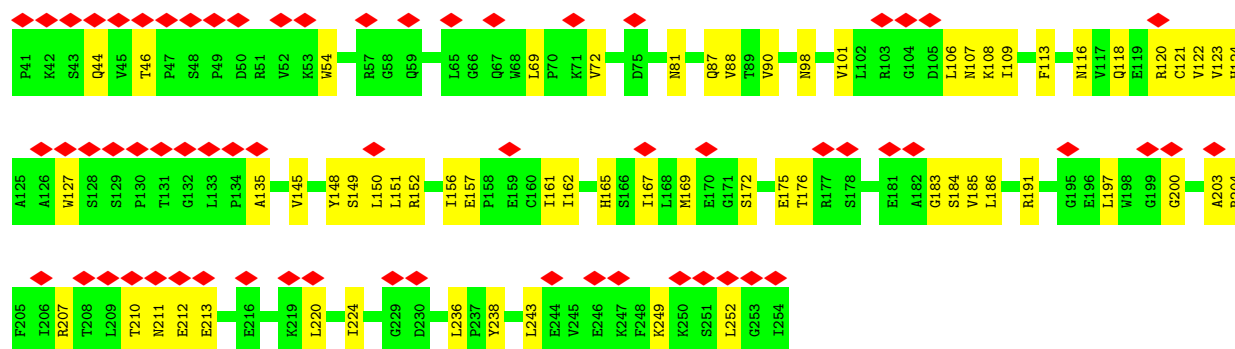


- Molecule 43: Uncharacterized protein At2g27730, mitochondrial

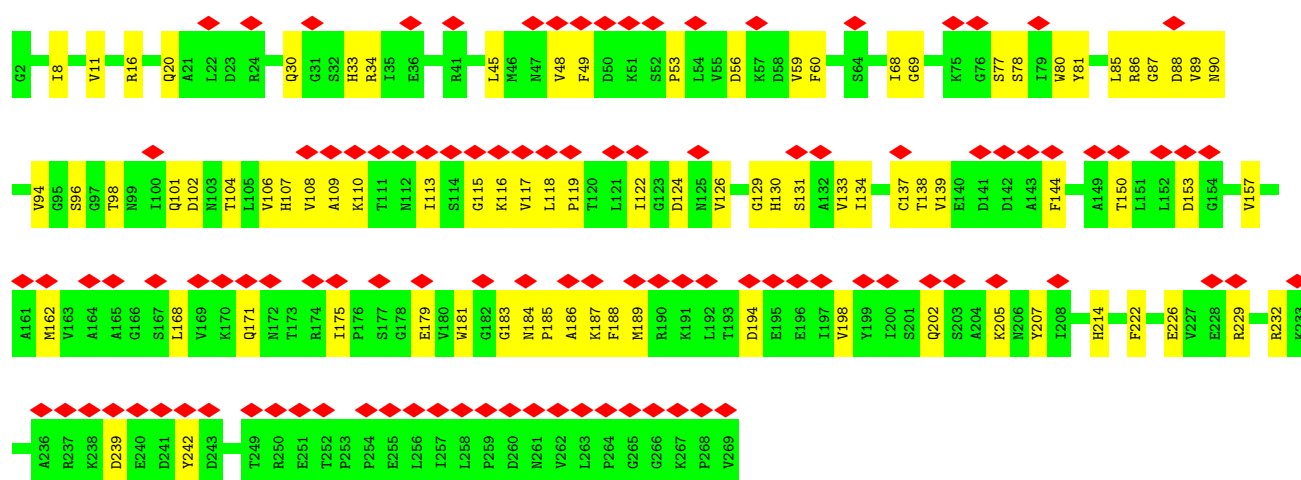
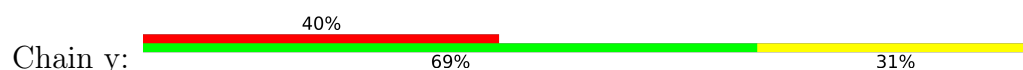


- Molecule 44: Gamma carbonic anhydrase-like 2, mitochondrial

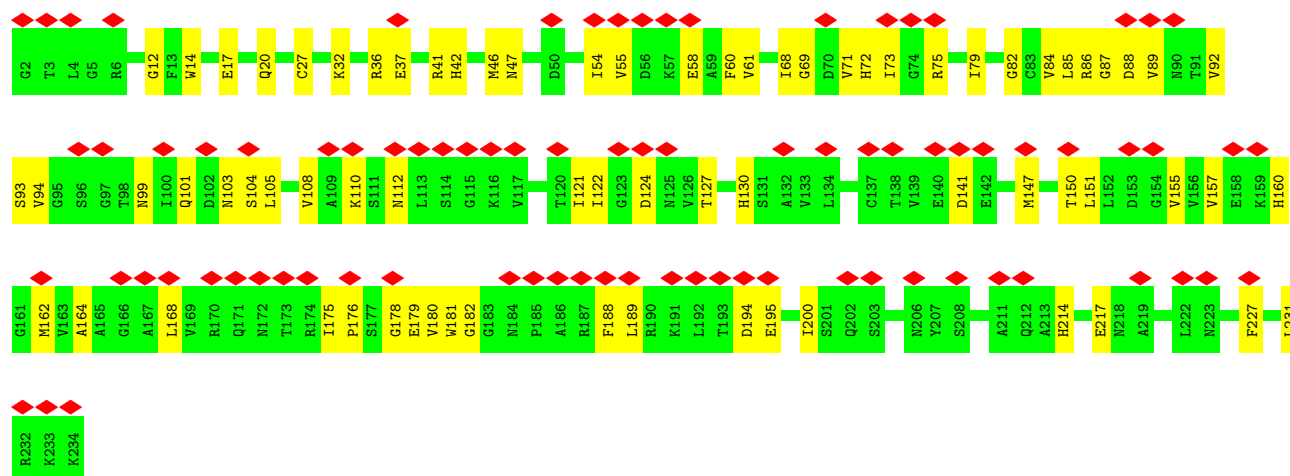




• Molecule 45: Gamma carbonic anhydrase 2, mitochondrial



• Molecule 46: 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	48933	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	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.011	Depositor
Map size ($\text{\AA}$)	502.2, 502.2, 502.2	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.837, 0.837, 0.837	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.15	0/813	0.33	0/1103
2	B	0.14	0/1279	0.28	0/1734
3	C	0.13	0/1629	0.30	0/2207
4	D	0.15	0/3147	0.33	0/4256
5	E	0.13	0/1535	0.36	0/2084
6	F	0.12	0/3441	0.32	0/4641
7	G	0.12	0/5347	0.31	0/7242
8	H	0.17	0/2609	0.42	0/3553
9	I	0.15	0/1410	0.33	0/1904
10	J	0.14	0/1118	0.30	0/1523
11	K	0.15	0/702	0.35	0/948
12	L	0.14	0/4938	0.39	1/6706 (0.0%)
13	M	0.15	0/3996	0.36	0/5431
14	N	0.14	0/3924	0.33	0/5327
15	P	0.14	0/2613	0.37	0/3539
16	Q	0.15	0/966	0.34	1/1305 (0.1%)
17	R	0.11	0/493	0.28	0/668
18	S	0.13	0/740	0.34	0/996
19	T	0.11	0/679	0.30	0/922
20	U	0.14	0/660	0.38	0/892
21	V	0.14	0/1146	0.33	0/1555
22	W	0.13	0/899	0.37	0/1218
23	X	0.14	0/777	0.42	0/1044
24	Z	0.14	0/1027	0.38	0/1392
25	a	0.15	0/482	0.40	0/646
26	b	0.14	0/300	0.34	0/407
27	c	0.11	0/637	0.34	0/860
28	d	0.15	0/605	0.36	0/815
29	e	0.11	0/559	0.27	0/745
30	f	0.15	0/768	0.35	0/1038
31	g	0.12	0/606	0.35	0/826
32	i	0.14	0/757	0.35	0/1019

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	j	0.13	0/433	0.31	0/592
34	k	0.13	0/384	0.39	0/515
35	l	0.09	0/370	0.23	0/504
36	m	0.11	0/580	0.30	0/778
37	n	0.10	0/938	0.30	0/1273
38	o	0.17	0/666	0.52	0/886
39	p	0.13	0/799	0.33	0/1074
40	q	0.10	0/537	0.30	0/728
41	r	0.21	0/89	0.73	0/119
43	v	0.09	0/230	0.22	0/311
44	x	0.13	0/1700	0.34	0/2320
45	y	0.11	0/2066	0.31	0/2800
46	z	0.12	0/1804	0.32	0/2441
All	All	0.14	0/61198	0.34	2/82887 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	Q	46	PRO	CA-N-CD	-6.63	102.72	112.00
12	L	461	ILE	CB-CA-C	-5.92	108.07	114.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	785	0	807	24	0
2	B	1244	0	1231	36	0
3	C	1581	0	1529	38	0
4	D	3077	0	3043	92	0
5	E	1500	0	1472	41	0
6	F	3368	0	3353	64	0
7	G	5252	0	5241	118	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	2536	0	2641	104	0
9	I	1381	0	1328	38	0
10	J	1093	0	1171	35	0
11	K	692	0	753	28	0
12	L	4807	0	4847	204	0
13	M	3887	0	4037	143	0
14	N	3820	0	3925	107	0
15	P	2556	0	2598	64	0
16	Q	939	0	928	19	0
17	R	482	0	478	7	0
18	S	728	0	759	18	0
19	T	667	0	648	14	0
20	U	650	0	635	17	0
21	V	1123	0	1112	33	0
22	W	880	0	873	16	0
23	X	763	0	761	19	0
24	Z	997	0	979	32	0
25	a	470	0	472	21	0
26	b	295	0	322	7	0
27	c	617	0	619	24	0
28	d	592	0	610	18	0
29	e	546	0	512	8	0
30	f	752	0	754	21	0
31	g	586	0	572	24	0
32	i	737	0	705	13	0
33	j	415	0	406	16	0
34	k	374	0	369	20	0
35	l	360	0	364	8	0
36	m	565	0	555	15	0
37	n	911	0	879	27	0
38	o	657	0	671	29	0
39	p	778	0	768	30	0
40	q	520	0	478	6	0
41	r	87	0	98	13	0
42	u	150	0	34	0	0
43	v	226	0	235	1	0
44	x	1659	0	1673	46	0
45	y	2032	0	2044	64	0
46	z	1772	0	1768	60	0
47	B	8	0	0	2	0
47	F	8	0	0	2	0
47	G	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	I	16	0	0	1	0
48	E	4	0	0	2	0
48	G	4	0	0	0	0
49	F	31	0	19	2	0
50	H	35	0	40	5	0
51	I	50	0	77	7	0
51	M	50	0	79	3	0
51	N	50	0	79	4	0
52	M	52	0	77	6	0
52	f	52	0	82	3	0
53	M	69	0	88	6	0
54	P	48	0	22	0	0
55	R	1	0	0	0	0
55	y	1	0	0	0	0
56	W	35	0	0	1	0
56	n	35	0	0	0	0
57	y	41	0	52	1	0
58	z	30	0	32	1	0
59	z	61	0	0	0	0
All	All	60606	0	60704	1504	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 12.

All (1504) 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)
13:M:389:MET:HE1	13:M:430:LEU:HG	1.54	0.89
7:G:596:LYS:HA	7:G:613:ARG:NH2	1.89	0.88
41:r:86:ARG:HH12	41:r:88:VAL:HG22	1.40	0.87
13:M:38:ARG:HH21	13:M:112:MET:HB2	1.40	0.86
12:L:369:GLY:HA3	12:L:446:THR:HA	1.58	0.85
7:G:613:ARG:HG3	7:G:613:ARG:HH11	1.42	0.85
17:R:82:HIS:CD2	17:R:100:CYS:SG	2.70	0.85
37:n:115:ASP:HB3	46:z:112:ASN:HD21	1.42	0.84
21:V:123:ASP:O	41:r:82:PRO:HD3	1.76	0.83
12:L:230:VAL:HG23	12:L:235:GLN:HB2	1.62	0.82
12:L:460:PRO:HD2	12:L:463:MET:HE2	1.63	0.81
21:V:120:ILE:HG13	41:r:86:ARG:HG3	1.64	0.80
10:J:37:THR:HG21	11:K:40:LEU:HD11	1.63	0.79
8:H:143:GLN:NE2	8:H:196:ALA:O	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:101:ILE:HG13	13:M:127:GLU:HB2	1.66	0.78
12:L:376:PRO:HG2	33:j:25:THR:HG22	1.66	0.78
38:o:35:ILE:HG22	38:o:39:LYS:HZ3	1.49	0.78
11:K:42:VAL:HG11	14:N:191:LEU:HG	1.66	0.77
41:r:82:PRO:N	41:r:83:PRO:HD2	2.00	0.77
7:G:658:ARG:HH12	7:G:662:GLU:HB2	1.47	0.76
13:M:237:LEU:O	13:M:241:HIS:HB2	1.84	0.76
34:k:24:LEU:HA	34:k:27:GLN:HE21	1.51	0.76
7:G:512:PRO:HG2	7:G:542:VAL:HG12	1.67	0.76
15:P:282:LEU:HD22	15:P:360:PHE:HE1	1.51	0.76
20:U:88:GLU:OE2	22:W:56:ARG:NH1	2.18	0.76
7:G:596:LYS:HA	7:G:613:ARG:HH21	1.50	0.75
12:L:13:SER:HB2	12:L:118:SER:HB3	1.68	0.75
5:E:132:THR:HG23	5:E:134:PRO:HD2	1.67	0.74
7:G:629:THR:HG22	7:G:639:GLN:HG2	1.70	0.74
4:D:150:GLY:HA3	9:I:108:ARG:HG3	1.68	0.73
7:G:658:ARG:NH1	7:G:662:GLU:HB2	2.04	0.73
13:M:46:LEU:HD22	31:g:69:THR:HG21	1.70	0.73
39:p:56:LYS:HG3	39:p:60:ARG:HH12	1.53	0.73
12:L:58:TYR:O	27:c:60:GLN:NE2	2.21	0.73
37:n:76:ASN:HA	37:n:79:ARG:HE	1.53	0.73
8:H:185:PRO:HB3	51:I:303:PTY:H352	1.71	0.73
24:Z:86:LEU:HD23	24:Z:87:PRO:HD3	1.68	0.73
12:L:102:SER:HB3	12:L:462:PRO:HB2	1.71	0.73
1:A:88:ILE:HD12	1:A:92:GLY:HA3	1.69	0.73
4:D:87:GLU:OE1	21:V:129:HIS:NE2	2.19	0.73
41:r:82:PRO:CD	41:r:83:PRO:HD2	2.19	0.73
45:y:81:TYR:HH	45:y:214:HIS:HD1	1.34	0.73
1:A:8:ILE:HD11	8:H:103:LEU:HD11	1.71	0.72
8:H:205:LEU:HD13	8:H:291:ARG:HA	1.72	0.72
13:M:229:PRO:HB2	13:M:313:VAL:HG13	1.71	0.72
4:D:80:HIS:NE2	4:D:240:ASP:OD2	2.22	0.72
7:G:111:LEU:HD11	7:G:267:ILE:HD11	1.71	0.72
12:L:596:ILE:HA	12:L:601:GLY:HA3	1.71	0.72
25:a:18:MET:HA	25:a:21:ILE:HG12	1.72	0.72
13:M:38:ARG:NH1	37:n:114:GLU:OE1	2.23	0.71
14:N:203:ALA:HB1	14:N:208:GLN:HG3	1.71	0.71
14:N:244:VAL:HG11	14:N:304:LEU:HD12	1.71	0.71
7:G:581:VAL:HB	7:G:600:VAL:HG12	1.73	0.71
8:H:105:ILE:HG13	8:H:106:GLY:H	1.56	0.71
12:L:328:ILE:HG23	12:L:330:ASN:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:613:ARG:HG3	7:G:613:ARG:O	1.91	0.71
11:K:76:GLY:HA2	14:N:180:LEU:HD21	1.72	0.71
13:M:322:GLY:HA3	13:M:403:ILE:HG23	1.73	0.71
3:C:21:LYS:HB3	3:C:32:ASP:HB3	1.73	0.70
14:N:65:THR:HG23	14:N:101:LEU:HD21	1.72	0.70
9:I:71:LEU:HG	51:I:303:PTY:H362	1.70	0.70
13:M:299:LEU:HD12	13:M:300:ARG:HG2	1.72	0.70
8:H:263:ILE:HB	8:H:267:ILE:HD11	1.72	0.70
8:H:254:ILE:HG13	8:H:255:LEU:H	1.56	0.70
8:H:38:LYS:HG2	9:I:93:THR:HG21	1.73	0.70
12:L:303:LEU:HD12	12:L:559:PHE:HB2	1.74	0.70
44:x:123:VAL:HG12	44:x:151:LEU:HB2	1.73	0.70
33:j:56:PRO:O	38:o:56:HIS:ND1	2.24	0.70
46:z:55:VAL:HG22	46:z:73:ILE:HD12	1.73	0.70
15:P:246:ILE:HG21	15:P:344:ILE:HD12	1.73	0.69
3:C:61:GLY:O	4:D:352:ARG:NH1	2.25	0.69
15:P:219:PRO:HA	15:P:282:LEU:HB2	1.72	0.69
45:y:90:ASN:HB2	45:y:108:VAL:HG11	1.73	0.69
5:E:77:LEU:HD22	5:E:88:LEU:HD21	1.75	0.69
8:H:98:MET:HG3	25:a:27:TYR:HB2	1.74	0.69
24:Z:112:MET:HE3	29:e:60:GLU:HG3	1.75	0.69
44:x:88:VAL:HG23	44:x:109:ILE:HB	1.73	0.69
6:F:248:LEU:HD21	7:G:115:GLY:HA3	1.75	0.69
7:G:96:GLU:OE2	7:G:104:ARG:NH2	2.25	0.69
46:z:61:VAL:HA	46:z:79:ILE:HB	1.73	0.69
12:L:356:ILE:HG12	12:L:361:ASP:HA	1.75	0.69
41:r:82:PRO:HD2	41:r:83:PRO:HD2	1.74	0.69
4:D:147:ARG:NH1	4:D:174:ASP:OD2	2.26	0.68
6:F:427:ALA:HB1	6:F:431:GLU:HG3	1.75	0.68
9:I:58:LYS:HE2	26:b:8:ARG:HE	1.55	0.68
22:W:95:GLN:HG2	22:W:98:HIS:HB2	1.74	0.68
23:X:14:THR:OG1	25:a:53:ASP:OD1	2.10	0.68
4:D:22:ALA:HB1	4:D:26:LEU:HD23	1.76	0.68
12:L:358:ALA:HA	12:L:455:ARG:HH21	1.57	0.68
45:y:187:LYS:HG2	45:y:189:MET:HE3	1.75	0.68
12:L:124:MET:HE1	12:L:256:ILE:HD11	1.74	0.68
12:L:256:ILE:HG13	12:L:261:MET:HG2	1.75	0.68
13:M:295:SER:HB2	13:M:424:LEU:HD22	1.75	0.67
6:F:418:ILE:HG22	6:F:422:MET:HE2	1.75	0.67
14:N:282:ILE:HG13	14:N:497:LEU:HD13	1.76	0.67
15:P:360:PHE:HD2	15:P:367:PRO:HG3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:156:ARG:HD2	15:P:63:ARG:HD2	1.77	0.67
31:g:48:ARG:HH22	31:g:57:ARG:HH21	1.39	0.67
32:i:23:ASP:HB3	32:i:27:ARG:HH21	1.59	0.67
4:D:80:HIS:ND1	4:D:106:CYS:SG	2.68	0.67
45:y:80:TRP:HD1	45:y:101:GLN:HA	1.59	0.67
12:L:446:THR:HG23	34:k:19:ARG:HD2	1.77	0.67
9:I:155:TYR:HB3	9:I:197:LYS:HG3	1.76	0.67
13:M:305:LYS:HE3	13:M:362:ARG:HH12	1.60	0.67
1:A:70:ILE:HG21	10:J:163:MET:HE2	1.77	0.66
13:M:53:LEU:HD12	31:g:77:LEU:HD21	1.76	0.66
13:M:399:GLY:O	13:M:403:ILE:HG13	1.95	0.66
6:F:233:THR:HG21	6:F:247:ARG:HG2	1.76	0.66
12:L:173:VAL:HG22	13:M:423:ILE:HD11	1.76	0.66
41:r:86:ARG:NH1	41:r:88:VAL:HG22	2.09	0.66
15:P:320:ALA:HB2	15:P:341:LEU:HD13	1.77	0.66
14:N:14:ASN:ND2	30:f:20:PRO:O	2.26	0.66
5:E:124:LYS:HD2	5:E:187:SER:HA	1.77	0.66
4:D:276:VAL:HG21	24:Z:33:VAL:HG21	1.78	0.66
6:F:422:MET:HE1	6:F:435:LEU:HD22	1.77	0.66
13:M:413:LEU:O	13:M:416:THR:OG1	2.12	0.66
20:U:109:ILE:HG21	20:U:114:LEU:HB3	1.76	0.66
3:C:72:GLU:OE2	3:C:89:GLN:NE2	2.28	0.65
12:L:609:LEU:HG	12:L:612:ARG:HD2	1.78	0.65
14:N:119:ARG:HG3	45:y:239:ASP:HB2	1.76	0.65
31:g:94:HIS:HA	39:p:46:GLU:HG2	1.78	0.65
46:z:71:VAL:HG22	46:z:92:VAL:HB	1.78	0.65
11:K:79:ILE:HD12	14:N:180:LEU:HD22	1.77	0.65
46:z:86:ARG:HH22	46:z:110:LYS:HZ1	1.44	0.65
7:G:176:GLY:O	7:G:182:GLN:NE2	2.29	0.65
15:P:186:LEU:O	15:P:218:ARG:NH2	2.29	0.65
9:I:178:VAL:HG21	9:I:211:ILE:HG21	1.79	0.65
14:N:210:ALA:HB2	14:N:283:TYR:HB3	1.76	0.65
37:n:62:ASP:OD1	37:n:66:LYS:NZ	2.30	0.65
12:L:488:LEU:HA	12:L:506:LEU:HD21	1.78	0.65
44:x:148:TYR:OH	46:z:103:ASN:O	2.14	0.65
52:M:501:PC7:H71	27:c:16:ARG:HD2	1.77	0.65
39:p:24:TYR:HA	39:p:30:MET:HE1	1.77	0.65
16:Q:111:GLU:OE2	16:Q:129:LYS:NZ	2.30	0.65
3:C:1:MET:N	3:C:82:TYR:O	2.31	0.64
23:X:43:ASP:OD2	23:X:45:ASN:ND2	2.29	0.64
4:D:299:ARG:NH2	9:I:175:ASP:OD1	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:k:23:MET:O	34:k:27:GLN:NE2	2.31	0.64
12:L:262:VAL:HB	12:L:319:LEU:HD11	1.80	0.64
8:H:176:GLN:NE2	24:Z:63:GLN:OE1	2.30	0.64
23:X:18:LEU:HB3	24:Z:85:ILE:HD11	1.77	0.64
46:z:68:ILE:HB	46:z:86:ARG:HG2	1.78	0.64
1:A:105:ILE:HD12	14:N:34:ILE:HD11	1.79	0.64
51:M:502:PTY:H362	31:g:77:LEU:HD12	1.79	0.64
22:W:121:THR:HG23	22:W:123:PHE:H	1.63	0.64
5:E:128:LEU:HB2	5:E:182:THR:HB	1.79	0.64
12:L:180:LEU:HB3	12:L:224:LEU:HD13	1.79	0.64
13:M:432:LEU:HA	13:M:435:ARG:HD3	1.79	0.64
22:W:79:ILE:HG22	22:W:83:MET:HE1	1.79	0.64
30:f:33:ASP:OD2	30:f:84:ARG:NH2	2.31	0.64
44:x:203:ALA:O	44:x:204:ARG:NH1	2.31	0.64
5:E:202:THR:HB	5:E:205:LYS:HB2	1.80	0.64
8:H:154:ILE:HG21	8:H:190:PHE:HB2	1.79	0.63
12:L:120:PHE:CZ	12:L:256:ILE:HG12	2.34	0.63
31:g:78:GLY:O	31:g:82:ASN:ND2	2.31	0.63
44:x:69:LEU:HB2	45:y:232:ARG:HD3	1.80	0.63
8:H:195:LEU:HG	8:H:201:ALA:HB2	1.80	0.63
13:M:92:PHE:HB3	13:M:339:LEU:HD21	1.80	0.63
20:U:63:LYS:NZ	20:U:79:LEU:O	2.29	0.63
45:y:101:GLN:HB2	45:y:130:HIS:H	1.63	0.63
7:G:435:GLU:OE2	7:G:457:ARG:NH1	2.32	0.63
44:x:249:LYS:HD3	46:z:231:LEU:HD21	1.81	0.63
4:D:110:ARG:NH2	4:D:332:GLU:O	2.32	0.63
3:C:9:TYR:OH	3:C:48:HIS:NE2	2.28	0.62
4:D:225:ARG:NH2	4:D:267:GLU:OE2	2.32	0.62
8:H:67:SER:HA	8:H:219:GLU:HG3	1.80	0.62
8:H:93:PRO:HD2	8:H:245:LEU:HD21	1.81	0.62
13:M:452:LEU:HB3	13:M:456:GLU:HG3	1.81	0.62
8:H:261:LYS:HE3	8:H:261:LYS:HA	1.82	0.62
3:C:52:ARG:HD2	21:V:92:GLU:HG2	1.81	0.62
8:H:182:PRO:HG3	24:Z:60:GLY:HA3	1.79	0.62
12:L:6:VAL:HG12	12:L:125:LEU:HB3	1.80	0.62
12:L:277:GLU:HG3	12:L:500:LEU:HD22	1.80	0.62
21:V:44:ILE:HD13	21:V:57:VAL:HG11	1.80	0.62
46:z:101:GLN:HB3	46:z:130:HIS:CD2	2.34	0.62
2:B:186:PRO:HG2	9:I:185:PHE:HD2	1.65	0.62
12:L:49:GLU:HG2	27:c:69:ILE:HB	1.81	0.62
5:E:32:LEU:O	5:E:119:ARG:NH2	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:15:PHE:HZ	4:D:375:LEU:HD11	1.65	0.62
6:F:423:LYS:O	6:F:472:ARG:NH1	2.32	0.62
14:N:467:LEU:HG	14:N:471:MET:HE3	1.80	0.62
27:c:17:ALA:HA	31:g:42:LYS:HD3	1.81	0.62
7:G:445:THR:HG23	7:G:447:PRO:HD3	1.80	0.61
12:L:197:ILE:O	12:L:201:ALA:HB2	1.99	0.61
13:M:242:VAL:HA	13:M:305:LYS:HG2	1.82	0.61
13:M:420:LEU:O	13:M:423:ILE:HG22	2.00	0.61
5:E:205:LYS:O	5:E:209:ILE:HG13	2.00	0.61
13:M:103:ILE:HG23	13:M:459:ILE:HD11	1.82	0.61
14:N:390:THR:HG1	28:d:19:TYR:HH	1.49	0.61
44:x:118:GLN:HE22	46:z:110:LYS:HD2	1.64	0.61
13:M:29:ILE:O	13:M:117:LYS:NZ	2.33	0.61
2:B:164:TYR:OH	4:D:65:PRO:HG2	2.00	0.61
3:C:1:MET:HG2	21:V:138:LEU:HD21	1.82	0.61
7:G:258:SER:HB3	7:G:261:SER:HB3	1.83	0.61
15:P:192:SER:O	15:P:198:ARG:NH1	2.34	0.61
44:x:197:LEU:HD21	44:x:207:ARG:HE	1.66	0.61
3:C:60:CYS:HB3	3:C:74:VAL:HB	1.83	0.61
12:L:168:MET:HG2	13:M:430:LEU:HD12	1.82	0.61
13:M:341:HIS:HA	13:M:344:VAL:HG22	1.83	0.61
14:N:346:LEU:HD13	14:N:493:MET:HE2	1.83	0.61
4:D:71:ASP:OD1	4:D:335:LYS:NZ	2.32	0.61
5:E:153:VAL:HG11	5:E:159:THR:HA	1.81	0.61
15:P:348:THR:HG23	15:P:349:THR:HG23	1.82	0.61
27:c:45:PHE:O	27:c:49:ILE:HG12	2.01	0.61
3:C:173:GLN:OE1	9:I:161:LYS:NZ	2.34	0.61
8:H:274:LEU:HB2	25:a:12:LEU:HD12	1.83	0.61
46:z:94:VAL:HA	46:z:122:ILE:HB	1.81	0.61
7:G:299:VAL:HG11	7:G:453:MET:HB2	1.82	0.61
13:M:391:LEU:O	13:M:394:THR:OG1	2.18	0.61
23:X:90:ASP:HA	23:X:93:ARG:HH21	1.66	0.61
11:K:53:LEU:HD22	29:e:45:LEU:HD22	1.83	0.60
6:F:64:ILE:O	6:F:160:LYS:NZ	2.34	0.60
13:M:237:LEU:O	13:M:241:HIS:CB	2.48	0.60
2:B:166:HIS:O	2:B:166:HIS:ND1	2.35	0.60
12:L:96:VAL:HG11	12:L:255:LEU:HB2	1.84	0.60
15:P:142:ILE:HD11	15:P:269:LEU:HD11	1.83	0.60
2:B:148:GLU:HB2	8:H:62:GLU:HG2	1.82	0.60
7:G:613:ARG:HH11	7:G:613:ARG:CG	2.14	0.60
12:L:29:ALA:HA	12:L:114:MET:HG3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:59:LYS:NZ	19:T:81:ASP:OD2	2.33	0.60
20:U:118:PHE:O	20:U:122:HIS:ND1	2.33	0.60
12:L:399:TYR:HB3	12:L:482:LYS:HD3	1.84	0.60
7:G:520:LEU:HD23	7:G:529:ILE:HG21	1.83	0.60
37:n:15:ALA:O	37:n:19:ARG:HB2	2.02	0.60
40:q:100:ILE:HG22	40:q:101:THR:HG23	1.82	0.60
7:G:264:VAL:HA	7:G:267:ILE:HG22	1.82	0.59
12:L:3:LEU:HB2	27:c:55:SER:HB2	1.84	0.59
12:L:278:TYR:OH	39:p:67:TYR:OH	2.19	0.59
31:g:40:ARG:HE	31:g:41:PRO:HD2	1.65	0.59
5:E:128:LEU:HB3	5:E:169:MET:HB3	1.85	0.59
6:F:185:TYR:HB3	6:F:188:GLU:HB2	1.83	0.59
49:F:500:FMN:O4'	49:F:500:FMN:O2'	2.19	0.59
12:L:81:LEU:HB2	12:L:496:SER:HB3	1.84	0.59
22:W:22:ALA:HB1	22:W:75:ILE:HG21	1.84	0.59
4:D:139:GLU:OE1	4:D:152:ARG:NH2	2.36	0.59
19:T:56:SER:O	34:k:14:ARG:NH1	2.35	0.59
37:n:31:THR:HG23	37:n:41:PHE:HE1	1.68	0.59
44:x:211:ASN:OD1	44:x:212:GLU:N	2.36	0.59
6:F:155:ARG:HG3	6:F:188:GLU:HG3	1.85	0.59
12:L:172:ARG:HH21	13:M:422:MET:HB2	1.68	0.59
16:Q:47:GLU:HA	16:Q:50:LEU:HD23	1.85	0.59
44:x:81:ASN:OD1	46:z:42:HIS:ND1	2.35	0.59
5:E:129:VAL:HG22	5:E:130:CYS:H	1.68	0.59
44:x:238:TYR:OH	46:z:36:ARG:NH1	2.36	0.59
46:z:71:VAL:HG11	46:z:85:LEU:HD13	1.85	0.59
8:H:135:LEU:O	8:H:139:ARG:HG3	2.03	0.59
12:L:282:ALA:O	12:L:286:ILE:HG12	2.03	0.59
27:c:16:ARG:HE	27:c:26:PRO:HG3	1.68	0.59
44:x:172:SER:HB2	44:x:186:LEU:HD11	1.85	0.59
12:L:166:LYS:HA	12:L:169:LEU:HD12	1.84	0.59
12:L:306:ASP:OD2	12:L:309:ARG:NH1	2.35	0.59
27:c:48:CYS:HA	27:c:51:ILE:HD12	1.85	0.58
3:C:158:ASP:OD2	15:P:86:GLN:NE2	2.36	0.58
12:L:274:PRO:HB3	12:L:498:LEU:HD13	1.85	0.58
13:M:307:ILE:HD12	13:M:432:LEU:HD21	1.85	0.58
11:K:57:MET:HE3	11:K:57:MET:HA	1.84	0.58
2:B:99:MET:HG2	4:D:135:PHE:HE2	1.67	0.58
41:r:84:ILE:HG22	41:r:84:ILE:O	2.03	0.58
45:y:94:VAL:HA	45:y:122:ILE:HB	1.86	0.58
6:F:319:LEU:HD21	6:F:340:ILE:HD13	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:489:VAL:HG23	28:d:56:LEU:HD21	1.86	0.58
10:J:121:SER:O	24:Z:96:ARG:NH2	2.37	0.58
12:L:256:ILE:HG13	12:L:261:MET:CG	2.33	0.58
38:o:51:CYS:SG	38:o:55:ARG:NH1	2.77	0.58
7:G:386:GLN:N	7:G:411:GLU:OE1	2.36	0.58
7:G:582:TYR:HD1	7:G:601:VAL:HG13	1.69	0.58
12:L:411:LYS:HB2	12:L:505:ILE:HD13	1.85	0.58
44:x:124:HIS:HB3	44:x:152:ARG:HG3	1.86	0.58
27:c:30:PRO:HG2	27:c:33:TRP:HB3	1.86	0.58
6:F:337:LEU:HD23	6:F:352:LYS:HG3	1.86	0.58
12:L:451:ARG:NH2	19:T:94:LYS:O	2.37	0.58
8:H:105:ILE:HG13	8:H:106:GLY:N	2.19	0.57
27:c:31:LYS:HZ3	31:g:35:PRO:HB2	1.68	0.57
1:A:78:PHE:HZ	1:A:100:LEU:HD11	1.69	0.57
12:L:183:LEU:HD13	13:M:408:PHE:CD2	2.40	0.57
15:P:161:HIS:NE2	15:P:165:GLU:OE2	2.37	0.57
45:y:30:GLN:HG3	46:z:12:GLY:HA3	1.86	0.57
5:E:136:MET:SD	5:E:141:ARG:NH2	2.74	0.57
12:L:307:LEU:HD21	12:L:352:ALA:HB1	1.85	0.57
13:M:26:LEU:HD22	13:M:121:ILE:HG12	1.85	0.57
13:M:425:GLY:HA2	13:M:428:TYR:CE1	2.39	0.57
15:P:360:PHE:CD2	15:P:367:PRO:HG3	2.37	0.57
39:p:41:LYS:O	39:p:45:ILE:HG12	2.05	0.57
44:x:87:GLN:HG3	44:x:108:LYS:HA	1.86	0.57
8:H:177:ILE:HD11	24:Z:64:VAL:HG23	1.85	0.57
12:L:197:ILE:HD11	12:L:275:LEU:HD13	1.87	0.57
45:y:33:HIS:O	46:z:47:ASN:ND2	2.37	0.57
4:D:70:LEU:HD11	4:D:355:ILE:HD13	1.87	0.57
6:F:161:LEU:HD13	6:F:268:VAL:HG23	1.84	0.57
6:F:428:LYS:NZ	6:F:431:GLU:OE2	2.37	0.57
8:H:109:TYR:HA	10:J:51:MET:HE2	1.86	0.57
8:H:135:LEU:HD23	8:H:139:ARG:HD2	1.87	0.57
34:k:8:THR:HB	37:n:49:ARG:HH11	1.70	0.57
12:L:172:ARG:HG3	13:M:423:ILE:HA	1.85	0.57
15:P:324:PHE:HE2	15:P:336:PRO:HB3	1.69	0.57
19:T:71:PHE:HB3	19:T:77:LEU:HD13	1.86	0.57
39:p:39:ARG:O	39:p:43:ILE:HG12	2.05	0.57
7:G:412:GLY:HA3	7:G:556:TYR:HE2	1.69	0.57
21:V:86:VAL:HA	21:V:89:LEU:HD12	1.86	0.57
8:H:254:ILE:HG13	8:H:255:LEU:N	2.19	0.57
14:N:125:PHE:O	14:N:129:ILE:HG12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:m:46:ILE:O	36:m:50:LYS:HG2	2.05	0.57
46:z:162:MET:HB3	46:z:180:VAL:HG12	1.87	0.57
12:L:102:SER:HB3	12:L:462:PRO:CB	2.35	0.57
27:c:37:THR:O	27:c:41:MET:HG2	2.04	0.57
38:o:23:ALA:HA	39:p:64:VAL:HG11	1.87	0.57
18:S:84:LYS:O	18:S:88:ASN:ND2	2.38	0.56
33:j:31:LEU:HA	33:j:34:VAL:HG12	1.87	0.56
5:E:174:CYS:H	6:F:148:CYS:HB3	1.70	0.56
13:M:147:GLU:HG3	14:N:402:PRO:HG2	1.86	0.56
45:y:226:GLU:OE2	45:y:229:ARG:NH2	2.38	0.56
12:L:58:TYR:HE1	12:L:77:LEU:HG	1.70	0.56
13:M:408:PHE:CE1	13:M:415:ALA:HB3	2.40	0.56
14:N:139:MET:HE1	14:N:155:GLN:NE2	2.20	0.56
2:B:91:LEU:HB2	4:D:25:VAL:HB	1.87	0.56
6:F:350:ILE:HG23	6:F:354:ILE:HG13	1.87	0.56
12:L:86:LEU:O	12:L:90:THR:HG22	2.05	0.56
12:L:379:TYR:HA	12:L:382:MET:HE2	1.86	0.56
20:U:109:ILE:HG12	20:U:114:LEU:HD23	1.87	0.56
40:q:62:TYR:HE2	40:q:77:GLU:HB2	1.71	0.56
3:C:60:CYS:SG	3:C:61:GLY:N	2.77	0.56
7:G:429:THR:OG1	7:G:548:ASN:O	2.22	0.56
21:V:123:ASP:O	41:r:82:PRO:CD	2.49	0.56
7:G:293:ILE:HD13	7:G:638:GLN:HG3	1.87	0.56
37:n:24:TYR:HA	37:n:52:PHE:HE2	1.71	0.56
39:p:41:LYS:HE2	39:p:85:GLY:HA2	1.85	0.56
3:C:1:MET:HE3	3:C:6:ILE:HD11	1.87	0.56
8:H:296:MET:HE3	8:H:296:MET:HA	1.87	0.56
10:J:127:TYR:HE1	24:Z:89:LEU:HD23	1.71	0.56
11:K:50:SER:HB2	11:K:58:GLY:HA3	1.86	0.56
13:M:358:ARG:HG3	37:n:111:TYR:HE2	1.71	0.56
24:Z:99:SER:HA	24:Z:102:LYS:NZ	2.20	0.56
15:P:76:ALA:HB3	15:P:97:VAL:HG13	1.86	0.56
34:k:16:ASP:OD2	37:n:38:ARG:NH1	2.39	0.56
38:o:67:MET:HA	38:o:70:MET:HG2	1.88	0.56
44:x:122:VAL:HB	44:x:150:LEU:HD13	1.88	0.56
2:B:162:GLY:HA3	2:B:166:HIS:CD2	2.41	0.55
5:E:35:HIS:ND1	5:E:37:ASP:OD1	2.39	0.55
14:N:78:ILE:HA	30:f:7:ALA:HA	1.89	0.55
27:c:13:GLY:HA2	37:n:101:PRO:HG3	1.88	0.55
39:p:81:THR:HA	39:p:84:VAL:HG23	1.89	0.55
2:B:88:THR:HG23	2:B:98:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:MET:HB3	3:C:143:LEU:HB2	1.88	0.55
12:L:4:LEU:HD12	12:L:8:LEU:HD21	1.88	0.55
39:p:77:TYR:HD2	39:p:78:LEU:HD22	1.70	0.55
45:y:80:TRP:CD1	45:y:101:GLN:HA	2.41	0.55
7:G:523:ARG:HH22	7:G:713:THR:HB	1.72	0.55
7:G:587:ASP:OD2	7:G:730:ARG:NH1	2.39	0.55
11:K:61:PHE:CG	14:N:146:ILE:HG12	2.41	0.55
14:N:124:GLU:HA	14:N:127:VAL:HG12	1.88	0.55
15:P:60:THR:O	15:P:65:SER:OG	2.19	0.55
15:P:299:ASP:OD1	15:P:300:MET:N	2.39	0.55
19:T:43:ARG:HE	19:T:112:ILE:HG12	1.71	0.55
4:D:112:LEU:HD21	4:D:141:LEU:HB2	1.89	0.55
7:G:326:GLU:OE1	16:Q:61:ARG:NH2	2.40	0.55
12:L:235:GLN:O	12:L:239:HIS:ND1	2.38	0.55
1:A:4:GLU:O	8:H:101:SER:OG	2.21	0.55
7:G:139:LEU:H	7:G:142:MET:HE2	1.71	0.55
8:H:89:TRP:HZ2	8:H:237:ILE:HG22	1.71	0.55
12:L:392:PHE:HB3	12:L:395:LEU:HD12	1.88	0.55
12:L:481:ALA:HA	12:L:484:MET:HG3	1.88	0.55
21:V:57:VAL:HA	21:V:60:PHE:CE2	2.41	0.55
28:d:32:PRO:HD2	46:z:17:GLU:OE2	2.06	0.55
7:G:613:ARG:HG3	7:G:613:ARG:NH1	2.17	0.55
12:L:96:VAL:HG21	12:L:255:LEU:HB2	1.87	0.55
15:P:63:ARG:NH1	15:P:114:ASP:OD1	2.39	0.55
33:j:48:PRO:HB2	33:j:54:ARG:HG2	1.89	0.55
15:P:150:GLU:HG2	15:P:156:PHE:CE2	2.42	0.55
38:o:63:TYR:CD2	38:o:67:MET:HE1	2.42	0.55
41:r:82:PRO:N	41:r:83:PRO:CD	2.69	0.55
5:E:147:LEU:HD21	5:E:206:VAL:HG21	1.89	0.55
9:I:172:CYS:SG	9:I:177:ILE:HG22	2.47	0.55
12:L:322:MET:HE1	12:L:338:LEU:HA	1.89	0.55
15:P:98:PRO:HB2	15:P:123:PHE:CD1	2.42	0.55
45:y:98:THR:HG22	45:y:126:VAL:H	1.72	0.55
12:L:4:LEU:O	12:L:8:LEU:HG	2.06	0.55
12:L:102:SER:CB	12:L:462:PRO:HB2	2.36	0.55
14:N:108:ILE:HD11	14:N:126:ILE:HG23	1.89	0.55
14:N:144:ASP:OD1	14:N:145:LEU:N	2.40	0.55
38:o:35:ILE:HG22	38:o:39:LYS:NZ	2.19	0.55
45:y:133:VAL:HB	45:y:150:THR:HA	1.89	0.55
46:z:130:HIS:HB2	46:z:147:MET:SD	2.47	0.55
4:D:210:THR:HA	21:V:21:VAL:HG13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:18:LEU:HB2	25:a:18:MET:HE1	1.87	0.54
9:I:154:ARG:NH1	16:Q:89:MET:O	2.40	0.54
12:L:172:ARG:HH12	12:L:176:PHE:HB2	1.72	0.54
13:M:433:TYR:CZ	13:M:437:VAL:HG11	2.42	0.54
8:H:100:LEU:O	25:a:38:LYS:NZ	2.40	0.54
12:L:48:TYR:HA	12:L:52:LEU:HD13	1.89	0.54
12:L:195:SER:HB2	39:p:56:LYS:HD3	1.88	0.54
20:U:70:THR:HG22	20:U:73:ALA:HB2	1.89	0.54
46:z:162:MET:HE3	46:z:200:ILE:HD11	1.88	0.54
5:E:132:THR:HA	5:E:136:MET:HE2	1.89	0.54
13:M:347:ALA:HB1	13:M:384:PHE:CE2	2.43	0.54
37:n:22:ILE:O	37:n:26:ARG:HG2	2.07	0.54
14:N:189:ILE:HG23	14:N:232:PHE:HD1	1.72	0.54
24:Z:119:LYS:HG2	24:Z:119:LYS:O	2.08	0.54
2:B:153:ILE:HD11	2:B:202:LEU:HD22	1.89	0.54
3:C:159:ASP:HB2	15:P:112:MET:HE1	1.89	0.54
8:H:195:LEU:HD21	8:H:283:VAL:HG11	1.88	0.54
31:g:75:VAL:O	31:g:79:VAL:HG12	2.07	0.54
8:H:298:LEU:O	8:H:302:VAL:HG22	2.08	0.54
44:x:243:LEU:HD11	45:y:20:GLN:HE22	1.71	0.54
7:G:443:ILE:HD13	7:G:472:VAL:HB	1.90	0.54
8:H:302:VAL:HG12	26:b:16:VAL:HG21	1.90	0.54
10:J:123:ARG:HH21	24:Z:135:THR:HG21	1.72	0.54
45:y:85:LEU:HD13	45:y:106:VAL:HB	1.88	0.54
12:L:116:TYR:HB3	12:L:150:LEU:HD21	1.89	0.54
12:L:154:TRP:CE2	37:n:97:ARG:HD2	2.43	0.54
14:N:302:MET:HB3	14:N:432:THR:HG21	1.88	0.54
5:E:109:GLU:OE2	7:G:239:ILE:N	2.39	0.54
12:L:66:SER:HB3	13:M:475:LYS:HG3	1.90	0.54
24:Z:74:LEU:O	24:Z:77:GLU:HG3	2.08	0.54
6:F:402:CYS:HA	7:G:242:ARG:HG3	1.89	0.54
7:G:489:PRO:HB3	7:G:710:MET:HE2	1.90	0.54
53:M:503:LMN:HCJ	28:d:5:ALA:HB2	1.90	0.54
14:N:338:THR:C	32:i:48:ILE:HD13	2.33	0.54
35:l:105:VAL:O	38:o:77:ARG:NH2	2.40	0.54
39:p:15:PRO:HG2	39:p:33:MET:HE2	1.89	0.54
4:D:219:PHE:HZ	4:D:365:GLY:HA3	1.73	0.53
15:P:213:GLU:HB3	15:P:276:MET:HE2	1.88	0.53
45:y:144:PHE:HD2	45:y:162:MET:HG3	1.74	0.53
14:N:205:HIS:HB3	14:N:208:GLN:HG2	1.90	0.53
21:V:18:THR:HG23	21:V:25:VAL:HG12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:375:LEU:HD21	8:H:213:VAL:HG11	1.90	0.53
7:G:529:ILE:HA	7:G:710:MET:HE3	1.91	0.53
13:M:316:MET:HE2	13:M:316:MET:HA	1.88	0.53
9:I:59:ASP:HB2	9:I:62:THR:HG22	1.89	0.53
24:Z:88:ILE:HG23	24:Z:89:LEU:HD12	1.89	0.53
5:E:130:CYS:HB2	5:E:140:SER:OG	2.09	0.53
7:G:394:MET:SD	7:G:683:VAL:HG11	2.48	0.53
13:M:184:MET:O	13:M:188:ILE:HG12	2.08	0.53
15:P:217:MET:HG3	15:P:282:LEU:HD11	1.91	0.53
12:L:140:TRP:HE1	12:L:232:LYS:HG2	1.73	0.53
12:L:183:LEU:HD13	13:M:408:PHE:HD2	1.73	0.53
17:R:71:ALA:HB1	17:R:84:ILE:HD11	1.91	0.53
18:S:7:ILE:HB	18:S:43:ASN:HD21	1.74	0.53
20:U:81:LEU:HD21	20:U:89:VAL:HG21	1.91	0.53
20:U:87:VAL:HA	20:U:90:VAL:HG12	1.90	0.53
44:x:167:ILE:HG22	44:x:169:MET:HE3	1.91	0.53
4:D:296:PRO:HB3	4:D:315:LEU:HD11	1.89	0.53
8:H:119:TYR:OH	10:J:58:ILE:O	2.24	0.53
4:D:26:LEU:HD13	4:D:389:PHE:HZ	1.74	0.53
7:G:337:ASP:HB2	7:G:734:ILE:HD12	1.91	0.53
7:G:600:VAL:HG23	7:G:614:ALA:HA	1.91	0.53
8:H:5:VAL:O	8:H:9:ILE:HG12	2.08	0.53
28:d:55:LYS:O	28:d:58:GLU:HG2	2.09	0.53
34:k:16:ASP:HB2	34:k:19:ARG:HG2	1.90	0.53
3:C:109:GLY:HA2	3:C:126:HIS:HE1	1.73	0.53
8:H:282:TRP:NE1	9:I:83:THR:OG1	2.41	0.53
12:L:302:ILE:O	12:L:436:ARG:NH1	2.41	0.53
13:M:228:VAL:HG23	13:M:260:GLY:HA3	1.91	0.53
14:N:492:GLN:NE2	28:d:59:ASP:OD2	2.41	0.53
30:f:80:ASN:HA	30:f:89:PHE:HE2	1.72	0.53
37:n:93:SER:O	37:n:97:ARG:NH2	2.41	0.53
45:y:115:GLY:C	45:y:116:LYS:HD3	2.34	0.53
4:D:119:THR:HG21	4:D:134:ALA:CB	2.39	0.53
6:F:143:SER:HG	6:F:227:TYR:HD1	1.56	0.53
8:H:98:MET:HG2	25:a:23:GLY:C	2.34	0.53
12:L:314:SER:O	12:L:318:GLN:HG2	2.09	0.53
12:L:452:ASP:OD2	19:T:94:LYS:NZ	2.37	0.53
13:M:80:ILE:HD12	13:M:140:LEU:HD23	1.90	0.53
14:N:442:ARG:O	14:N:445:LYS:HG2	2.08	0.53
3:C:176:ARG:NH2	9:I:138:ILE:O	2.42	0.52
14:N:143:TYR:HE1	14:N:283:TYR:HE2	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:W:40:ILE:HA	22:W:43:ILE:HG22	1.90	0.52
2:B:93:CYS:HB2	4:D:153:MET:HE1	1.92	0.52
8:H:183:LEU:HB3	8:H:186:VAL:HB	1.91	0.52
13:M:209:SER:HB2	13:M:212:ARG:HB2	1.92	0.52
38:o:17:MET:SD	38:o:27:ARG:HD3	2.49	0.52
7:G:278:PHE:HE1	7:G:313:MET:HB3	1.74	0.52
8:H:13:ILE:HD12	8:H:86:LEU:HD13	1.92	0.52
10:J:130:LYS:HG2	25:a:44:GLU:OE2	2.09	0.52
12:L:236:ILE:HD13	12:L:292:MET:HG2	1.91	0.52
12:L:567:GLN:NE2	12:L:571:ASP:OD2	2.43	0.52
45:y:86:ARG:HE	45:y:107:HIS:CD2	2.27	0.52
12:L:211:CYS:HB2	13:M:413:LEU:HD13	1.90	0.52
12:L:366:ARG:HA	37:n:36:VAL:HG13	1.91	0.52
13:M:65:LYS:HE2	32:i:26:ALA:HB1	1.92	0.52
21:V:15:LYS:O	21:V:16:GLN:HG3	2.10	0.52
44:x:157:GLU:HB3	44:x:176:THR:HG22	1.90	0.52
45:y:16:ARG:HH11	46:z:27:CYS:HB2	1.75	0.52
7:G:420:ASP:OD2	18:S:36:TYR:OH	2.27	0.52
12:L:147:SER:O	12:L:151:ILE:HG12	2.10	0.52
13:M:411:ASN:ND2	36:m:52:ILE:HG23	2.24	0.52
13:M:445:PHE:HB3	36:m:8:ASN:HB2	1.92	0.52
30:f:84:ARG:HB3	30:f:94:GLU:OE2	2.10	0.52
1:A:116:LEU:HD11	8:H:300:TRP:HB3	1.92	0.52
5:E:65:PRO:HG2	5:E:68:TYR:HB2	1.92	0.52
15:P:301:ILE:O	15:P:302:ARG:HG2	2.09	0.52
26:b:7:LEU:O	26:b:11:VAL:HG23	2.10	0.52
35:l:108:THR:O	38:o:69:ARG:NH2	2.42	0.52
45:y:175:ILE:HD11	45:y:179:GLU:HB2	1.91	0.52
5:E:106:ARG:NH1	7:G:235:GLN:OE1	2.43	0.52
12:L:55:SER:OG	27:c:63:HIS:O	2.21	0.52
12:L:170:VAL:HG21	12:L:241:TRP:CD1	2.45	0.52
13:M:147:GLU:OE1	13:M:181:SER:HB2	2.10	0.52
14:N:249:TRP:O	14:N:253:ILE:HG12	2.10	0.52
1:A:71:PHE:HZ	1:A:107:PHE:HB2	1.74	0.51
4:D:311:HIS:ND1	7:G:186:MET:SD	2.80	0.51
9:I:110:GLU:HA	9:I:185:PHE:HZ	1.74	0.51
19:T:107:SER:HB2	19:T:110:LEU:HD13	1.92	0.51
44:x:183:GLY:HA3	46:z:168:LEU:HD21	1.92	0.51
5:E:138:ARG:NH2	6:F:303:GLY:O	2.43	0.51
11:K:27:ASN:C	11:K:29:LEU:H	2.19	0.51
12:L:172:ARG:HD2	12:L:175:ASP:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:103:ASP:HB2	37:m:21:ARG:HE	1.75	0.51
3:C:7:PHE:CG	3:C:24:ARG:HD3	2.45	0.51
4:D:197:ARG:O	4:D:201:GLN:HG3	2.10	0.51
7:G:703:LYS:O	18:S:37:LYS:NZ	2.35	0.51
12:L:36:VAL:HG21	12:L:97:HIS:HD2	1.76	0.51
15:P:55:LEU:HD13	15:P:69:ILE:HD11	1.92	0.51
46:z:164:ALA:HB3	46:z:182:GLY:HA3	1.92	0.51
3:C:1:MET:HG2	21:V:138:LEU:HD11	1.93	0.51
3:C:29:ASN:HB3	3:C:86:ILE:HD12	1.93	0.51
12:L:165:ILE:HD13	13:M:431:TRP:HD1	1.75	0.51
12:L:318:GLN:O	12:L:322:MET:HG3	2.11	0.51
24:Z:92:GLU:OE2	25:a:52:ARG:NH1	2.43	0.51
30:f:57:ILE:O	30:f:57:ILE:HG13	2.11	0.51
8:H:57:LYS:HE2	8:H:58:LEU:HD22	1.91	0.51
12:L:14:SER:HA	52:M:501:PC7:H181	1.92	0.51
12:L:235:GLN:HA	12:L:293:THR:HG21	1.92	0.51
12:L:251:PRO:O	12:L:255:LEU:N	2.36	0.51
12:L:584:VAL:HG12	36:m:36:LEU:HD11	1.93	0.51
12:L:596:ILE:O	12:L:602:ILE:N	2.43	0.51
15:P:131:ILE:HD12	15:P:167:LEU:HD23	1.92	0.51
45:y:68:ILE:HD11	45:y:86:ARG:HG2	1.92	0.51
2:B:157:SER:N	47:B:500:SF4:S4	2.84	0.51
4:D:168:PRO:HG2	4:D:171:LEU:HB2	1.92	0.51
39:p:54:LYS:HB3	39:p:73:LEU:HD21	1.92	0.51
12:L:217:ALA:O	12:L:221:ILE:HG12	2.11	0.51
12:L:505:ILE:O	12:L:505:ILE:HG13	2.10	0.51
30:f:63:VAL:HG11	52:f:201:PC7:H341	1.91	0.51
44:x:161:ILE:HD12	44:x:220:LEU:HD23	1.93	0.51
4:D:245:LEU:HD13	4:D:274:ILE:HG23	1.92	0.51
4:D:250:PRO:HB3	4:D:266:GLU:HG2	1.93	0.51
6:F:182:ARG:NE	6:F:184:GLU:OE1	2.36	0.51
7:G:439:LEU:HD22	7:G:506:LEU:HD13	1.93	0.51
7:G:472:VAL:HG22	7:G:485:LEU:HB2	1.93	0.51
13:M:299:LEU:HD23	13:M:424:LEU:HD21	1.93	0.51
14:N:346:LEU:HB2	14:N:490:THR:HG23	1.92	0.51
29:e:16:ASP:OD2	29:e:16:ASP:N	2.44	0.51
36:m:48:VAL:O	36:m:52:ILE:HD12	2.11	0.51
4:D:84:LEU:HD13	21:V:131:PRO:HD3	1.92	0.51
13:M:112:MET:HE3	13:M:112:MET:HA	1.92	0.51
15:P:68:GLY:O	15:P:139:ASN:ND2	2.35	0.51
15:P:242:PHE:HA	15:P:306:ARG:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:105:PHE:O	7:G:223:ARG:NH2	2.43	0.51
7:G:257:THR:HG22	7:G:742:LEU:HD22	1.93	0.51
7:G:266:ASP:OD2	7:G:333:ARG:NH2	2.37	0.51
13:M:284:TYR:HB3	13:M:414:VAL:HG21	1.93	0.51
20:U:61:PHE:CE2	20:U:89:VAL:HG22	2.46	0.51
8:H:313:SER:HA	26:b:27:GLY:HA3	1.93	0.50
12:L:258:ALA:HB1	12:L:345:LYS:HG3	1.92	0.50
22:W:86:LEU:O	22:W:90:VAL:HG23	2.11	0.50
38:o:24:LEU:HG	39:p:64:VAL:HG12	1.93	0.50
44:x:81:ASN:HB2	44:x:98:ASN:HB2	1.94	0.50
46:z:157:VAL:HG22	46:z:175:ILE:HD12	1.93	0.50
5:E:180:MET:HG2	5:E:199:GLU:HA	1.92	0.50
12:L:150:LEU:HD12	12:L:252:VAL:HG11	1.92	0.50
14:N:39:PHE:CZ	30:f:60:PRO:HB3	2.47	0.50
14:N:369:THR:HG21	14:N:458:TYR:HA	1.92	0.50
21:V:36:LEU:HD21	21:V:94:ARG:HG3	1.92	0.50
25:a:45:TRP:CE2	25:a:49:MET:HE3	2.47	0.50
39:p:19:ASP:OD1	39:p:19:ASP:N	2.43	0.50
2:B:155:MET:HE3	2:B:195:LEU:HB2	1.93	0.50
2:B:165:TYR:C	2:B:167:TYR:H	2.18	0.50
4:D:182:PHE:CE2	4:D:186:ILE:HD11	2.46	0.50
7:G:106:CYS:O	7:G:226:ARG:NH2	2.34	0.50
7:G:613:ARG:CG	7:G:613:ARG:NH1	2.73	0.50
10:J:154:VAL:HG11	14:N:150:LEU:HB3	1.91	0.50
15:P:363:LEU:O	15:P:363:LEU:HD23	2.11	0.50
25:a:25:SER:O	25:a:29:ILE:HG13	2.10	0.50
31:g:85:PRO:HG2	31:g:87:LEU:HD22	1.93	0.50
38:o:22:ILE:O	38:o:27:ARG:NH2	2.43	0.50
44:x:236:LEU:O	46:z:41:ARG:NH2	2.43	0.50
6:F:410:GLU:OE1	7:G:165:ASN:ND2	2.42	0.50
12:L:51:ALA:HB1	12:L:492:PHE:HE1	1.77	0.50
13:M:389:MET:HE2	13:M:426:ALA:HB1	1.93	0.50
36:m:42:ILE:O	36:m:46:ILE:HG12	2.12	0.50
45:y:101:GLN:HG3	45:y:129:GLY:HA2	1.93	0.50
4:D:76:MET:HE1	4:D:157:PHE:HB3	1.94	0.50
16:Q:52:ARG:HH12	16:Q:96:ASP:CG	2.19	0.50
21:V:37:TYR:HB2	21:V:65:LEU:HD13	1.93	0.50
43:v:79:ASP:O	43:v:83:ASN:ND2	2.44	0.50
44:x:236:LEU:HD23	44:x:236:LEU:H	1.75	0.50
4:D:246:ASP:O	4:D:277:GLN:NE2	2.43	0.50
7:G:489:PRO:HG2	7:G:711:SER:OG	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:341:HIS:HA	12:L:344:PHE:CE2	2.46	0.50
14:N:362:ILE:HG21	14:N:391:PHE:CD1	2.47	0.50
33:j:13:LYS:HE3	34:k:18:TRP:H	1.76	0.50
3:C:111:TRP:O	3:C:114:GLU:HG3	2.12	0.50
8:H:94:PHE:HB2	8:H:98:MET:HB3	1.92	0.50
44:x:106:LEU:HD22	44:x:127:TRP:NE1	2.26	0.50
46:z:176:PRO:HB2	46:z:179:GLU:OE2	2.11	0.50
1:A:99:PHE:CD2	10:J:156:SER:HB3	2.46	0.50
2:B:211:ASP:OD1	2:B:211:ASP:N	2.45	0.50
5:E:136:MET:HG2	5:E:140:SER:HB3	1.93	0.50
6:F:251:PRO:HG3	16:Q:140:TYR:HD2	1.77	0.50
7:G:169:ASP:CG	7:G:217:ARG:HH21	2.20	0.50
7:G:252:VAL:HG23	7:G:254:LYS:HG2	1.94	0.50
7:G:338:GLY:O	7:G:606:HIS:NE2	2.40	0.50
11:K:78:ALA:O	11:K:82:ILE:HG12	2.12	0.50
12:L:581:GLY:HA2	13:M:296:LEU:HB3	1.93	0.50
1:A:57:PHE:HA	10:J:71:MET:HG2	1.93	0.49
2:B:160:ASN:HB2	2:B:184:TYR:HD2	1.77	0.49
4:D:32:MET:HG2	4:D:37:VAL:HA	1.93	0.49
4:D:188:GLU:OE2	9:I:86:TYR:OH	2.30	0.49
7:G:367:VAL:O	7:G:371:ILE:HG12	2.12	0.49
8:H:21:ALA:HB2	50:H:500:UQ9:H12	1.94	0.49
11:K:12:ILE:HA	11:K:15:ILE:HG12	1.94	0.49
4:D:209:VAL:HG22	4:D:260:ARG:HH21	1.77	0.49
7:G:447:PRO:O	7:G:455:ASN:HB2	2.11	0.49
9:I:141:GLU:HB2	9:I:154:ARG:HB3	1.94	0.49
10:J:154:VAL:HG13	14:N:154:LEU:HD11	1.94	0.49
14:N:358:ASP:HB2	14:N:472:THR:HG21	1.93	0.49
38:o:22:ILE:HD11	38:o:35:ILE:HG12	1.95	0.49
45:y:56:ASP:HB3	45:y:59:VAL:HG23	1.94	0.49
6:F:163:GLU:HG2	6:F:275:PRO:HB3	1.94	0.49
8:H:257:LEU:O	8:H:259:ILE:N	2.40	0.49
12:L:183:LEU:HD12	12:L:184:GLY:N	2.27	0.49
13:M:171:TYR:OH	14:N:445:LYS:HD3	2.11	0.49
6:F:248:LEU:HD11	7:G:118:ARG:HH12	1.78	0.49
6:F:251:PRO:HG3	16:Q:140:TYR:CD2	2.47	0.49
12:L:60:ARG:HA	12:L:75:GLY:HA2	1.95	0.49
53:M:503:LMN:HAZ	51:N:501:PTY:H281	1.93	0.49
14:N:499:LEU:HD13	28:d:66:LYS:HD2	1.94	0.49
23:X:88:GLU:HG2	23:X:91:LEU:HG	1.94	0.49
2:B:176:ASP:OD1	2:B:176:ASP:N	2.40	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:215:TRP:CE2	15:P:332:PRO:HB2	2.47	0.49
8:H:14:LEU:HB3	50:H:500:UQ9:H26	1.94	0.49
11:K:24:ASN:HD21	11:K:30:ILE:HB	1.77	0.49
15:P:226:GLU:HA	15:P:231:ASN:ND2	2.27	0.49
24:Z:125:TYR:HE2	24:Z:131:MET:HB2	1.77	0.49
29:e:33:ASP:OD1	29:e:34:CYS:N	2.46	0.49
1:A:77:PHE:O	10:J:145:TYR:OH	2.24	0.49
7:G:259:GLU:HG2	7:G:260:LEU:N	2.27	0.49
12:L:57:CYS:HB3	27:c:61:ARG:NE	2.27	0.49
12:L:227:ILE:O	12:L:230:VAL:HG12	2.13	0.49
13:M:287:SER:OG	13:M:317:ASN:O	2.31	0.49
14:N:402:PRO:HA	14:N:407:PHE:CG	2.46	0.49
24:Z:68:ASN:OD1	24:Z:71:ARG:NH1	2.46	0.49
45:y:175:ILE:HD12	45:y:181:TRP:HB2	1.95	0.49
7:G:172:ILE:HG23	9:I:124:ILE:HD12	1.95	0.49
7:G:723:TYR:HB2	7:G:739:SER:HB3	1.95	0.49
8:H:27:GLU:HG3	8:H:31:MET:HE3	1.95	0.49
12:L:461:ILE:N	12:L:462:PRO:CD	2.75	0.49
53:M:503:LMN:HBK	28:d:3:ILE:HD11	1.94	0.49
14:N:113:ASP:HB2	14:N:462:ASP:OD2	2.12	0.49
14:N:366:LEU:HB2	14:N:371:VAL:HG11	1.95	0.49
2:B:80:ARG:NH1	2:B:211:ASP:OD2	2.44	0.49
6:F:56:GLY:HA2	6:F:317:ILE:HD13	1.93	0.49
6:F:305:VAL:HG12	6:F:330:VAL:HA	1.94	0.49
6:F:343:GLY:HA2	6:F:376:ALA:H	1.78	0.49
6:F:474:ARG:O	6:F:478:GLU:HG3	2.12	0.49
12:L:13:SER:OG	12:L:119:ILE:HG23	2.13	0.49
14:N:491:HIS:CD2	28:d:64:LEU:HD21	2.48	0.49
15:P:69:ILE:HB	15:P:93:SER:HB2	1.95	0.49
46:z:180:VAL:HG23	46:z:189:LEU:HB2	1.94	0.49
8:H:82:PHE:CE1	8:H:86:LEU:HD11	2.47	0.49
12:L:86:LEU:HA	12:L:89:VAL:HG12	1.94	0.49
12:L:172:ARG:HH21	13:M:422:MET:CB	2.26	0.49
13:M:320:THR:HA	13:M:323:MET:HE3	1.94	0.49
14:N:78:ILE:HD12	30:f:5:ILE:HD11	1.94	0.49
15:P:324:PHE:CE2	15:P:336:PRO:HB3	2.48	0.49
21:V:113:ASP:OD1	41:r:91:LYS:NZ	2.37	0.49
39:p:62:GLU:HB3	39:p:66:HIS:HA	1.95	0.49
46:z:124:ASP:H	46:z:141:ASP:HB3	1.77	0.49
3:C:18:TRP:HH2	21:V:103:MET:HE1	1.77	0.49
6:F:169:GLY:HA3	6:F:216:PHE:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:187:LEU:HD21	51:I:303:PTY:H261	1.94	0.49
8:H:200:ARG:NE	8:H:236:MET:SD	2.85	0.49
9:I:110:GLU:O	9:I:180:GLY:N	2.44	0.49
13:M:331:ILE:O	13:M:335:ILE:HD12	2.12	0.49
31:g:96:LYS:HA	31:g:99:GLU:HG3	1.95	0.49
36:m:50:LYS:HA	36:m:53:VAL:HG12	1.94	0.49
44:x:167:ILE:HB	44:x:185:VAL:HG13	1.95	0.49
44:x:175:GLU:OE1	44:x:191:ARG:NH2	2.46	0.49
45:y:118:LEU:HD11	45:y:138:THR:HG21	1.94	0.49
6:F:162:LEU:HD12	6:F:205:LEU:HD11	1.94	0.48
7:G:448:ARG:NH2	7:G:479:ASN:OD1	2.35	0.48
10:J:30:PHE:CZ	10:J:34:PHE:HE2	2.30	0.48
12:L:68:GLU:HB3	13:M:329:GLN:OE1	2.13	0.48
12:L:318:GLN:HA	12:L:321:TYR:CD2	2.47	0.48
12:L:394:PHE:CE2	33:j:43:ALA:HA	2.47	0.48
12:L:484:MET:HB2	38:o:46:TYR:HD1	1.78	0.48
13:M:158:GLY:HA3	14:N:449:PHE:CZ	2.48	0.48
28:d:26:LEU:HD23	28:d:30:ARG:HG2	1.95	0.48
14:N:93:THR:HG23	14:N:140:ILE:HG22	1.95	0.48
14:N:292:GLN:N	14:N:292:GLN:OE1	2.45	0.48
44:x:72:VAL:HG23	44:x:90:VAL:HB	1.95	0.48
6:F:257:GLY:HA3	6:F:263:THR:HG22	1.94	0.48
8:H:26:ALA:HB2	25:a:11:PRO:HB2	1.95	0.48
13:M:332:GLY:O	13:M:336:LEU:HD23	2.13	0.48
14:N:139:MET:HE3	14:N:272:SER:HB2	1.96	0.48
14:N:498:TYR:OH	32:i:48:ILE:HG13	2.14	0.48
22:W:80:PHE:HA	22:W:83:MET:HE2	1.96	0.48
45:y:45:LEU:HD13	45:y:53:PRO:HG2	1.94	0.48
4:D:234:ARG:HH11	4:D:332:GLU:HG2	1.78	0.48
6:F:54:HIS:O	6:F:54:HIS:ND1	2.44	0.48
8:H:317:LEU:HD23	24:Z:61:MET:HG3	1.95	0.48
13:M:386:LEU:HD21	52:M:501:PC7:H441	1.96	0.48
13:M:431:TRP:O	13:M:435:ARG:HD2	2.13	0.48
14:N:436:GLY:HA2	14:N:439:TYR:CE1	2.47	0.48
45:y:101:GLN:HE22	45:y:207:TYR:HD2	1.59	0.48
6:F:164:GLY:HA2	6:F:275:PRO:HD3	1.96	0.48
13:M:347:ALA:HB1	13:M:384:PHE:CD2	2.48	0.48
15:P:58:LYS:HG2	16:Q:84:TRP:HB2	1.95	0.48
28:d:27:PRO:HG2	28:d:30:ARG:HE	1.79	0.48
37:n:87:PRO:HA	37:n:93:SER:H	1.77	0.48
40:q:51:LEU:HD11	40:q:60:LYS:HE2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:427:MET:HA	7:G:551:ASN:HB2	1.95	0.48
14:N:290:LEU:HA	14:N:293:ILE:HG22	1.95	0.48
15:P:58:LYS:HB3	15:P:66:VAL:HB	1.94	0.48
15:P:311:PRO:HB2	15:P:314:ILE:HG22	1.94	0.48
37:n:13:ARG:HH22	37:n:64:ILE:HD13	1.78	0.48
45:y:124:ASP:OD1	45:y:124:ASP:N	2.44	0.48
12:L:13:SER:HB2	12:L:118:SER:CB	2.39	0.48
12:L:68:GLU:HB2	13:M:328:ILE:HD13	1.95	0.48
12:L:552:CYS:HA	12:L:555:LEU:HD12	1.94	0.48
14:N:352:TYR:HA	14:N:355:MET:HE2	1.95	0.48
20:U:82:ASP:O	20:U:86:SER:N	2.43	0.48
33:j:12:TYR:HD2	34:k:18:TRP:HA	1.79	0.48
12:L:76:PHE:HB3	12:L:129:THR:HG22	1.95	0.48
12:L:140:TRP:HZ3	12:L:175:ASP:HA	1.78	0.48
12:L:165:ILE:HD13	13:M:431:TRP:CD1	2.48	0.48
13:M:350:LEU:HD12	13:M:463:PHE:HE2	1.79	0.48
14:N:344:SER:HB3	14:N:412:TYR:HD1	1.79	0.48
20:U:85:ASP:O	20:U:89:VAL:HG23	2.14	0.48
27:c:58:LEU:O	27:c:58:LEU:HD12	2.14	0.48
4:D:26:LEU:HD13	4:D:389:PHE:CZ	2.48	0.48
4:D:166:ASP:OD2	24:Z:22:GLN:NE2	2.43	0.48
8:H:324:LEU:O	24:Z:72:ARG:NH2	2.39	0.48
12:L:252:VAL:O	12:L:256:ILE:HG22	2.14	0.48
14:N:348:GLY:HA2	14:N:409:SER:HB2	1.96	0.48
35:l:89:PHE:O	35:l:93:GLY:N	2.39	0.48
38:o:34:LEU:HD13	38:o:58:TYR:CZ	2.48	0.48
11:K:55:ASP:OD1	11:K:56:MET:N	2.47	0.48
12:L:3:LEU:HD21	12:L:61:ILE:HD11	1.95	0.48
12:L:99:TYR:CD2	12:L:463:MET:HB2	2.49	0.48
12:L:209:ILE:O	12:L:211:CYS:N	2.40	0.48
12:L:353:GLY:HA2	12:L:356:ILE:HG22	1.96	0.48
13:M:146:PHE:CE1	13:M:259:PHE:HB3	2.49	0.48
13:M:217:TRP:CZ2	13:M:283:ILE:HD11	2.49	0.48
15:P:340:ASN:O	15:P:344:ILE:HG12	2.13	0.48
45:y:109:ALA:HB1	45:y:113:ILE:HB	1.95	0.48
4:D:113:ASN:ND2	4:D:334:PRO:HB2	2.29	0.47
6:F:366:LYS:HB3	6:F:366:LYS:HE2	1.63	0.47
8:H:136:GLY:HA2	8:H:139:ARG:HD3	1.96	0.47
14:N:388:ALA:HB1	14:N:447:MET:HE3	1.96	0.47
21:V:143:TYR:O	21:V:147:GLU:HG2	2.14	0.47
23:X:83:TYR:CE2	25:a:36:ARG:HD3	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:p:34:ARG:O	39:p:38:VAL:HG23	2.13	0.47
45:y:8:ILE:HA	45:y:11:VAL:HG22	1.95	0.47
46:z:87:GLY:HA2	46:z:108:VAL:HG21	1.96	0.47
13:M:78:GLU:OE2	53:M:503:LMN:OAS	2.31	0.47
14:N:491:HIS:HD2	28:d:60:LEU:HD11	1.79	0.47
21:V:34:ILE:HD11	21:V:69:LYS:HG2	1.96	0.47
23:X:94:LYS:HA	23:X:97:GLU:OE2	2.14	0.47
30:f:36:ARG:HA	30:f:39:THR:HG22	1.95	0.47
34:k:8:THR:HB	37:n:49:ARG:HD2	1.96	0.47
38:o:37:LEU:O	38:o:41:ARG:HG3	2.14	0.47
4:D:113:ASN:HD22	4:D:334:PRO:HB2	1.79	0.47
4:D:148:VAL:O	9:I:106:ARG:NH1	2.47	0.47
7:G:380:ILE:HA	7:G:580:PHE:HB3	1.96	0.47
13:M:38:ARG:HD3	13:M:109:TRP:CZ2	2.50	0.47
15:P:179:ARG:NH2	15:P:268:ALA:O	2.45	0.47
1:A:62:TYR:O	1:A:66:ILE:HG12	2.14	0.47
6:F:339:ALA:HB1	6:F:349:LEU:HD11	1.95	0.47
8:H:119:TYR:O	8:H:123:ILE:HG12	2.14	0.47
12:L:130:GLY:HA2	12:L:135:GLN:HE21	1.78	0.47
13:M:10:PHE:CD2	13:M:54:VAL:HG11	2.49	0.47
14:N:428:VAL:HA	14:N:431:VAL:HG12	1.96	0.47
17:R:52:SER:OG	17:R:55:GLU:OE1	2.31	0.47
3:C:7:PHE:CE1	3:C:22:MET:HE1	2.48	0.47
11:K:24:ASN:ND2	11:K:27:ASN:OD1	2.46	0.47
12:L:588:ALA:HB1	36:m:37:ILE:HB	1.96	0.47
13:M:440:ASN:OD1	13:M:442:LYS:NZ	2.36	0.47
14:N:437:CYS:O	14:N:441:ILE:HG12	2.15	0.47
38:o:35:ILE:HA	38:o:38:ASN:ND2	2.29	0.47
4:D:212:GLN:NE2	4:D:216:ASP:OD2	2.48	0.47
12:L:9:PRO:O	12:L:118:SER:OG	2.32	0.47
12:L:206:ASN:OD1	12:L:207:SER:N	2.47	0.47
12:L:373:SER:OG	34:k:27:GLN:OE1	2.28	0.47
16:Q:61:ARG:HB2	16:Q:71:LEU:HD11	1.97	0.47
30:f:94:GLU:HA	30:f:97:SER:HB3	1.96	0.47
1:A:85:LEU:HD22	8:H:324:LEU:HD11	1.96	0.47
2:B:101:THR:HG21	2:B:195:LEU:HD23	1.95	0.47
6:F:305:VAL:HG13	6:F:379:VAL:HG21	1.96	0.47
7:G:331:LYS:HG3	7:G:729:THR:HG21	1.97	0.47
10:J:6:LEU:HD21	10:J:36:ASP:O	2.14	0.47
12:L:59:LEU:HB2	27:c:58:LEU:HD12	1.97	0.47
12:L:69:MET:H	39:p:49:LYS:HZ3	1.61	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:240:THR:HA	12:L:562:ARG:NH1	2.29	0.47
13:M:179:LEU:HD12	13:M:180:GLY:N	2.30	0.47
14:N:74:PRO:HB2	30:f:88:PHE:HB3	1.97	0.47
14:N:362:ILE:HD13	14:N:469:LEU:HD21	1.97	0.47
15:P:145:ILE:HG21	15:P:163:ILE:HG21	1.97	0.47
20:U:70:THR:HG23	20:U:72:LYS:H	1.80	0.47
20:U:97:PHE:HD2	20:U:99:PHE:HD1	1.62	0.47
26:b:34:VAL:O	26:b:38:LEU:HG	2.15	0.47
33:j:11:THR:HB	33:j:16:THR:HB	1.95	0.47
45:y:88:ASP:OD1	45:y:88:ASP:N	2.47	0.47
46:z:150:THR:OG1	46:z:168:LEU:HA	2.15	0.47
1:A:23:LEU:HD11	8:H:227:LEU:HD22	1.96	0.47
2:B:130:THR:HG21	4:D:49:ARG:HG3	1.97	0.47
8:H:63:PRO:HA	8:H:222:SER:HB3	1.96	0.47
11:K:36:GLU:OE1	11:K:73:SER:OG	2.33	0.47
12:L:544:ARG:O	12:L:544:ARG:NH1	2.39	0.47
14:N:343:GLN:HA	14:N:490:THR:HG22	1.97	0.47
33:j:32:CYS:HB3	34:k:34:GLY:HA3	1.97	0.47
12:L:95:LEU:HB3	12:L:466:PRO:HB3	1.96	0.47
13:M:238:PRO:HB3	13:M:306:LYS:HG2	1.97	0.47
15:P:369:LYS:HZ1	15:P:371:LYS:HD2	1.79	0.47
21:V:139:PRO:HG2	21:V:142:PHE:CE2	2.49	0.47
45:y:48:VAL:HG13	45:y:49:PHE:N	2.30	0.47
2:B:165:TYR:O	2:B:167:TYR:N	2.47	0.47
2:B:170:SER:OG	4:D:48:HIS:O	2.32	0.47
7:G:208:GLY:H	7:G:255:LEU:HB3	1.80	0.47
7:G:379:GLU:HB3	7:G:578:ALA:HA	1.97	0.47
12:L:335:VAL:HG11	12:L:493:TRP:CH2	2.49	0.47
31:g:88:SER:OG	31:g:89:ILE:N	2.48	0.47
32:i:83:LEU:HD23	32:i:83:LEU:H	1.80	0.47
44:x:145:VAL:HA	44:x:162:ILE:HB	1.96	0.47
45:y:189:MET:HA	45:y:189:MET:HE2	1.96	0.47
4:D:106:CYS:O	4:D:109:THR:OG1	2.28	0.46
7:G:364:ALA:O	7:G:368:VAL:HG23	2.15	0.46
8:H:219:GLU:O	8:H:219:GLU:HG2	2.15	0.46
10:J:157:LEU:O	10:J:161:VAL:HG23	2.15	0.46
11:K:77:LEU:O	11:K:81:VAL:HG13	2.15	0.46
15:P:79:PHE:HA	15:P:226:GLU:OE2	2.14	0.46
24:Z:142:VAL:HG23	24:Z:143:TRP:CD1	2.50	0.46
45:y:104:THR:HA	45:y:131:SER:HA	1.97	0.46
12:L:11:LEU:O	12:L:15:VAL:HG12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:469:LEU:HD13	12:L:472:LEU:HD21	1.98	0.46
13:M:285:THR:O	13:M:289:ILE:HG12	2.15	0.46
14:N:139:MET:HE1	14:N:155:GLN:CD	2.40	0.46
15:P:297:MET:O	15:P:301:ILE:HG12	2.15	0.46
4:D:73:VAL:HG11	4:D:116:LEU:HD22	1.97	0.46
4:D:90:LEU:HG	4:D:322:VAL:HG22	1.96	0.46
6:F:249:LYS:N	6:F:250:PRO:HD2	2.29	0.46
8:H:140:SER:O	8:H:144:MET:HG3	2.15	0.46
8:H:162:VAL:HG11	8:H:170:ILE:HG12	1.96	0.46
16:Q:115:LYS:HD2	16:Q:127:VAL:HG21	1.96	0.46
22:W:41:MET:HE1	22:W:55:LEU:HD12	1.97	0.46
30:f:17:ASP:OD2	30:f:24:LYS:HE3	2.15	0.46
37:n:113:LEU:HD23	37:n:113:LEU:H	1.81	0.46
45:y:90:ASN:HB3	45:y:119:PRO:HB3	1.97	0.46
5:E:136:MET:HE3	6:F:392:ARG:HD2	1.97	0.46
6:F:161:LEU:HD23	6:F:192:LEU:HD11	1.97	0.46
12:L:260:THR:O	12:L:264:ALA:N	2.49	0.46
12:L:531:VAL:O	12:L:535:VAL:HG23	2.15	0.46
18:S:74:LEU:HA	18:S:77:LEU:HD13	1.98	0.46
18:S:84:LYS:HE2	18:S:87:GLU:HG3	1.98	0.46
40:q:83:ARG:O	40:q:85:ASN:N	2.48	0.46
45:y:150:THR:HB	45:y:168:LEU:HD12	1.97	0.46
2:B:65:ALA:O	2:B:69:ILE:HD12	2.16	0.46
2:B:189:PRO:HD3	4:D:154:HIS:CD2	2.51	0.46
4:D:16:GLY:H	4:D:17:PRO:HD3	1.81	0.46
10:J:6:LEU:HD22	10:J:40:LEU:HD13	1.96	0.46
11:K:14:PHE:CE1	11:K:38:MET:HE3	2.51	0.46
12:L:430:THR:HA	12:L:433:TYR:CE2	2.51	0.46
13:M:284:TYR:CG	13:M:414:VAL:HG11	2.50	0.46
14:N:18:ALA:O	14:N:89:ARG:NH1	2.49	0.46
14:N:143:TYR:HE2	14:N:207:ASP:HB2	1.81	0.46
22:W:49:VAL:HG23	22:W:50:VAL:HG22	1.98	0.46
44:x:121:CYS:SG	44:x:149:SER:OG	2.72	0.46
45:y:134:ILE:HG23	45:y:137:CYS:HB3	1.98	0.46
46:z:27:CYS:SG	46:z:32:LYS:HG3	2.55	0.46
3:C:107:SER:HB3	4:D:217:TRP:HA	1.97	0.46
4:D:388:VAL:HG23	4:D:391:GLU:HG2	1.96	0.46
7:G:425:TYR:OH	7:G:564:ASP:OD1	2.26	0.46
7:G:495:ILE:HA	7:G:500:HIS:NE2	2.30	0.46
8:H:108:LEU:HD11	10:J:52:ILE:HD11	1.97	0.46
13:M:468:VAL:O	13:M:472:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:M:503:LMN:HAAA	53:M:503:LMN:HBFA	1.97	0.46
14:N:25:ILE:HD12	14:N:65:THR:HG21	1.98	0.46
18:S:64:TYR:HD2	18:S:68:VAL:HG23	1.80	0.46
19:T:83:VAL:HG21	37:n:25:ARG:HB2	1.98	0.46
44:x:220:LEU:O	44:x:224:ILE:HG12	2.15	0.46
46:z:88:ASP:OD1	46:z:89:VAL:N	2.46	0.46
4:D:175:ILE:HG22	4:D:279:LEU:HD11	1.97	0.46
7:G:92:LEU:O	7:G:96:GLU:HG2	2.16	0.46
9:I:160:THR:HG21	9:I:190:HIS:CE1	2.51	0.46
10:J:54:LEU:HG	10:J:58:ILE:HD11	1.97	0.46
13:M:153:MET:HE2	13:M:153:MET:HB3	1.72	0.46
13:M:433:TYR:O	13:M:437:VAL:HG12	2.16	0.46
45:y:48:VAL:HG23	46:z:214:HIS:NE2	2.30	0.46
45:y:113:ILE:HG22	45:y:117:VAL:HG22	1.97	0.46
3:C:154:GLN:HG3	3:C:169:ILE:HA	1.98	0.46
4:D:71:ASP:HB3	4:D:78:GLN:CD	2.40	0.46
4:D:165:GLN:NE2	9:I:106:ARG:HD3	2.31	0.46
7:G:178:GLU:HB3	7:G:284:ASN:HD22	1.80	0.46
12:L:370:GLY:N	12:L:444:VAL:O	2.48	0.46
13:M:143:TYR:CE2	13:M:185:LEU:HD13	2.51	0.46
37:n:26:ARG:HD2	37:n:75:TYR:CZ	2.50	0.46
2:B:123:ASP:OD2	8:H:57:LYS:HD2	2.16	0.46
5:E:34:TYR:CD1	5:E:36:LEU:HD13	2.51	0.46
7:G:292:THR:HG22	7:G:641:VAL:H	1.80	0.46
8:H:128:SER:HA	8:H:219:GLU:OE2	2.16	0.46
14:N:113:ASP:OD2	14:N:117:GLN:HB2	2.15	0.46
15:P:280:TYR:HA	15:P:358:LEU:HB2	1.98	0.46
18:S:61:TRP:CE3	18:S:71:CYS:HB3	2.51	0.46
20:U:83:SER:OG	56:W:200:8Q1:O3	2.30	0.46
21:V:117:CYS:HB3	41:r:89:LEU:HB2	1.98	0.46
23:X:65:LYS:O	23:X:69:GLN:HG2	2.16	0.46
25:a:45:TRP:CZ2	25:a:49:MET:HE3	2.51	0.46
30:f:21:ALA:O	30:f:25:VAL:HG22	2.15	0.46
31:g:70:SER:O	31:g:74:ILE:HG12	2.15	0.46
3:C:163:ARG:CZ	3:C:165:VAL:HG12	2.45	0.46
5:E:84:ASN:ND2	5:E:87:TRP:NE1	2.64	0.46
12:L:593:ALA:O	12:L:597:LEU:HG	2.16	0.46
14:N:84:ASN:ND2	32:i:61:ALA:O	2.49	0.46
32:i:38:LYS:HD3	32:i:38:LYS:HA	1.67	0.46
44:x:120:ARG:NH1	46:z:82:GLY:O	2.49	0.46
45:y:222:PHE:CE1	46:z:37:GLU:HA	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:52:ARG:NH2	21:V:95:ASP:OD2	2.43	0.45
6:F:172:MET:O	6:F:174:ALA:N	2.48	0.45
7:G:486:GLY:HA3	7:G:491:THR:OG1	2.15	0.45
8:H:84:LEU:HA	8:H:87:VAL:HG12	1.97	0.45
12:L:36:VAL:HG21	12:L:97:HIS:CD2	2.51	0.45
12:L:235:GLN:CD	12:L:323:ILE:HG13	2.40	0.45
12:L:282:ALA:O	12:L:285:VAL:HG12	2.16	0.45
13:M:198:THR:HA	13:M:203:LEU:HD11	1.97	0.45
14:N:22:GLU:O	14:N:25:ILE:HG22	2.16	0.45
15:P:242:PHE:HD2	15:P:308:VAL:HG21	1.81	0.45
16:Q:149:ASN:O	16:Q:151:GLN:N	2.48	0.45
45:y:168:LEU:HB3	45:y:184:ASN:O	2.16	0.45
7:G:210:LEU:HD12	7:G:211:VAL:HG23	1.98	0.45
8:H:14:LEU:HB2	8:H:15:PRO:HD3	1.98	0.45
8:H:244:THR:HA	8:H:248:LEU:HB2	1.98	0.45
13:M:231:VAL:HG21	13:M:289:ILE:HG13	1.98	0.45
16:Q:39:ILE:HA	16:Q:42:VAL:HG22	1.97	0.45
25:a:10:LEU:O	25:a:14:ILE:HG12	2.16	0.45
26:b:19:ALA:O	26:b:23:ILE:HG13	2.16	0.45
34:k:6:GLY:O	37:n:49:ARG:HD3	2.16	0.45
44:x:252:LEU:HD12	44:x:252:LEU:O	2.16	0.45
9:I:168:CYS:HB3	47:I:301:SF4:S2	2.56	0.45
10:J:29:PHE:HA	10:J:32:LEU:HD12	1.98	0.45
12:L:67:SER:HA	13:M:482:HIS:HE2	1.82	0.45
13:M:103:ILE:O	13:M:107:VAL:HG13	2.16	0.45
13:M:281:PRO:O	13:M:285:THR:HG23	2.17	0.45
15:P:183:VAL:HG22	15:P:217:MET:HB3	1.97	0.45
38:o:13:THR:HB	38:o:17:MET:HE3	1.99	0.45
39:p:37:ILE:O	39:p:41:LYS:HG2	2.16	0.45
45:y:144:PHE:CD2	45:y:162:MET:HG3	2.50	0.45
46:z:54:ILE:HD12	46:z:72:HIS:CE1	2.51	0.45
4:D:141:LEU:HD21	4:D:178:PHE:CE2	2.51	0.45
4:D:191:GLU:OE2	9:I:78:ARG:NH1	2.49	0.45
4:D:313:PHE:CE2	9:I:128:LEU:HD21	2.52	0.45
8:H:4:ALA:HB2	25:a:33:TYR:HD1	1.82	0.45
13:M:146:PHE:HE1	13:M:259:PHE:HB3	1.81	0.45
14:N:113:ASP:OD2	14:N:368:GLN:NE2	2.47	0.45
31:g:62:TRP:C	31:g:65:PRO:HD2	2.41	0.45
36:m:9:LYS:HG2	36:m:14:GLU:OE2	2.17	0.45
39:p:82:ARG:O	39:p:90:HIS:ND1	2.50	0.45
45:y:34:ARG:HA	46:z:47:ASN:HD21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:368:VAL:HG12	6:F:368:VAL:O	2.16	0.45
51:I:303:PTY:H382	51:I:303:PTY:H351	1.69	0.45
13:M:10:PHE:HB3	13:M:51:TYR:CZ	2.51	0.45
27:c:82:ASP:OD1	27:c:82:ASP:N	2.50	0.45
29:e:39:GLU:O	29:e:43:GLU:HG3	2.17	0.45
31:g:69:THR:O	31:g:73:THR:HG23	2.16	0.45
46:z:99:ASN:OD1	46:z:127:THR:HA	2.16	0.45
46:z:151:LEU:HD23	46:z:155:VAL:HG11	1.98	0.45
7:G:88:GLY:HA3	16:Q:137:VAL:HG13	1.99	0.45
7:G:159:MET:HE3	7:G:185:SER:HA	1.99	0.45
14:N:50:LEU:HD23	14:N:50:LEU:H	1.81	0.45
30:f:49:TYR:CE1	30:f:53:ILE:HD11	2.51	0.45
3:C:136:TYR:CD2	22:W:93:ALA:HB1	2.51	0.45
12:L:292:MET:HE3	35:l:89:PHE:CD2	2.52	0.45
4:D:306:MET:HE3	4:D:310:ILE:HG13	1.99	0.45
10:J:47:ASP:OD1	10:J:47:ASP:N	2.47	0.45
12:L:102:SER:HB3	12:L:462:PRO:HG2	1.99	0.45
12:L:366:ARG:HG2	37:n:36:VAL:HG22	1.98	0.45
13:M:83:TYR:HD1	13:M:137:LEU:HB2	1.81	0.45
13:M:465:VAL:HG23	51:M:502:PTY:H171	1.97	0.45
14:N:464:ASN:OD1	14:N:465:LYS:N	2.46	0.45
23:X:104:PRO:O	23:X:105:LEU:HD23	2.17	0.45
28:d:21:ASN:ND2	28:d:28:TYR:O	2.48	0.45
33:j:13:LYS:HE3	34:k:18:TRP:N	2.31	0.45
4:D:133:TRP:O	4:D:136:GLU:HG3	2.16	0.45
4:D:176:ASP:O	4:D:180:GLN:HG2	2.16	0.45
4:D:266:GLU:O	4:D:270:GLN:HG2	2.17	0.45
6:F:443:GLU:OE2	6:F:456:TRP:NE1	2.39	0.45
8:H:249:GLY:O	8:H:272:LYS:NZ	2.33	0.45
9:I:119:GLY:HA3	17:R:56:LEU:HD22	1.99	0.45
12:L:18:PHE:HA	27:c:22:MET:HE2	1.99	0.45
14:N:100:LEU:HD13	14:N:140:ILE:HD11	1.98	0.45
38:o:64:GLU:HA	38:o:67:MET:HE2	1.98	0.45
46:z:84:VAL:HG12	46:z:84:VAL:O	2.17	0.45
4:D:119:THR:HB	4:D:131:PHE:HA	1.98	0.45
4:D:182:PHE:HD2	4:D:272:LEU:HD13	1.81	0.45
13:M:382:PHE:CD2	52:M:501:PC7:H361	2.51	0.45
57:y:302:PGT:H122	57:y:302:PGT:H151	1.76	0.45
46:z:99:ASN:HB2	46:z:101:GLN:HE21	1.81	0.45
4:D:241:VAL:O	4:D:241:VAL:HG13	2.15	0.44
6:F:360:MET:SD	6:F:365:LEU:HD11	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:412:GLY:O	7:G:559:GLN:NE2	2.47	0.44
12:L:541:GLN:CD	12:L:541:GLN:H	2.25	0.44
13:M:258:LYS:HG3	13:M:338:MET:HG2	1.99	0.44
15:P:184:SER:O	15:P:219:PRO:HD2	2.16	0.44
15:P:329:VAL:HB	15:P:330:PRO:HD3	1.98	0.44
19:T:112:ILE:HA	19:T:115:VAL:HG22	1.99	0.44
21:V:141:GLN:O	21:V:141:GLN:NE2	2.41	0.44
5:E:135:CYS:HB2	48:E:500:FES:S2	2.56	0.44
7:G:427:MET:HE2	7:G:427:MET:HB2	1.88	0.44
13:M:359:HIS:HB3	36:m:7:THR:HG23	1.98	0.44
18:S:7:ILE:HB	18:S:43:ASN:ND2	2.33	0.44
21:V:30:ARG:HG3	21:V:68:CYS:SG	2.58	0.44
45:y:89:VAL:HG21	45:y:110:LYS:HA	1.98	0.44
3:C:162:LYS:HD2	3:C:162:LYS:N	2.31	0.44
4:D:233:LEU:HA	4:D:233:LEU:HD23	1.84	0.44
12:L:487:GLY:HA3	38:o:41:ARG:HH22	1.83	0.44
14:N:467:LEU:HD11	51:N:501:PTY:H171	2.00	0.44
15:P:246:ILE:HD11	15:P:339:PHE:CE1	2.52	0.44
15:P:298:TYR:OH	15:P:304:TRP:O	2.22	0.44
27:c:57:LYS:HD3	27:c:57:LYS:HA	1.70	0.44
28:d:33:TRP:HE1	58:z:301:PSF:H132	1.82	0.44
30:f:35:LEU:HD23	30:f:35:LEU:HA	1.85	0.44
1:A:101:PHE:O	1:A:105:ILE:HG12	2.18	0.44
2:B:98:MET:HB2	2:B:155:MET:SD	2.57	0.44
4:D:381:ILE:O	4:D:385:GLN:HG2	2.18	0.44
5:E:111:ALA:HA	5:E:117:PHE:HD2	1.82	0.44
5:E:135:CYS:HB2	5:E:175:CYS:SG	2.58	0.44
5:E:136:MET:HA	5:E:140:SER:H	1.82	0.44
8:H:257:LEU:HG	8:H:258:PRO:HD2	2.00	0.44
10:J:40:LEU:HG	11:K:6:TYR:HE1	1.82	0.44
12:L:240:THR:HA	12:L:562:ARG:HH12	1.82	0.44
13:M:176:TYR:CD2	13:M:236:TRP:HB3	2.52	0.44
15:P:282:LEU:HD22	15:P:360:PHE:CE1	2.41	0.44
18:S:4:ARG:HG2	18:S:4:ARG:HH11	1.82	0.44
39:p:76:GLN:HA	39:p:79:ASP:OD2	2.17	0.44
4:D:16:GLY:H	4:D:17:PRO:CD	2.30	0.44
6:F:147:THR:HG22	6:F:376:ALA:HB3	1.99	0.44
7:G:416:GLY:HA3	7:G:526:LYS:HE2	1.99	0.44
50:H:500:UQ9:H10B	50:H:500:UQ9:H12A	1.81	0.44
11:K:40:LEU:O	11:K:44:LEU:HD23	2.17	0.44
12:L:127:LEU:HD12	12:L:140:TRP:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:431:VAL:O	14:N:435:ILE:HD12	2.18	0.44
16:Q:88:LEU:HG	16:Q:89:MET:HG2	1.99	0.44
21:V:44:ILE:HB	21:V:100:ILE:HD13	1.99	0.44
24:Z:100:GLU:OE2	24:Z:103:LYS:NZ	2.38	0.44
6:F:446:THR:HG21	6:F:451:GLY:HA3	2.00	0.44
9:I:78:ARG:HH11	9:I:78:ARG:HG2	1.82	0.44
12:L:484:MET:HB3	38:o:46:TYR:HB3	2.00	0.44
13:M:190:LEU:HD12	14:N:418:LEU:HD13	1.99	0.44
14:N:90:ASP:H	14:N:93:THR:HB	1.83	0.44
21:V:66:ASN:O	21:V:69:LYS:N	2.50	0.44
30:f:89:PHE:HB3	30:f:90:PRO:HD2	1.99	0.44
45:y:183:GLY:HA3	45:y:187:LYS:HE3	1.98	0.44
6:F:334:TRP:CE2	6:F:337:LEU:HD22	2.53	0.44
8:H:18:LEU:CB	25:a:18:MET:HE1	2.48	0.44
8:H:20:VAL:O	8:H:24:VAL:HG23	2.17	0.44
13:M:26:LEU:HD21	13:M:117:LYS:HB2	2.00	0.44
13:M:241:HIS:CD2	13:M:249:SER:HB3	2.52	0.44
13:M:315:HIS:O	13:M:319:VAL:HG23	2.18	0.44
19:T:70:HIS:CD2	19:T:73:ASN:HB3	2.52	0.44
20:U:59:LYS:HA	20:U:64:VAL:HG21	2.00	0.44
31:g:68:ILE:O	31:g:72:LEU:HD23	2.18	0.44
45:y:139:VAL:HG23	45:y:157:VAL:HG23	2.00	0.44
45:y:202:GLN:OE1	45:y:205:LYS:NZ	2.45	0.44
46:z:175:ILE:HG23	46:z:181:TRP:CD1	2.52	0.44
1:A:11:TYR:CD1	8:H:9:ILE:HG23	2.52	0.44
1:A:14:ILE:HD12	8:H:9:ILE:HG13	2.00	0.44
2:B:146:MET:HE2	2:B:146:MET:HB3	1.88	0.44
2:B:209:ARG:NH1	15:P:104:ASP:OD2	2.51	0.44
7:G:178:GLU:HB3	7:G:284:ASN:ND2	2.33	0.44
7:G:389:ASP:OD1	7:G:389:ASP:N	2.51	0.44
12:L:148:TYR:CD1	12:L:164:ALA:HB1	2.53	0.44
12:L:325:ALA:O	12:L:328:ILE:HG22	2.18	0.44
12:L:377:LEU:HD11	12:L:468:ILE:HD11	1.98	0.44
14:N:446:ARG:HE	14:N:446:ARG:HB2	1.69	0.44
16:Q:149:ASN:OD1	16:Q:150:PRO:HD2	2.18	0.44
30:f:80:ASN:HA	30:f:89:PHE:CE2	2.52	0.44
52:f:201:PC7:H201	52:f:201:PC7:H232	1.84	0.44
45:y:60:PHE:HB3	45:y:78:SER:HB2	1.98	0.44
45:y:181:TRP:CD1	45:y:188:PHE:HD1	2.35	0.44
4:D:79:GLU:OE2	4:D:156:SER:HA	2.17	0.44
10:J:48:PHE:O	10:J:52:ILE:HG12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:185:CYS:SG	12:L:197:ILE:HD12	2.57	0.44
12:L:256:ILE:HD12	12:L:256:ILE:HA	1.75	0.44
12:L:386:SER:O	12:L:390:ILE:HG12	2.17	0.44
12:L:604:TYR:CE1	12:L:607:ARG:HB2	2.53	0.44
22:W:96:ARG:HG3	22:W:97:HIS:ND1	2.33	0.44
23:X:92:CYS:SG	23:X:93:ARG:N	2.87	0.44
33:j:13:LYS:HG2	34:k:18:TRP:HB3	2.00	0.44
38:o:35:ILE:HB	38:o:36:PRO:HD3	2.00	0.44
44:x:101:VAL:HG21	45:y:102:ASP:HB3	1.98	0.44
44:x:167:ILE:HB	44:x:185:VAL:HG22	2.00	0.44
3:C:42:LEU:HD12	3:C:105:PHE:HE2	1.83	0.43
7:G:419:ALA:HB2	7:G:563:LEU:HD22	1.99	0.43
7:G:567:LEU:HD12	7:G:567:LEU:O	2.18	0.43
12:L:120:PHE:HB2	12:L:146:ALA:HB1	2.00	0.43
13:M:195:THR:OG1	13:M:196:GLY:N	2.51	0.43
14:N:107:THR:HA	14:N:110:MET:HE2	2.00	0.43
51:N:501:PTY:H372	51:N:501:PTY:H402	1.73	0.43
19:T:66:THR:HG22	19:T:68:GLU:H	1.82	0.43
46:z:179:GLU:HB2	46:z:188:PHE:HE1	1.82	0.43
1:A:18:VAL:HA	1:A:21:ILE:HG22	2.00	0.43
2:B:93:CYS:HB3	4:D:72:TYR:CG	2.53	0.43
4:D:15:PHE:CZ	4:D:375:LEU:HD11	2.50	0.43
4:D:273:ARG:HD2	24:Z:35:TYR:CZ	2.52	0.43
7:G:438:ASP:HB2	7:G:510:LYS:O	2.18	0.43
12:L:52:LEU:H	12:L:52:LEU:HD12	1.83	0.43
12:L:261:MET:HA	12:L:264:ALA:HB2	1.99	0.43
13:M:171:TYR:HE1	14:N:441:ILE:HG22	1.83	0.43
13:M:312:SER:HA	13:M:341:HIS:HE2	1.83	0.43
14:N:17:LEU:HD21	30:f:78:TYR:HE1	1.83	0.43
51:N:501:PTY:H293	51:N:501:PTY:H262	1.79	0.43
20:U:61:PHE:O	20:U:62:GLN:HG2	2.18	0.43
21:V:138:LEU:HB2	21:V:143:TYR:CE2	2.53	0.43
23:X:93:ARG:O	23:X:96:GLN:HB3	2.18	0.43
4:D:125:VAL:O	8:H:289:ARG:HB3	2.18	0.43
7:G:350:ARG:HD2	7:G:354:GLY:HA2	1.99	0.43
7:G:413:THR:HG21	7:G:518:ALA:O	2.19	0.43
7:G:469:VAL:HG21	7:G:480:TYR:CE2	2.53	0.43
10:J:29:PHE:O	10:J:33:VAL:HG23	2.18	0.43
11:K:34:SER:O	11:K:38:MET:HG3	2.18	0.43
12:L:368:MET:SD	12:L:368:MET:N	2.91	0.43
13:M:149:VAL:HG21	13:M:256:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:273:PRO:HG2	13:M:274:GLU:OE1	2.18	0.43
18:S:19:CYS:SG	18:S:20:GLN:N	2.92	0.43
46:z:160:HIS:O	46:z:178:GLY:HA2	2.19	0.43
6:F:401:SER:C	6:F:403:GLY:H	2.27	0.43
8:H:182:PRO:HB2	8:H:183:LEU:HD12	2.01	0.43
10:J:130:LYS:HB2	25:a:45:TRP:HE3	1.83	0.43
12:L:266:VAL:HG13	12:L:326:CYS:SG	2.59	0.43
12:L:328:ILE:CD1	12:L:411:LYS:HD3	2.48	0.43
12:L:382:MET:HE1	12:L:442:PHE:CD2	2.54	0.43
12:L:590:ASP:OD1	13:M:234:HIS:NE2	2.52	0.43
13:M:411:ASN:OD1	13:M:412:SER:N	2.52	0.43
14:N:457:LEU:HD21	44:x:113:PHE:HB2	1.99	0.43
17:R:69:ILE:HG22	17:R:88:CYS:HA	2.01	0.43
17:R:94:PRO:HB2	17:R:103:ARG:HB3	1.99	0.43
2:B:87:MET:HE1	2:B:125:MET:HE3	2.01	0.43
4:D:219:PHE:CZ	4:D:365:GLY:HA3	2.52	0.43
5:E:174:CYS:HB3	6:F:300:CYS:SG	2.59	0.43
13:M:74:TRP:NE1	14:N:480:LEU:O	2.44	0.43
16:Q:38:GLU:HB2	22:W:74:VAL:HG11	2.00	0.43
19:T:58:PRO:HG3	34:k:14:ARG:NH2	2.33	0.43
21:V:12:ALA:N	21:V:75:GLU:OE2	2.51	0.43
44:x:151:LEU:HD11	44:x:156:ILE:HD11	2.00	0.43
46:z:69:GLY:HA3	46:z:87:GLY:O	2.19	0.43
6:F:67:ASN:HD22	6:F:156:HIS:HB3	1.84	0.43
51:M:502:PTY:H231	51:M:502:PTY:H261	1.74	0.43
14:N:17:LEU:HD23	14:N:20:PHE:CE2	2.53	0.43
27:c:31:LYS:HG3	27:c:32:HIS:CE1	2.54	0.43
31:g:100:ARG:HH22	39:p:47:LYS:HG3	1.83	0.43
32:i:36:ARG:O	32:i:40:ILE:HG12	2.18	0.43
3:C:38:LEU:HD21	3:C:75:TYR:CE1	2.54	0.43
3:C:172:THR:O	16:Q:93:SER:OG	2.29	0.43
4:D:185:ARG:HA	4:D:185:ARG:HD3	1.84	0.43
6:F:293:ASN:ND2	6:F:361:ASP:OD2	2.51	0.43
8:H:23:LEU:HB2	25:a:15:ILE:HD12	2.00	0.43
12:L:64:TRP:HZ3	12:L:134:LEU:HB3	1.84	0.43
12:L:392:PHE:O	12:L:398:PHE:HB2	2.19	0.43
12:L:430:THR:HA	12:L:433:TYR:CZ	2.54	0.43
15:P:105:SER:OG	15:P:106:PRO:HD3	2.19	0.43
15:P:228:ARG:HG3	15:P:228:ARG:HH11	1.83	0.43
32:i:43:MET:HE2	32:i:43:MET:HB3	1.83	0.43
44:x:204:ARG:HA	44:x:204:ARG:HD3	1.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:230:MET:O	13:M:234:HIS:ND1	2.48	0.43
34:k:21:HIS:CE1	34:k:23:MET:HB2	2.53	0.43
3:C:171:MET:HE3	3:C:171:MET:HB3	1.89	0.43
4:D:32:MET:HA	4:D:37:VAL:HA	2.01	0.43
5:E:180:MET:HE2	48:E:500:FES:S1	2.58	0.43
6:F:85:TRP:CE2	6:F:204:LEU:HD13	2.54	0.43
7:G:511:ASN:N	7:G:512:PRO:HD3	2.34	0.43
8:H:205:LEU:HA	8:H:289:ARG:HD3	2.01	0.43
9:I:58:LYS:CE	26:b:8:ARG:HE	2.28	0.43
12:L:68:GLU:OE2	39:p:45:ILE:HD12	2.19	0.43
12:L:356:ILE:HA	12:L:359:MET:HG2	2.01	0.43
15:P:88:LEU:O	15:P:93:SER:OG	2.36	0.43
28:d:63:MET:HE2	28:d:63:MET:HB2	1.97	0.43
38:o:75:LYS:HE2	38:o:79:GLU:OE2	2.19	0.43
46:z:99:ASN:HB2	46:z:101:GLN:NE2	2.34	0.43
2:B:129:GLY:HA2	47:B:500:SF4:S3	2.59	0.43
5:E:74:ILE:HB	5:E:75:PRO:HD3	1.99	0.43
6:F:348:PRO:HD2	6:F:370:SER:HA	2.00	0.43
6:F:446:THR:HB	47:F:501:SF4:S3	2.59	0.43
7:G:207:LEU:HA	7:G:255:LEU:HD22	2.00	0.43
8:H:105:ILE:HD11	10:J:51:MET:HG3	2.00	0.43
8:H:109:TYR:O	8:H:113:ILE:HG12	2.19	0.43
8:H:173:ALA:HA	24:Z:71:ARG:HD2	2.01	0.43
12:L:63:PRO:HB2	13:M:475:LYS:HE3	1.99	0.43
12:L:241:TRP:HH2	12:L:261:MET:HE1	1.84	0.43
12:L:606:PHE:HA	12:L:609:LEU:HB3	1.99	0.43
13:M:12:LEU:HD21	13:M:135:CYS:HB2	2.01	0.43
13:M:142:PHE:O	13:M:146:PHE:HB2	2.19	0.43
53:M:503:LMN:HAX	53:M:503:LMN:HBDA	1.58	0.43
14:N:341:GLY:HA2	14:N:416:ALA:HB1	2.01	0.43
27:c:59:GLU:O	27:c:77:ASN:HB2	2.19	0.43
39:p:74:VAL:O	39:p:78:LEU:HD23	2.19	0.43
44:x:184:SER:HA	44:x:200:GLY:O	2.19	0.43
8:H:71:PHE:HA	8:H:75:ARG:HH21	1.84	0.42
50:H:500:UQ9:H7	50:H:500:UQ9:H10	1.72	0.42
9:I:195:TYR:HB3	9:I:200:LEU:HD22	2.00	0.42
14:N:40:SER:HB2	14:N:50:LEU:HD21	2.00	0.42
14:N:291:GLN:O	14:N:295:PHE:HB2	2.19	0.42
45:y:113:ILE:H	45:y:117:VAL:HG21	1.83	0.42
7:G:743:LEU:HD23	7:G:743:LEU:HA	1.86	0.42
14:N:40:SER:OG	45:y:242:TYR:OH	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:a:44:GLU:HA	25:a:47:VAL:HG22	2.00	0.42
25:a:53:ASP:HA	25:a:56:VAL:HG12	2.00	0.42
36:m:35:ALA:O	36:m:39:ILE:HG12	2.19	0.42
46:z:104:SER:OG	46:z:105:LEU:N	2.52	0.42
4:D:252:GLY:N	4:D:263:ILE:HD11	2.34	0.42
5:E:132:THR:OG1	5:E:133:THR:N	2.51	0.42
6:F:342:PRO:HG3	6:F:350:ILE:HD12	2.01	0.42
7:G:503:CYS:SG	7:G:504:THR:N	2.92	0.42
50:H:500:UQ9:H20	50:H:500:UQ9:H17	1.68	0.42
9:I:197:LYS:H	9:I:200:LEU:HD23	1.84	0.42
11:K:14:PHE:HZ	14:N:189:ILE:HD13	1.84	0.42
12:L:377:LEU:O	12:L:381:MET:HG2	2.19	0.42
12:L:412:TYR:CE2	35:l:101:LYS:HE2	2.54	0.42
16:Q:82:LEU:HD13	22:W:132:TYR:CE2	2.54	0.42
6:F:449:ALA:HB3	49:F:500:FMN:HM82	2.02	0.42
7:G:112:SER:OG	7:G:230:GLU:OE2	2.25	0.42
7:G:234:VAL:HG11	7:G:258:SER:HB2	2.01	0.42
8:H:31:MET:HG2	8:H:285:ALA:HB2	2.00	0.42
8:H:96:TYR:OH	23:X:88:GLU:OE2	2.37	0.42
10:J:3:LEU:HD22	11:K:5:LYS:HE3	2.01	0.42
12:L:50:VAL:O	12:L:54:ALA:HA	2.19	0.42
12:L:120:PHE:HD2	12:L:146:ALA:HB3	1.83	0.42
12:L:394:PHE:HE2	33:j:43:ALA:HA	1.84	0.42
12:L:584:VAL:HA	36:m:36:LEU:HD21	2.02	0.42
13:M:43:CYS:O	13:M:47:ILE:HG22	2.19	0.42
15:P:300:MET:HB3	15:P:382:ARG:NH2	2.34	0.42
20:U:75:PHE:HB2	20:U:110:GLN:OE1	2.20	0.42
40:q:83:ARG:C	40:q:85:ASN:H	2.26	0.42
45:y:106:VAL:HG22	45:y:134:ILE:HB	2.00	0.42
45:y:153:ASP:OD1	45:y:153:ASP:N	2.52	0.42
45:y:153:ASP:OD1	45:y:171:GLN:HG3	2.20	0.42
2:B:81:THR:HG21	2:B:207:ASN:OD1	2.19	0.42
3:C:97:ARG:HG2	3:C:122:SER:HB2	2.01	0.42
8:H:9:ILE:O	8:H:13:ILE:HG12	2.20	0.42
12:L:239:HIS:C	12:L:562:ARG:HH22	2.27	0.42
12:L:347:LEU:HD12	12:L:467:LEU:HD13	2.02	0.42
12:L:447:ASN:HA	34:k:19:ARG:HH21	1.85	0.42
12:L:600:TYR:OH	13:M:171:TYR:HB3	2.19	0.42
13:M:208:PHE:HB2	13:M:213:GLN:HE21	1.85	0.42
52:M:501:PC7:H372	52:M:501:PC7:H131	2.02	0.42
32:i:25:LYS:HB3	32:i:25:LYS:HE2	1.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:PHE:HD2	10:J:156:SER:HB3	1.85	0.42
2:B:165:TYR:HE1	4:D:51:THR:HG22	1.85	0.42
7:G:116:ASN:O	7:G:117:CYS:SG	2.77	0.42
7:G:368:VAL:HG22	7:G:616:VAL:HG11	2.01	0.42
8:H:146:SER:O	8:H:149:VAL:HG22	2.19	0.42
12:L:3:LEU:HD23	12:L:3:LEU:HA	1.92	0.42
13:M:20:VAL:O	13:M:24:ILE:HG12	2.19	0.42
13:M:344:VAL:O	13:M:348:LEU:HG	2.20	0.42
32:i:17:GLU:OE2	32:i:22:ARG:NH1	2.52	0.42
7:G:161:PHE:O	7:G:164:MET:HG2	2.19	0.42
7:G:210:LEU:HD13	7:G:334:PHE:CE2	2.54	0.42
7:G:222:THR:O	7:G:226:ARG:HG3	2.19	0.42
12:L:133:PHE:HB3	12:L:182:ILE:HG12	2.02	0.42
12:L:281:THR:HA	12:L:284:ILE:HD12	2.01	0.42
12:L:395:LEU:HD11	33:j:39:ILE:HD11	2.02	0.42
12:L:410:THR:HG21	12:L:509:SER:HA	2.01	0.42
12:L:514:PRO:HB2	12:L:516:ILE:HG22	2.01	0.42
13:M:107:VAL:HG11	13:M:350:LEU:HD22	2.02	0.42
13:M:266:ARG:HD3	13:M:266:ARG:HA	1.94	0.42
14:N:412:TYR:CD2	14:N:487:PHE:HE2	2.38	0.42
18:S:29:ARG:O	18:S:33:GLU:HG2	2.20	0.42
21:V:73:ASP:OD1	21:V:76:MET:HG2	2.20	0.42
27:c:31:LYS:HB2	31:g:39:GLU:HA	2.01	0.42
37:n:82:ASP:OD1	37:n:82:ASP:N	2.49	0.42
44:x:44:GLN:HE22	44:x:46:THR:HG22	1.83	0.42
46:z:58:GLU:HB2	46:z:75:ARG:HG2	2.02	0.42
1:A:62:TYR:OH	11:K:74:ALA:O	2.37	0.42
4:D:192:MET:HG3	9:I:82:LEU:HD23	2.02	0.42
4:D:256:ASP:O	4:D:258:TYR:N	2.52	0.42
13:M:272:PHE:HB3	13:M:275:ALA:HB3	2.01	0.42
18:S:78:THR:H	18:S:81:GLN:HB2	1.83	0.42
21:V:57:VAL:O	21:V:61:THR:OG1	2.30	0.42
28:d:32:PRO:HA	28:d:35:HIS:HB2	2.02	0.42
39:p:82:ARG:HG3	39:p:90:HIS:CE1	2.54	0.42
7:G:423:TYR:OH	7:G:700:PRO:HA	2.20	0.42
8:H:203:PHE:CZ	51:I:303:PTY:H141	2.55	0.42
51:I:303:PTY:H132	51:I:303:PTY:H162	1.82	0.42
12:L:120:PHE:HE2	12:L:143:VAL:HB	1.84	0.42
12:L:546:PHE:HZ	12:L:556:TYR:HB2	1.85	0.42
13:M:307:ILE:HD12	13:M:432:LEU:HD11	2.01	0.42
13:M:404:LEU:HD11	13:M:422:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:P:97:VAL:HG11	15:P:109:LEU:HD22	2.02	0.42
39:p:77:TYR:CD2	39:p:78:LEU:HD22	2.51	0.42
44:x:54:TRP:HZ3	46:z:227:PHE:HB2	1.84	0.42
4:D:75:MET:SD	4:D:75:MET:N	2.90	0.42
6:F:80:MET:SD	6:F:85:TRP:HB2	2.59	0.42
8:H:78:PRO:HB2	8:H:227:LEU:HD23	2.02	0.42
8:H:178:TRP:HB3	8:H:247:PHE:O	2.20	0.42
13:M:450:SER:OG	13:M:451:ASP:N	2.52	0.42
14:N:32:LEU:HD21	14:N:57:LEU:HB3	2.01	0.42
15:P:99:PHE:CD1	15:P:106:PRO:HG3	2.55	0.42
15:P:131:ILE:O	15:P:135:MET:HE3	2.20	0.42
15:P:313:PRO:HA	15:P:316:LYS:HG2	2.01	0.42
18:S:25:SER:OG	18:S:58:PRO:HG3	2.20	0.42
23:X:77:ASP:OD1	23:X:78:TYR:N	2.53	0.42
31:g:81:LEU:HD22	31:g:84:LYS:NZ	2.35	0.42
45:y:96:SER:H	45:y:124:ASP:HB3	1.84	0.42
4:D:309:LEU:HD21	7:G:170:CYS:HB2	2.01	0.41
4:D:310:ILE:HG23	7:G:182:GLN:HB2	2.01	0.41
5:E:84:ASN:HD21	5:E:87:TRP:NE1	2.18	0.41
7:G:599:PHE:HA	7:G:615:ASN:ND2	2.35	0.41
11:K:61:PHE:CD2	14:N:146:ILE:HG23	2.55	0.41
13:M:408:PHE:HA	13:M:411:ASN:O	2.20	0.41
52:M:501:PC7:H382	52:M:501:PC7:H411	1.78	0.41
14:N:404:LEU:HD22	14:N:476:ILE:HG22	2.02	0.41
15:P:74:PHE:HB3	15:P:145:ILE:HG13	2.02	0.41
31:g:64:LEU:HB3	31:g:65:PRO:HD3	2.02	0.41
33:j:36:TRP:HZ2	34:k:32:LEU:HD22	1.85	0.41
33:j:58:ASP:O	38:o:60:LYS:HA	2.20	0.41
45:y:77:SER:HB3	45:y:98:THR:H	1.85	0.41
46:z:175:ILE:HG23	46:z:181:TRP:HD1	1.84	0.41
4:D:105:PHE:HZ	4:D:148:VAL:HG11	1.84	0.41
4:D:203:LEU:HD13	4:D:257:CYS:O	2.20	0.41
8:H:38:LYS:HD2	8:H:38:LYS:HA	1.80	0.41
8:H:77:ALA:HB2	8:H:123:ILE:HG13	2.02	0.41
8:H:256:ASP:OD1	8:H:260:PHE:HB2	2.20	0.41
12:L:318:GLN:HA	12:L:321:TYR:HD2	1.85	0.41
15:P:246:ILE:HG23	15:P:315:ALA:HB1	2.02	0.41
15:P:379:ILE:O	15:P:382:ARG:HG2	2.21	0.41
18:S:4:ARG:HG2	18:S:4:ARG:NH1	2.35	0.41
18:S:84:LYS:O	18:S:87:GLU:HB2	2.20	0.41
21:V:134:ARG:O	21:V:134:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:X:18:LEU:HD13	24:Z:89:LEU:HD11	2.02	0.41
32:i:41:LYS:HD2	32:i:41:LYS:HA	1.68	0.41
34:k:21:HIS:O	34:k:23:MET:N	2.52	0.41
36:m:40:PHE:HA	36:m:44:LEU:HD13	2.02	0.41
7:G:341:ARG:HD2	7:G:341:ARG:HA	1.80	0.41
9:I:156:ASP:OD1	9:I:156:ASP:N	2.49	0.41
12:L:82:THR:O	12:L:86:LEU:HG	2.19	0.41
29:e:18:TRP:HB2	29:e:41:TYR:CE1	2.54	0.41
39:p:33:MET:O	39:p:37:ILE:HG13	2.21	0.41
41:r:82:PRO:CD	41:r:83:PRO:CD	2.94	0.41
45:y:81:TYR:OH	45:y:214:HIS:ND1	2.31	0.41
3:C:18:TRP:CZ2	3:C:40:GLN:HB3	2.56	0.41
6:F:85:TRP:CD2	6:F:204:LEU:HD13	2.54	0.41
6:F:293:ASN:O	6:F:315:MET:HG2	2.20	0.41
7:G:284:ASN:OD1	7:G:285:TRP:N	2.54	0.41
7:G:685:PRO:O	7:G:688:VAL:HG22	2.21	0.41
8:H:8:GLU:O	8:H:12:ILE:HG12	2.20	0.41
8:H:258:PRO:HA	8:H:261:LYS:HD3	2.03	0.41
11:K:22:LEU:HD23	11:K:22:LEU:HA	1.90	0.41
12:L:172:ARG:HD2	12:L:172:ARG:HA	1.86	0.41
13:M:425:GLY:HA2	13:M:428:TYR:HE1	1.81	0.41
14:N:60:LEU:O	14:N:64:ILE:HG13	2.21	0.41
23:X:46:PRO:HG2	24:Z:97:PHE:CD2	2.55	0.41
23:X:97:GLU:HA	23:X:100:GLU:CD	2.45	0.41
36:m:30:THR:O	36:m:34:PHE:N	2.49	0.41
46:z:14:TRP:O	46:z:17:GLU:HG3	2.20	0.41
1:A:79:PHE:CG	8:H:108:LEU:HD12	2.55	0.41
2:B:76:MET:HG2	8:H:60:LEU:HD13	2.01	0.41
2:B:186:PRO:HG2	9:I:185:PHE:CD2	2.50	0.41
4:D:55:ILE:HG12	4:D:66:TYR:HD2	1.86	0.41
6:F:288:PHE:O	6:F:295:GLY:N	2.43	0.41
8:H:95:ASP:H	8:H:98:MET:HB2	1.85	0.41
9:I:178:VAL:HG11	9:I:215:LEU:HD11	2.02	0.41
12:L:157:ARG:HH21	12:L:247:GLU:CD	2.27	0.41
13:M:50:LEU:HD21	31:g:69:THR:HG23	2.03	0.41
13:M:153:MET:O	13:M:157:ILE:HG12	2.20	0.41
14:N:426:ALA:O	14:N:430:VAL:HG23	2.21	0.41
38:o:38:ASN:O	38:o:42:GLN:HG2	2.20	0.41
44:x:165:HIS:CE1	46:z:150:THR:HG22	2.55	0.41
7:G:170:CYS:N	7:G:171:PRO:HD2	2.36	0.41
7:G:237:LEU:HD12	7:G:237:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:162:VAL:HG21	8:H:170:ILE:HA	2.02	0.41
10:J:37:THR:CG2	11:K:44:LEU:HD21	2.51	0.41
10:J:167:ILE:O	10:J:171:MET:HG2	2.20	0.41
14:N:159:PHE:CE2	14:N:269:PRO:HG3	2.56	0.41
44:x:107:ASN:ND2	44:x:135:ALA:O	2.53	0.41
44:x:210:THR:HG23	44:x:213:GLU:H	1.85	0.41
45:y:184:ASN:HB3	45:y:185:PRO:HD3	2.02	0.41
7:G:440:PHE:HB2	7:G:469:VAL:HG22	2.03	0.41
8:H:206:PRO:HG3	8:H:292:TYR:HD1	1.85	0.41
10:J:38:SER:OG	10:J:50:ALA:O	2.25	0.41
12:L:300:THR:HG21	12:L:562:ARG:HG3	2.01	0.41
12:L:563:TRP:CH2	35:l:89:PHE:HZ	2.39	0.41
13:M:59:PHE:HE2	13:M:480:CYS:HB3	1.85	0.41
14:N:76:LEU:HG	14:N:89:ARG:HH11	1.86	0.41
18:S:85:ALA:HA	18:S:88:ASN:HD21	1.85	0.41
23:X:92:CYS:C	23:X:94:LYS:H	2.28	0.41
40:q:55:ASP:OD1	40:q:56:LYS:N	2.54	0.41
44:x:236:LEU:HD11	46:z:20:GLN:OE1	2.20	0.41
5:E:84:ASN:ND2	5:E:87:TRP:CD1	2.89	0.41
6:F:284:TRP:O	6:F:287:SER:OG	2.35	0.41
7:G:280:PHE:CD2	9:I:144:GLU:HB2	2.56	0.41
7:G:409:TRP:CE3	7:G:569:GLN:HG3	2.56	0.41
7:G:603:GLN:NE2	7:G:653:ASP:HA	2.35	0.41
9:I:54:LYS:HA	9:I:54:LYS:HD2	1.87	0.41
10:J:132:ARG:HH21	24:Z:83:ARG:HH22	1.68	0.41
12:L:398:PHE:CZ	12:L:522:ILE:HD11	2.55	0.41
14:N:95:PHE:O	14:N:98:ILE:HG22	2.21	0.41
14:N:485:PRO:O	14:N:489:VAL:HG23	2.21	0.41
24:Z:118:TRP:CH2	29:e:53:ARG:HD2	2.56	0.41
52:f:201:PC7:H182	52:f:201:PC7:H212	1.74	0.41
44:x:81:ASN:HD21	46:z:42:HIS:CE1	2.38	0.41
1:A:115:ALA:HB2	10:J:171:MET:SD	2.60	0.41
2:B:148:GLU:HB2	8:H:62:GLU:CG	2.48	0.41
4:D:357:ALA:HB1	4:D:391:GLU:HB2	2.03	0.41
5:E:66:SER:O	5:E:69:LYS:HG3	2.20	0.41
5:E:148:LEU:HD11	5:E:154:LYS:HD2	2.03	0.41
6:F:309:CYS:HB3	6:F:311:VAL:HG13	2.03	0.41
7:G:198:MET:HG3	17:R:86:PHE:CE1	2.56	0.41
8:H:205:LEU:N	8:H:206:PRO:HD2	2.36	0.41
10:J:157:LEU:HD22	14:N:131:LEU:HD11	2.03	0.41
12:L:224:LEU:HD23	12:L:224:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:343:PHE:HB3	12:L:474:SER:HB3	2.03	0.41
12:L:505:ILE:HA	35:l:110:ARG:NH2	2.36	0.41
13:M:52:SER:HB3	13:M:98:THR:HG21	2.03	0.41
13:M:93:PHE:CZ	13:M:338:MET:HE3	2.56	0.41
13:M:119:TYR:OH	13:M:247:ALA:HB3	2.21	0.41
13:M:237:LEU:HB3	13:M:238:PRO:HD3	2.03	0.41
13:M:241:HIS:HE1	13:M:253:ALA:HB2	1.85	0.41
13:M:371:VAL:HB	13:M:437:VAL:HG22	2.01	0.41
14:N:148:MET:CG	14:N:276:ASN:HD21	2.34	0.41
14:N:339:ILE:HD12	14:N:339:ILE:H	1.84	0.41
14:N:404:LEU:HD23	14:N:477:THR:HA	2.01	0.41
15:P:236:PHE:HE1	15:P:240:TYR:CD2	2.39	0.41
27:c:61:ARG:HG2	27:c:78:PHE:CE2	2.56	0.41
35:l:77:GLU:OE2	35:l:81:TRP:NE1	2.54	0.41
46:z:93:SER:HB3	46:z:121:ILE:HA	2.02	0.41
6:F:408:CYS:HB2	47:F:501:SF4:S3	2.60	0.41
8:H:290:TYR:CE2	8:H:294:GLN:HG3	2.56	0.41
12:L:493:TRP:HE3	12:L:496:SER:HB2	1.86	0.41
29:e:55:ASN:O	29:e:59:LYS:HG2	2.21	0.41
38:o:8:LYS:NZ	38:o:29:MET:HB2	2.35	0.41
39:p:62:GLU:CD	39:p:69:LYS:HZ2	2.29	0.41
4:D:194:THR:O	4:D:200:LYS:HE2	2.21	0.40
7:G:653:ASP:O	7:G:657:VAL:HG23	2.21	0.40
11:K:4:ILE:O	11:K:8:THR:HG23	2.21	0.40
11:K:9:PHE:O	11:K:13:ILE:HG12	2.21	0.40
12:L:250:THR:N	12:L:251:PRO:HD2	2.36	0.40
12:L:372:ALA:HB2	12:L:442:PHE:HB3	2.02	0.40
13:M:56:TRP:HB2	13:M:95:ILE:HD11	2.03	0.40
13:M:82:PHE:CD1	13:M:141:LEU:HD13	2.56	0.40
13:M:288:ALA:HB2	13:M:414:VAL:HG23	2.03	0.40
14:N:309:ALA:HB2	14:N:321:TYR:HB3	2.02	0.40
18:S:78:THR:O	18:S:82:ILE:N	2.47	0.40
23:X:94:LYS:HA	23:X:94:LYS:HD3	1.91	0.40
31:g:61:ASP:OD1	31:g:62:TRP:N	2.54	0.40
44:x:116:ASN:ND2	44:x:224:ILE:HG21	2.35	0.40
45:y:115:GLY:O	45:y:116:LYS:HD3	2.21	0.40
1:A:112:LYS:HE3	1:A:112:LYS:HB3	1.89	0.40
3:C:21:LYS:NZ	21:V:120:ILE:HD11	2.35	0.40
4:D:169:LEU:HD11	24:Z:21:LEU:HG	2.02	0.40
4:D:269:ARG:HD3	24:Z:35:TYR:O	2.21	0.40
5:E:122:VAL:HG13	5:E:165:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:181:ILE:HG22	5:E:198:PHE:HB2	2.03	0.40
6:F:142:GLU:OE2	6:F:142:GLU:HA	2.21	0.40
12:L:295:PHE:CG	12:L:422:LEU:HD22	2.57	0.40
12:L:484:MET:CB	38:o:46:TYR:HB3	2.51	0.40
13:M:113:ARG:HH12	46:z:112:ASN:ND2	2.19	0.40
14:N:368:GLN:HB3	14:N:459:GLU:OE2	2.21	0.40
15:P:161:HIS:HA	15:P:203:ALA:HB2	2.03	0.40
23:X:10:ASN:HB2	23:X:11:PRO:HD3	2.03	0.40
27:c:17:ALA:O	31:g:42:LYS:HB2	2.21	0.40
33:j:55:HIS:HD1	33:j:58:ASP:H	1.68	0.40
37:n:13:ARG:HH12	37:n:64:ILE:HD13	1.86	0.40
39:p:51:LEU:HD13	39:p:77:TYR:HA	2.03	0.40
45:y:181:TRP:CE3	45:y:186:ALA:HB1	2.56	0.40
46:z:217:GLU:H	46:z:217:GLU:HG3	1.79	0.40
1:A:113:ARG:HA	1:A:113:ARG:HD3	1.90	0.40
5:E:129:VAL:HG22	5:E:130:CYS:N	2.35	0.40
7:G:90:THR:O	7:G:93:GLN:N	2.53	0.40
7:G:208:GLY:N	7:G:255:LEU:HB3	2.37	0.40
12:L:97:HIS:HE1	12:L:117:LEU:CB	2.35	0.40
13:M:174:PHE:O	13:M:178:LEU:HG	2.22	0.40
13:M:441:LEU:C	13:M:443:PRO:HD3	2.46	0.40
32:i:9:GLU:O	32:i:13:LEU:HD23	2.21	0.40
37:n:24:TYR:HA	37:n:52:PHE:CE2	2.54	0.40
39:p:30:MET:HE2	39:p:30:MET:HB2	1.79	0.40
45:y:69:GLY:HA3	45:y:87:GLY:O	2.21	0.40
3:C:58:ASP:OD2	3:C:58:ASP:C	2.64	0.40
3:C:99:SER:HA	3:C:124:ILE:HB	2.03	0.40
5:E:138:ARG:HH21	6:F:303:GLY:H	1.69	0.40
7:G:444:GLY:HA3	7:G:520:LEU:HD11	2.03	0.40
8:H:55:GLY:O	8:H:59:ILE:HG13	2.21	0.40
8:H:179:PHE:O	8:H:183:LEU:HB2	2.21	0.40
9:I:72:PHE:HD1	51:I:303:PTY:H361	1.56	0.40
9:I:195:TYR:HB3	9:I:200:LEU:CD2	2.52	0.40
10:J:132:ARG:NH2	24:Z:83:ARG:HH22	2.19	0.40
12:L:77:LEU:HD13	12:L:194:PHE:HD2	1.86	0.40
12:L:209:ILE:HG13	36:m:59:GLN:HG2	2.04	0.40
13:M:169:ALA:HB2	13:M:243:GLU:OE1	2.21	0.40
19:T:87:MET:O	19:T:90:GLU:HB2	2.22	0.40
28:d:60:LEU:O	28:d:64:LEU:HD23	2.21	0.40
30:f:5:ILE:HG23	30:f:5:ILE:O	2.21	0.40
45:y:194:ASP:O	45:y:198:VAL:HG23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
46:z:46:MET:HE3	46:z:46:MET:HB2	1.99	0.40
46:z:60:PHE:O	46:z:79:ILE:N	2.50	0.40
46:z:194:ASP:OD1	46:z:195:GLU:N	2.54	0.40
7:G:113:ILE:HG22	16:Q:140:TYR:HD1	1.86	0.40
12:L:350:LEU:HB3	12:L:467:LEU:HD21	2.03	0.40
13:M:74:TRP:HZ2	14:N:480:LEU:HD22	1.86	0.40
13:M:348:LEU:HD23	13:M:384:PHE:HB3	2.04	0.40
14:N:489:VAL:CG2	28:d:56:LEU:HD21	2.51	0.40
22:W:44:TYR:HB2	22:W:46:LEU:HD22	2.02	0.40
22:W:62:GLN:HA	22:W:62:GLN:OE1	2.22	0.40
24:Z:105:LEU:HD23	24:Z:105:LEU:HA	1.92	0.40
30:f:36:ARG:HD3	30:f:76:TYR:CD2	2.57	0.40
38:o:66:VAL:HG12	38:o:70:MET:CE	2.51	0.40
38:o:73:MET:O	38:o:76:ILE:HG22	2.22	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	155/157 (99%)	142 (92%)	13 (8%)	0	100	100
3	C	183/185 (99%)	174 (95%)	9 (5%)	0	100	100
4	D	383/385 (100%)	356 (93%)	27 (7%)	0	100	100
5	E	190/192 (99%)	170 (90%)	20 (10%)	0	100	100
6	F	432/434 (100%)	408 (94%)	24 (6%)	0	100	100
7	G	686/688 (100%)	637 (93%)	49 (7%)	0	100	100
8	H	322/324 (99%)	291 (90%)	31 (10%)	0	100	100
9	I	167/169 (99%)	162 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	134/205 (65%)	131 (98%)	3 (2%)	0	100	100
11	K	86/88 (98%)	85 (99%)	0	1 (1%)	10	39
12	L	613/615 (100%)	559 (91%)	54 (9%)	0	100	100
13	M	485/487 (100%)	465 (96%)	20 (4%)	0	100	100
14	N	486/488 (100%)	466 (96%)	20 (4%)	0	100	100
15	P	329/331 (99%)	309 (94%)	20 (6%)	0	100	100
16	Q	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
17	R	60/62 (97%)	59 (98%)	1 (2%)	0	100	100
18	S	91/93 (98%)	82 (90%)	9 (10%)	0	100	100
19	T	82/84 (98%)	80 (98%)	2 (2%)	0	100	100
20	U	81/83 (98%)	76 (94%)	5 (6%)	0	100	100
21	V	138/140 (99%)	134 (97%)	4 (3%)	0	100	100
22	W	104/133 (78%)	100 (96%)	4 (4%)	0	100	100
23	X	94/96 (98%)	89 (95%)	5 (5%)	0	100	100
24	Z	123/125 (98%)	114 (93%)	8 (6%)	1 (1%)	16	47
25	a	56/58 (97%)	56 (100%)	0	0	100	100
26	b	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
27	c	74/76 (97%)	59 (80%)	15 (20%)	0	100	100
28	d	73/75 (97%)	71 (97%)	2 (3%)	0	100	100
29	e	62/64 (97%)	60 (97%)	2 (3%)	0	100	100
30	f	98/100 (98%)	94 (96%)	4 (4%)	0	100	100
31	g	70/72 (97%)	65 (93%)	5 (7%)	0	100	100
32	i	83/85 (98%)	77 (93%)	6 (7%)	0	100	100
33	j	49/51 (96%)	45 (92%)	4 (8%)	0	100	100
34	k	45/47 (96%)	39 (87%)	6 (13%)	0	100	100
35	l	44/46 (96%)	43 (98%)	1 (2%)	0	100	100
36	m	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
37	n	107/109 (98%)	98 (92%)	9 (8%)	0	100	100
38	o	78/80 (98%)	70 (90%)	8 (10%)	0	100	100
39	p	91/93 (98%)	86 (94%)	5 (6%)	0	100	100
40	q	61/63 (97%)	53 (87%)	8 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	r	8/10 (80%)	7 (88%)	1 (12%)	0	100	100
43	v	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
44	x	212/214 (99%)	196 (92%)	16 (8%)	0	100	100
45	y	266/268 (99%)	239 (90%)	27 (10%)	0	100	100
46	z	231/233 (99%)	212 (92%)	19 (8%)	0	100	100
All	All	7468/7683 (97%)	6980 (94%)	486 (6%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	28	ILE
24	Z	120	VAL

5.3.2 Protein sidechains [i](#)

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	132/132 (100%)	132 (100%)	0	100	100
3	C	175/175 (100%)	175 (100%)	0	100	100
4	D	331/331 (100%)	331 (100%)	0	100	100
5	E	166/166 (100%)	166 (100%)	0	100	100
6	F	353/353 (100%)	353 (100%)	0	100	100
7	G	571/571 (100%)	570 (100%)	1 (0%)	87	86
8	H	271/271 (100%)	271 (100%)	0	100	100
9	I	151/151 (100%)	151 (100%)	0	100	100
10	J	123/186 (66%)	123 (100%)	0	100	100
11	K	76/76 (100%)	76 (100%)	0	100	100
12	L	518/518 (100%)	517 (100%)	1 (0%)	87	86
13	M	426/426 (100%)	426 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	406/406 (100%)	406 (100%)	0	100	100
15	P	273/273 (100%)	273 (100%)	0	100	100
16	Q	100/100 (100%)	100 (100%)	0	100	100
17	R	55/55 (100%)	55 (100%)	0	100	100
18	S	82/82 (100%)	82 (100%)	0	100	100
19	T	79/79 (100%)	79 (100%)	0	100	100
20	U	75/75 (100%)	75 (100%)	0	100	100
21	V	123/123 (100%)	123 (100%)	0	100	100
22	W	96/114 (84%)	96 (100%)	0	100	100
23	X	87/87 (100%)	87 (100%)	0	100	100
24	Z	100/100 (100%)	100 (100%)	0	100	100
25	a	48/48 (100%)	48 (100%)	0	100	100
26	b	33/33 (100%)	33 (100%)	0	100	100
27	c	66/66 (100%)	66 (100%)	0	100	100
28	d	60/60 (100%)	60 (100%)	0	100	100
29	e	59/59 (100%)	59 (100%)	0	100	100
30	f	80/80 (100%)	80 (100%)	0	100	100
31	g	62/62 (100%)	62 (100%)	0	100	100
32	i	77/77 (100%)	77 (100%)	0	100	100
33	j	42/42 (100%)	42 (100%)	0	100	100
34	k	38/38 (100%)	38 (100%)	0	100	100
35	l	37/37 (100%)	37 (100%)	0	100	100
36	m	58/58 (100%)	58 (100%)	0	100	100
37	n	92/92 (100%)	92 (100%)	0	100	100
38	o	70/70 (100%)	70 (100%)	0	100	100
39	p	83/83 (100%)	83 (100%)	0	100	100
40	q	52/52 (100%)	52 (100%)	0	100	100
41	r	10/10 (100%)	10 (100%)	0	100	100
43	v	23/23 (100%)	23 (100%)	0	100	100
44	x	183/183 (100%)	183 (100%)	0	100	100
45	y	223/223 (100%)	223 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	z	188/188 (100%)	188 (100%)	0	100	100
All	All	6437/6540 (98%)	6435 (100%)	2 (0%)	100	100

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

Mol	Chain	Res	Type
7	G	613	ARG
12	L	330	ASN

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

Mol	Chain	Res	Type
2	B	217	ASN
3	C	141	HIS
4	D	78	GLN
4	D	113	ASN
4	D	114	HIS
4	D	181	GLN
4	D	362	HIS
5	E	84	ASN
6	F	72	HIS
6	F	255	ASN
6	F	336	ASN
6	F	436	GLN
6	F	459	GLN
6	F	464	HIS
7	G	69	ASN
7	G	455	ASN
7	G	466	ASN
7	G	638	GLN
8	H	129	ASN
9	I	61	ASN
9	I	190	HIS
12	L	97	HIS
12	L	417	ASN
12	L	547	GLN
12	L	553	ASN
12	L	560	ASN
13	M	315	HIS
15	P	153	ASN
18	S	57	GLN

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Mol	Chain	Res	Type
18	S	81	GLN
18	S	88	ASN
21	V	132	GLN
22	W	66	ASN
23	X	87	ASN
25	a	39	HIS
25	a	42	HIS
27	c	60	GLN
28	d	21	ASN
29	e	46	HIS
30	f	80	ASN
32	i	71	GLN
39	p	44	GLN
39	p	68	GLN
43	v	83	ASN
44	x	81	ASN
44	x	116	ASN
44	x	165	HIS
45	y	107	HIS
45	y	224	GLN
46	z	47	ASN
46	z	101	GLN
46	z	112	ASN
46	z	130	HIS
46	z	218	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 24 ligands modelled in this entry, 2 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
47	SF4	I	301	9	0,12,12	-	-	-		
57	PGT	y	302	-	40,40,50	1.19	4 (10%)	43,46,56	1.10	2 (4%)
51	PTY	I	303	-	49,49,49	0.88	4 (8%)	52,54,54	1.08	2 (3%)
56	8Q1	n	200	-	32,34,34	1.64	6 (18%)	39,43,43	1.53	4 (10%)
48	FES	E	500	5	0,4,4	-	-	-		
58	PSF	z	301	-	28,29,29	1.20	4 (14%)	30,36,36	1.24	2 (6%)
54	NDP	P	500	-	51,52,52	2.38	6 (11%)	71,80,80	1.56	16 (22%)
59	T7X	z	302	-	61,61,61	0.85	4 (6%)	70,73,73	1.05	3 (4%)
50	UQ9	H	500	-	35,35,58	2.60	13 (37%)	43,45,73	1.55	8 (18%)
52	PC7	f	201	-	51,51,51	0.98	4 (7%)	57,59,59	1.04	2 (3%)
52	PC7	M	501	-	51,51,51	0.98	4 (7%)	57,59,59	1.10	3 (5%)
51	PTY	N	501	-	49,49,49	0.88	4 (8%)	52,54,54	1.08	2 (3%)
47	SF4	I	302	9	0,12,12	-	-	-		
49	FMN	F	500	-	33,33,33	1.06	2 (6%)	48,50,50	1.23	8 (16%)
47	SF4	B	500	2	0,12,12	-	-	-		
51	PTY	M	502	-	49,49,49	0.89	4 (8%)	52,54,54	1.11	2 (3%)
53	LMN	M	503	-	72,72,72	1.69	15 (20%)	92,98,98	1.15	5 (5%)
56	8Q1	W	200	-	32,34,34	1.62	6 (18%)	39,43,43	1.55	4 (10%)
47	SF4	F	501	6	0,12,12	-	-	-		
47	SF4	G	802	7	0,12,12	-	-	-		
47	SF4	G	803	7	0,12,12	-	-	-		
48	FES	G	801	7	0,4,4	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	SF4	I	301	9	-	-	0/6/5/5
57	PGT	y	302	-	-	27/45/45/55	-
51	PTY	I	303	-	-	19/53/53/53	-
56	8Q1	n	200	-	-	8/41/41/41	-
48	FES	E	500	5	-	-	0/1/1/1
58	PSF	z	301	-	-	9/35/35/35	-
54	NDP	P	500	-	-	4/34/77/77	0/5/5/5
59	T7X	z	302	-	-	24/56/80/80	0/1/1/1
50	UQ9	H	500	-	-	4/30/54/81	0/1/1/1
52	PC7	f	201	-	-	26/55/55/55	-
52	PC7	M	501	-	-	20/55/55/55	-
51	PTY	N	501	-	-	26/53/53/53	-
47	SF4	I	302	9	-	-	0/6/5/5
49	FMN	F	500	-	-	7/18/18/18	0/3/3/3
47	SF4	B	500	2	-	-	0/6/5/5
51	PTY	M	502	-	-	24/53/53/53	-
53	LMN	M	503	-	-	35/50/130/130	0/4/4/4
56	8Q1	W	200	-	-	22/41/41/41	-
47	SF4	F	501	6	-	-	0/6/5/5
47	SF4	G	802	7	-	-	0/6/5/5
47	SF4	G	803	7	-	-	0/6/5/5
48	FES	G	801	7	-	-	0/1/1/1

All (80) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	P	500	NDP	P2B-O2B	13.35	1.82	1.59
50	H	500	UQ9	C6-C1	10.42	1.53	1.35
56	W	200	8Q1	C34-N36	5.17	1.45	1.33
56	n	200	8Q1	C39-N41	5.16	1.45	1.33
56	n	200	8Q1	C34-N36	5.14	1.45	1.33
56	W	200	8Q1	C39-N41	5.10	1.45	1.33
50	H	500	UQ9	C4-C3	4.88	1.53	1.36
53	M	503	LMN	O5-C1	4.71	1.54	1.41
54	P	500	NDP	PA-O3	4.63	1.64	1.59
53	M	503	LMN	CBS-CCM	4.42	1.63	1.53
54	P	500	NDP	PN-O5D	4.30	1.76	1.59
53	M	503	LMN	CBT-CCM	4.30	1.63	1.53
50	H	500	UQ9	C7-C8	3.96	1.56	1.50
53	M	503	LMN	CBR-CCM	3.84	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	M	503	LMN	O1-C1	-3.47	1.34	1.40
49	F	500	FMN	C4A-N5	3.35	1.38	1.30
54	P	500	NDP	O2B-C2B	-3.07	1.33	1.44
57	y	302	PGT	O3-C11	3.07	1.42	1.33
57	y	302	PGT	O2-C31	2.97	1.42	1.34
53	M	503	LMN	OBZ-CCS	2.89	1.49	1.41
53	M	503	LMN	O4-C4	2.88	1.51	1.43
53	M	503	LMN	OBY-CCR	2.88	1.49	1.41
52	f	201	PC7	O2-C2	-2.75	1.40	1.46
51	I	303	PTY	O7-C6	-2.71	1.40	1.46
51	M	502	PTY	O7-C6	-2.69	1.40	1.46
58	z	301	PSF	O11-C3	-2.69	1.40	1.46
52	M	501	PC7	O2-C2	-2.68	1.40	1.46
53	M	503	LMN	OBX-CCF	2.65	1.50	1.44
50	H	500	UQ9	C11-C9	2.62	1.56	1.51
49	F	500	FMN	C10-N1	2.54	1.38	1.33
54	P	500	NDP	C5A-C4A	2.49	1.43	1.39
50	H	500	UQ9	C16-C14	2.49	1.56	1.51
56	W	200	8Q1	C1-S44	2.48	1.82	1.76
56	n	200	8Q1	C1-S44	2.47	1.82	1.76
53	M	503	LMN	OBX-CCJ	2.45	1.48	1.41
50	H	500	UQ9	C21-C19	2.42	1.56	1.51
50	H	500	UQ9	C26-C24	2.41	1.56	1.51
51	N	501	PTY	O4-C30	2.41	1.40	1.33
58	z	301	PSF	O52-C5	2.40	1.40	1.33
52	M	501	PC7	O3-C11	2.40	1.40	1.33
50	H	500	UQ9	O4-C4M	-2.40	1.39	1.45
59	z	302	T7X	O18-C11	2.39	1.40	1.33
51	I	303	PTY	O4-C30	2.39	1.40	1.33
51	M	502	PTY	O4-C30	2.39	1.40	1.33
52	f	201	PC7	O3-C11	2.37	1.40	1.33
51	N	501	PTY	O7-C6	-2.35	1.41	1.46
59	z	302	T7X	O16-C10	2.31	1.40	1.34
59	z	302	T7X	O16-C8	-2.31	1.41	1.46
56	n	200	8Q1	C6-C1	2.29	1.53	1.50
50	H	500	UQ9	C7-C6	2.29	1.55	1.51
56	W	200	8Q1	O40-C39	-2.27	1.18	1.23
56	n	200	8Q1	O35-C34	-2.27	1.19	1.23
51	N	501	PTY	O7-C8	2.26	1.40	1.34
57	y	302	PGT	P-O3P	2.26	1.68	1.59
56	W	200	8Q1	O35-C34	-2.26	1.19	1.23
52	f	201	PC7	O3-C3	-2.26	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	I	303	PTY	O4-C1	-2.24	1.40	1.45
52	M	501	PC7	O3-C3	-2.23	1.40	1.45
51	M	502	PTY	O4-C1	-2.22	1.40	1.45
53	M	503	LMN	C3-C4	-2.21	1.46	1.52
51	N	501	PTY	O4-C1	-2.20	1.40	1.45
56	n	200	8Q1	O40-C39	-2.20	1.18	1.23
50	H	500	UQ9	C17-C18	2.19	1.57	1.50
50	H	500	UQ9	C6-C5	2.19	1.52	1.46
58	z	301	PSF	O52-C4	-2.18	1.40	1.45
54	P	500	NDP	C2A-N1A	2.17	1.37	1.33
52	M	501	PC7	O2-C31	2.17	1.40	1.34
52	f	201	PC7	O2-C31	2.17	1.40	1.34
53	M	503	LMN	CBQ-CCM	2.16	1.58	1.54
59	z	302	T7X	O18-C9	-2.16	1.40	1.45
51	M	502	PTY	O7-C8	2.15	1.40	1.34
58	z	301	PSF	O11-C1	2.15	1.40	1.34
53	M	503	LMN	O5-C5	2.14	1.49	1.44
51	I	303	PTY	O7-C8	2.13	1.40	1.34
56	W	200	8Q1	C6-C1	2.13	1.53	1.50
57	y	302	PGT	O2-C2	-2.06	1.41	1.46
53	M	503	LMN	CBQ-CBK	2.02	1.59	1.52
53	M	503	LMN	OCB-CCQ	2.02	1.49	1.43
50	H	500	UQ9	O3-C3M	-2.01	1.40	1.45
50	H	500	UQ9	O5-C5	-2.01	1.18	1.23

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
56	n	200	8Q1	C6-C1-S44	5.47	119.92	113.40
56	W	200	8Q1	C6-C1-S44	5.35	119.78	113.40
54	P	500	NDP	P2B-O2B-C2B	-4.50	111.41	123.43
59	z	302	T7X	O16-C10-C12	4.13	120.41	111.48
52	M	501	PC7	O2-C31-C32	4.11	120.38	111.48
53	M	503	LMN	CCR-O4-C4	-4.06	108.35	117.98
50	H	500	UQ9	C7-C8-C9	-4.05	119.86	126.83
51	M	502	PTY	O7-C8-C11	4.02	120.19	111.48
51	N	501	PTY	O7-C8-C11	4.00	120.14	111.48
58	z	301	PSF	O11-C1-C13	3.99	120.11	111.48
57	y	302	PGT	O2-C31-C32	3.98	120.10	111.48
52	f	201	PC7	O2-C31-C32	3.92	119.97	111.48
51	I	303	PTY	O7-C8-C11	3.84	119.78	111.48
56	W	200	8Q1	O4-C1-C6	-3.67	119.75	123.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	P	500	NDP	O2B-P2B-O1X	-3.58	96.58	109.33
56	n	200	8Q1	O4-C1-C6	-3.40	120.06	123.98
50	H	500	UQ9	C12-C13-C14	-3.36	119.94	127.62
49	F	500	FMN	C4-N3-C2	-3.28	119.83	125.64
50	H	500	UQ9	C17-C18-C19	-3.28	120.13	127.62
54	P	500	NDP	O3-PA-O1A	-3.06	101.51	110.70
54	P	500	NDP	PA-O5B-C5B	-3.03	104.00	121.35
54	P	500	NDP	PN-O5D-C5D	-2.97	104.33	121.35
53	M	503	LMN	CCS-OCB-CCQ	-2.92	111.06	117.98
50	H	500	UQ9	C22-C23-C24	-2.90	120.98	127.62
56	W	200	8Q1	C43-S44-C1	2.81	110.14	101.84
51	M	502	PTY	O4-C30-C31	2.76	120.26	111.83
54	P	500	NDP	O2N-PN-O1N	2.74	125.17	112.44
54	P	500	NDP	O2N-PN-O3	2.72	114.63	107.27
50	H	500	UQ9	C15-C14-C16	2.71	119.94	115.23
51	I	303	PTY	O4-C30-C31	2.71	120.10	111.83
50	H	500	UQ9	C25-C24-C26	2.69	119.90	115.23
51	N	501	PTY	O4-C30-C31	2.69	120.05	111.83
49	F	500	FMN	O4-C4-C4A	-2.69	119.42	126.53
49	F	500	FMN	C4A-C4-N3	2.69	120.10	113.25
59	z	302	T7X	O18-C11-C31	2.66	119.96	111.83
52	M	501	PC7	O3-C11-C12	2.66	119.94	111.83
58	z	301	PSF	O52-C5-C6	2.65	119.92	111.83
57	y	302	PGT	O3-C11-C12	2.63	119.86	111.83
50	H	500	UQ9	C20-C19-C21	2.63	119.79	115.23
54	P	500	NDP	O5D-PN-O1N	-2.58	98.71	108.94
54	P	500	NDP	O3X-P2B-O2X	2.54	117.34	107.80
49	F	500	FMN	C5A-C9A-N10	2.53	120.25	117.97
52	f	201	PC7	O3-C11-C12	2.52	119.52	111.83
56	n	200	8Q1	C43-S44-C1	2.46	109.11	101.84
50	H	500	UQ9	C10-C9-C11	2.43	119.45	115.23
54	P	500	NDP	C2A-N1A-C6A	-2.43	114.75	118.73
49	F	500	FMN	C9A-C5A-N5	-2.34	119.97	122.45
49	F	500	FMN	C4A-C10-N10	2.32	119.80	116.48
54	P	500	NDP	C5D-C4D-C3D	-2.30	106.94	115.21
54	P	500	NDP	N3A-C4A-N9A	2.27	131.02	127.17
53	M	503	LMN	OBX-CCF-CCQ	2.25	114.37	109.72
53	M	503	LMN	OBX-CCJ-CCL	2.17	114.83	110.37
54	P	500	NDP	C5A-C4A-N3A	-2.16	123.74	126.72
49	F	500	FMN	C10-C4A-N5	-2.14	120.43	124.81
56	W	200	8Q1	C38-C39-N41	2.14	120.24	116.34
54	P	500	NDP	O3X-P2B-O2B	-2.10	97.65	105.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	F	500	FMN	C4A-C10-N1	-2.10	119.43	124.59
56	n	200	8Q1	O4-C1-S44	-2.10	120.02	122.68
54	P	500	NDP	C5B-C4B-C3B	-2.06	107.79	115.21
53	M	503	LMN	CBL-CBR-CCM	-2.06	110.93	117.19
54	P	500	NDP	C4B-O4B-C1B	-2.06	104.92	109.47
59	z	302	T7X	C6-C1-C2	2.01	113.65	110.86
52	M	501	PC7	C4-C5-N	-2.01	109.36	115.82

There are no chirality outliers.

All (255) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
49	F	500	FMN	N10-C1'-C2'-O2'
49	F	500	FMN	N10-C1'-C2'-C3'
49	F	500	FMN	C1'-C2'-C3'-O3'
49	F	500	FMN	C1'-C2'-C3'-C4'
51	I	303	PTY	N1-C2-C3-O11
51	I	303	PTY	O14-C5-C6-O7
51	I	303	PTY	C5-O14-P1-O11
51	I	303	PTY	C5-O14-P1-O13
51	M	502	PTY	O10-C8-O7-C6
51	M	502	PTY	C11-C8-O7-C6
51	M	502	PTY	C5-O14-P1-O11
51	M	502	PTY	C5-O14-P1-O13
51	N	501	PTY	O10-C8-O7-C6
51	N	501	PTY	C3-O11-P1-O13
51	N	501	PTY	C3-O11-P1-O14
51	N	501	PTY	C5-O14-P1-O11
51	N	501	PTY	C5-O14-P1-O13
52	M	501	PC7	C4-O4P-P-O3P
52	M	501	PC7	C4-O4P-P-O1P
52	M	501	PC7	C4-O4P-P-O2P
52	M	501	PC7	O4P-C4-C5-N
52	f	201	PC7	C32-C31-O2-C2
52	f	201	PC7	O31-C31-O2-C2
52	f	201	PC7	O2-C2-C3-O3
52	f	201	PC7	C1-O3P-P-O1P
52	f	201	PC7	C1-O3P-P-O4P
52	f	201	PC7	C4-O4P-P-O3P
52	f	201	PC7	C4-O4P-P-O1P
52	f	201	PC7	C5-C4-O4P-P
53	M	503	LMN	O5-C1-O1-CBS

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Mol	Chain	Res	Type	Atoms
53	M	503	LMN	CBK-CBQ-CCM-CBR
53	M	503	LMN	CBK-CBQ-CCM-CBS
53	M	503	LMN	CBK-CBQ-CCM-CBT
53	M	503	LMN	OBV-CBT-CCM-CBQ
53	M	503	LMN	OBV-CBT-CCM-CBR
54	P	500	NDP	C5B-O5B-PA-O3
56	W	200	8Q1	S44-C1-C6-C7
56	W	200	8Q1	O4-C1-S44-C43
56	W	200	8Q1	C6-C1-S44-C43
56	W	200	8Q1	C28-C29-C32-C34
56	W	200	8Q1	C31-C29-C32-C34
56	W	200	8Q1	C29-C32-C34-N36
56	W	200	8Q1	C29-C32-C34-O35
56	W	200	8Q1	O33-C32-C34-N36
56	W	200	8Q1	N36-C37-C38-C39
56	W	200	8Q1	C28-O27-P24-O2
56	W	200	8Q1	C28-O27-P24-O1
56	n	200	8Q1	O27-C28-C29-C30
56	n	200	8Q1	O27-C28-C29-C31
56	n	200	8Q1	O27-C28-C29-C32
56	n	200	8Q1	C42-C43-S44-C1
57	y	302	PGT	C32-C31-O2-C2
57	y	302	PGT	C1-O3P-P-O2P
57	y	302	PGT	C1-O3P-P-O4P
57	y	302	PGT	C4-O4P-P-O3P
57	y	302	PGT	C4-O4P-P-O1P
57	y	302	PGT	O4P-C4-C5-C6
58	z	301	PSF	CB-O1-P-O2
58	z	301	PSF	CB-O1-P-O4
58	z	301	PSF	CB-O1-P-O3
58	z	301	PSF	C13-C1-O11-C3
58	z	301	PSF	N-CA-CB-O1
58	z	301	PSF	C-CA-CB-O1
59	z	302	T7X	C1-O1-P1-O13
59	z	302	T7X	C12-C10-O16-C8
59	z	302	T7X	O17-C10-O16-C8
59	z	302	T7X	C21-C22-C23-C24
51	M	502	PTY	O30-C30-O4-C1
52	M	501	PC7	O11-C11-O3-C3
53	M	503	LMN	OBZ-CCS-OCB-CCQ
58	z	301	PSF	O12-C1-O11-C3
53	M	503	LMN	CCW-CCS-OCB-CCQ

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Mol	Chain	Res	Type	Atoms
52	M	501	PC7	C12-C11-O3-C3
51	N	501	PTY	C11-C8-O7-C6
50	H	500	UQ9	C12-C11-C9-C10
50	H	500	UQ9	C12-C11-C9-C8
51	M	502	PTY	C31-C30-O4-C1
57	y	302	PGT	O31-C31-O2-C2
54	P	500	NDP	O4D-C1D-N1N-C6N
53	M	503	LMN	OAJ-CBN-CCD-CCO
50	H	500	UQ9	C9-C11-C12-C13
53	M	503	LMN	OBX-CCJ-OBV-CBT
53	M	503	LMN	OAI-CBM-CCC-OBY
57	y	302	PGT	C14-C15-C16-C17
53	M	503	LMN	OAI-CBM-CCC-CCN
53	M	503	LMN	CCL-CCJ-OBV-CBT
57	y	302	PGT	O4P-C4-C5-O5
53	M	503	LMN	OAJ-CBN-CCD-OBZ
53	M	503	LMN	OAL-CBP-CCF-OBX
52	M	501	PC7	C11-C12-C13-C14
52	f	201	PC7	C18-C19-C20-C21
52	f	201	PC7	C31-C32-C33-C34
52	f	201	PC7	C11-C12-C13-C14
59	z	302	T7X	C11-C31-C32-C33
53	M	503	LMN	OBV-CBT-CCM-CBS
51	I	303	PTY	C35-C36-C37-C38
53	M	503	LMN	C2-C1-O1-CBS
53	M	503	LMN	CBJ-CBL-CBR-CCM
53	M	503	LMN	CBE-CBG-CBI-CBK
51	N	501	PTY	C15-C16-C17-C18
52	f	201	PC7	C40-C41-C42-C43
51	M	502	PTY	C22-C23-C24-C25
57	y	302	PGT	C18-C19-C20-C21
51	I	303	PTY	C23-C24-C25-C26
52	f	201	PC7	C13-C14-C15-C16
53	M	503	LMN	CBD-CBF-CBH-CBJ
57	y	302	PGT	C35-C36-C37-C38
51	M	502	PTY	C19-C20-C21-C22
49	F	500	FMN	O2'-C2'-C3'-C4'
53	M	503	LMN	CBC-CBE-CBG-CBI
52	f	201	PC7	C19-C20-C21-C22
53	M	503	LMN	OAL-CBP-CCF-CCQ
53	M	503	LMN	CCF-CCQ-OCB-CCS
51	I	303	PTY	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
57	y	302	PGT	C15-C16-C17-C18
53	M	503	LMN	CAY-CBA-CBC-CBE
51	M	502	PTY	O14-C5-C6-O7
53	M	503	LMN	CCH-CCQ-OCB-CCS
52	M	501	PC7	C32-C33-C34-C35
51	I	303	PTY	C12-C13-C14-C15
53	M	503	LMN	CBG-CBI-CBK-CBQ
56	W	200	8Q1	O33-C32-C34-O35
53	M	503	LMN	CBB-CBD-CBF-CBH
57	y	302	PGT	C17-C18-C19-C20
59	z	302	T7X	C12-C13-C14-C15
51	M	502	PTY	C18-C19-C20-C21
51	I	303	PTY	O14-C5-C6-C1
53	M	503	LMN	O5-C5-C6-O6
51	N	501	PTY	C32-C33-C34-C35
51	I	303	PTY	C30-C31-C32-C33
51	N	501	PTY	C31-C30-O4-C1
51	I	303	PTY	C37-C38-C39-C40
52	M	501	PC7	C35-C36-C37-C38
59	z	302	T7X	C33-C34-C35-C36
53	M	503	LMN	CBL-CBR-CCM-CBQ
56	n	200	8Q1	C13-C14-C15-C16
56	W	200	8Q1	C30-C29-C32-O33
56	W	200	8Q1	C31-C29-C32-O33
49	F	500	FMN	O2'-C2'-C3'-O3'
51	M	502	PTY	O14-C5-C6-C1
51	N	501	PTY	O14-C5-C6-C1
51	N	501	PTY	O4-C1-C6-C5
51	N	501	PTY	O30-C30-O4-C1
51	M	502	PTY	C21-C22-C23-C24
51	N	501	PTY	O14-C5-C6-O7
59	z	302	T7X	O13-C7-C8-O16
52	M	501	PC7	C41-C42-C43-C44
51	I	303	PTY	C11-C12-C13-C14
51	N	501	PTY	O4-C1-C6-O7
52	M	501	PC7	O2-C2-C3-O3
59	z	302	T7X	C15-C16-C17-C18
59	z	302	T7X	C16-C17-C18-C19
59	z	302	T7X	C19-C20-C21-C22
56	W	200	8Q1	O4-C1-C6-C7
51	N	501	PTY	C22-C23-C24-C25
59	z	302	T7X	C41-C42-C43-C44

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Mol	Chain	Res	Type	Atoms
53	M	503	LMN	OBY-CCR-O4-C4
57	y	302	PGT	C13-C14-C15-C16
57	y	302	PGT	O3P-C1-C2-C3
52	f	201	PC7	C36-C37-C38-C39
51	N	501	PTY	C1-C6-O7-C8
59	z	302	T7X	C9-C8-O16-C10
57	y	302	PGT	C16-C17-C18-C19
52	f	201	PC7	O3P-C1-C2-O2
52	f	201	PC7	C1-C2-C3-O3
52	f	201	PC7	O4P-C4-C5-N
51	I	303	PTY	C8-C11-C12-C13
52	f	201	PC7	O3P-C1-C2-C3
59	z	302	T7X	O13-C7-C8-C9
52	f	201	PC7	C33-C34-C35-C36
56	W	200	8Q1	C42-C43-S44-C1
52	M	501	PC7	C23-C24-C25-C26
57	y	302	PGT	C19-C20-C21-C22
57	y	302	PGT	O3P-C1-C2-O2
52	f	201	PC7	C42-C43-C44-C45
53	M	503	LMN	CCM-CBT-OBV-CCJ
51	M	502	PTY	O4-C1-C6-O7
57	y	302	PGT	O2-C2-C3-O3
51	N	501	PTY	C33-C34-C35-C36
56	n	200	8Q1	C43-C42-N41-C39
57	y	302	PGT	C1-C2-C3-O3
51	I	303	PTY	C18-C19-C20-C21
52	M	501	PC7	C19-C20-C21-C22
51	M	502	PTY	N1-C2-C3-O11
51	N	501	PTY	C3-O11-P1-O12
51	N	501	PTY	C5-O14-P1-O12
54	P	500	NDP	C5B-O5B-PA-O1A
54	P	500	NDP	C5D-O5D-PN-O1N
56	W	200	8Q1	C28-C29-C32-O33
59	z	302	T7X	C7-O13-P1-O1
59	z	302	T7X	C7-O13-P1-O11
53	M	503	LMN	CAX-CAZ-CBB-CBD
51	N	501	PTY	C14-C15-C16-C17
52	M	501	PC7	C18-C19-C20-C21
49	F	500	FMN	C5'-O5'-P-O1P
53	M	503	LMN	CCV-CCR-O4-C4
51	I	303	PTY	C15-C16-C17-C18
57	y	302	PGT	C12-C11-O3-C3

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Mol	Chain	Res	Type	Atoms
51	N	501	PTY	C30-C31-C32-C33
52	f	201	PC7	O3-C11-C12-C13
51	I	303	PTY	C13-C14-C15-C16
52	M	501	PC7	C36-C37-C38-C39
52	M	501	PC7	C38-C39-C40-C41
57	y	302	PGT	C33-C34-C35-C36
57	y	302	PGT	O11-C11-O3-C3
53	M	503	LMN	CBL-CBR-CCM-CBT
51	M	502	PTY	C37-C38-C39-C40
56	W	200	8Q1	C7-C8-C9-C10
52	M	501	PC7	O3P-C1-C2-O2
52	f	201	PC7	C16-C17-C18-C19
50	H	500	UQ9	C24-C26-C27-C28
59	z	302	T7X	C39-C40-C41-C42
51	N	501	PTY	C11-C12-C13-C14
52	f	201	PC7	C35-C36-C37-C38
57	y	302	PGT	C5-C4-O4P-P
59	z	302	T7X	C35-C36-C37-C38
56	n	200	8Q1	C9-C10-C11-C12
59	z	302	T7X	C43-C44-C45-C46
59	z	302	T7X	C13-C14-C15-C16
59	z	302	T7X	C31-C32-C33-C34
56	W	200	8Q1	C1-C6-C7-C8
56	W	200	8Q1	C12-C13-C14-C15
51	M	502	PTY	C8-C11-C12-C13
59	z	302	T7X	O18-C11-C31-C32
57	y	302	PGT	O3-C11-C12-C13
56	W	200	8Q1	C28-O27-P24-O3
52	M	501	PC7	C31-C32-C33-C34
53	M	503	LMN	CBL-CBR-CCM-CBS
51	N	501	PTY	C25-C26-C27-C28
51	M	502	PTY	O4-C1-C6-C5
56	W	200	8Q1	C30-C29-C32-C34
51	M	502	PTY	C33-C34-C35-C36
51	M	502	PTY	C39-C40-C41-C42
51	M	502	PTY	C34-C35-C36-C37
52	f	201	PC7	C32-C33-C34-C35
51	N	501	PTY	O4-C30-C31-C32
51	I	303	PTY	C38-C39-C40-C41
51	M	502	PTY	C31-C32-C33-C34
51	I	303	PTY	C40-C41-C42-C43
52	M	501	PC7	C1-C2-C3-O3

Continued on next page...

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Mol	Chain	Res	Type	Atoms
51	M	502	PTY	C12-C11-C8-O7
57	y	302	PGT	O2-C31-C32-C33
58	z	301	PSF	O11-C1-C13-C14
56	n	200	8Q1	C28-C29-C32-C34
59	z	302	T7X	O16-C10-C12-C13
51	N	501	PTY	C36-C37-C38-C39
51	N	501	PTY	O30-C30-C31-C32
51	M	502	PTY	C12-C11-C8-O10
51	I	303	PTY	C33-C34-C35-C36
52	f	201	PC7	C15-C16-C17-C18
51	M	502	PTY	C11-C12-C13-C14
57	y	302	PGT	O31-C31-C32-C33
58	z	301	PSF	O12-C1-C13-C14
59	z	302	T7X	O17-C10-C12-C13
52	M	501	PC7	O3P-C1-C2-C3

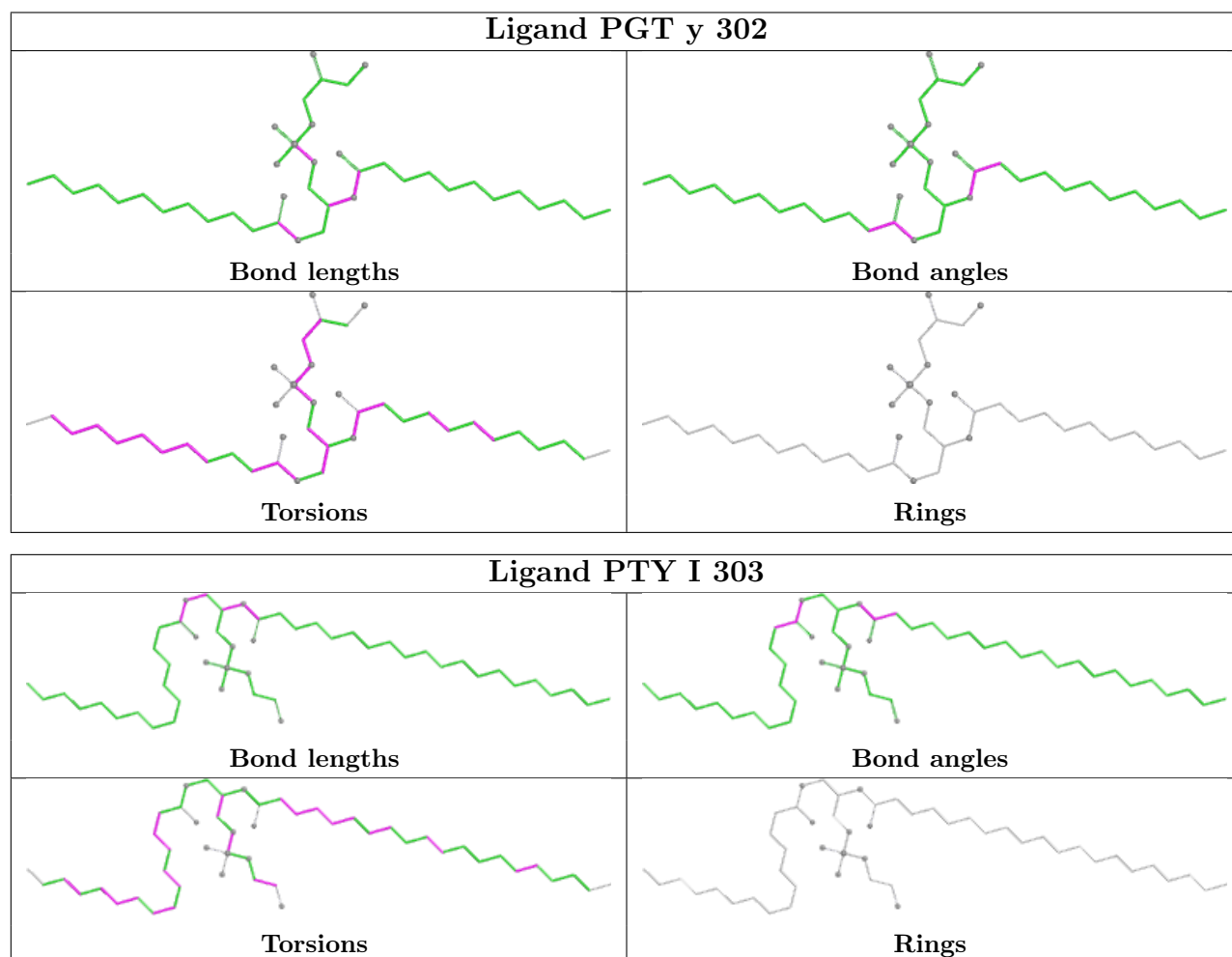
There are no ring outliers.

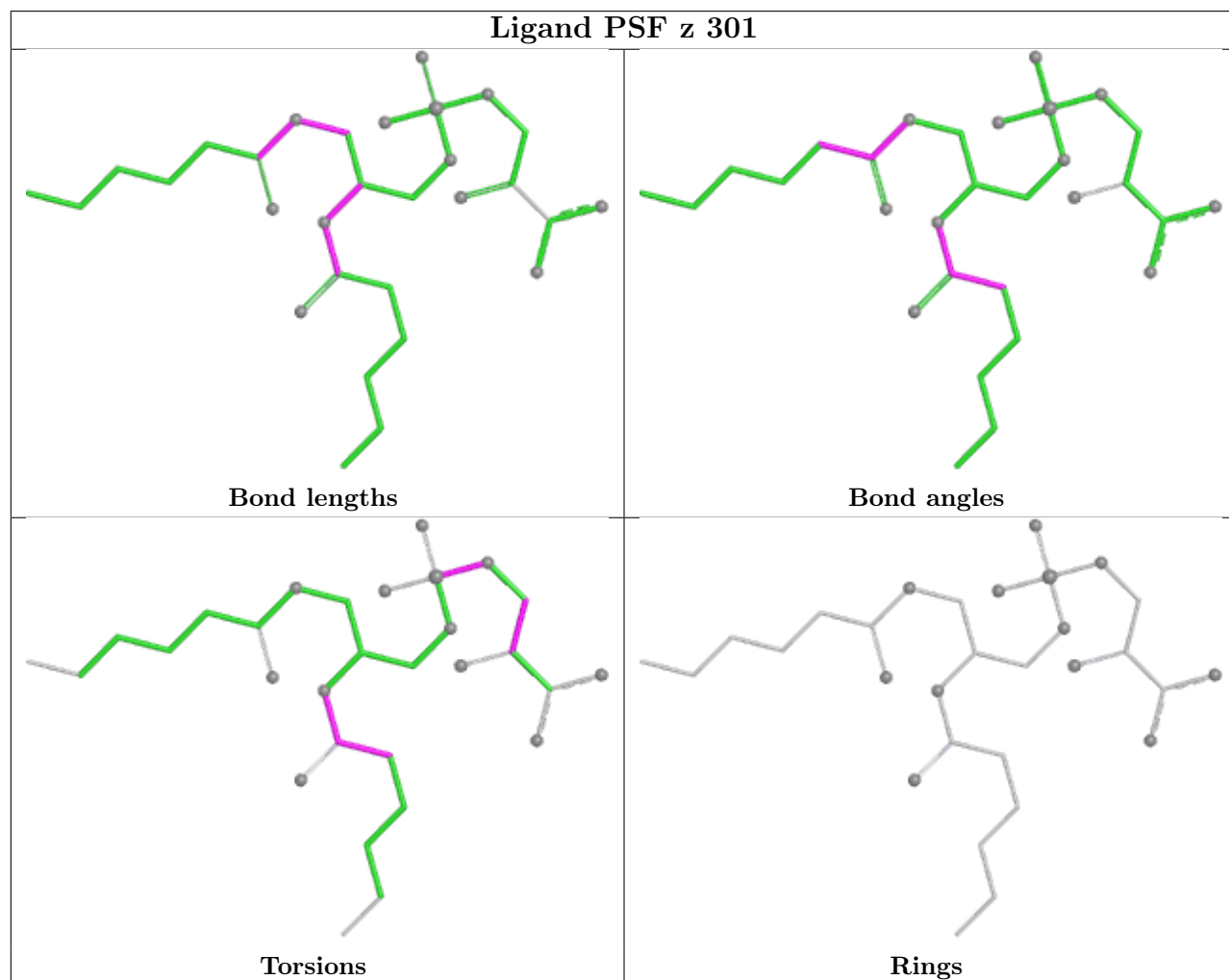
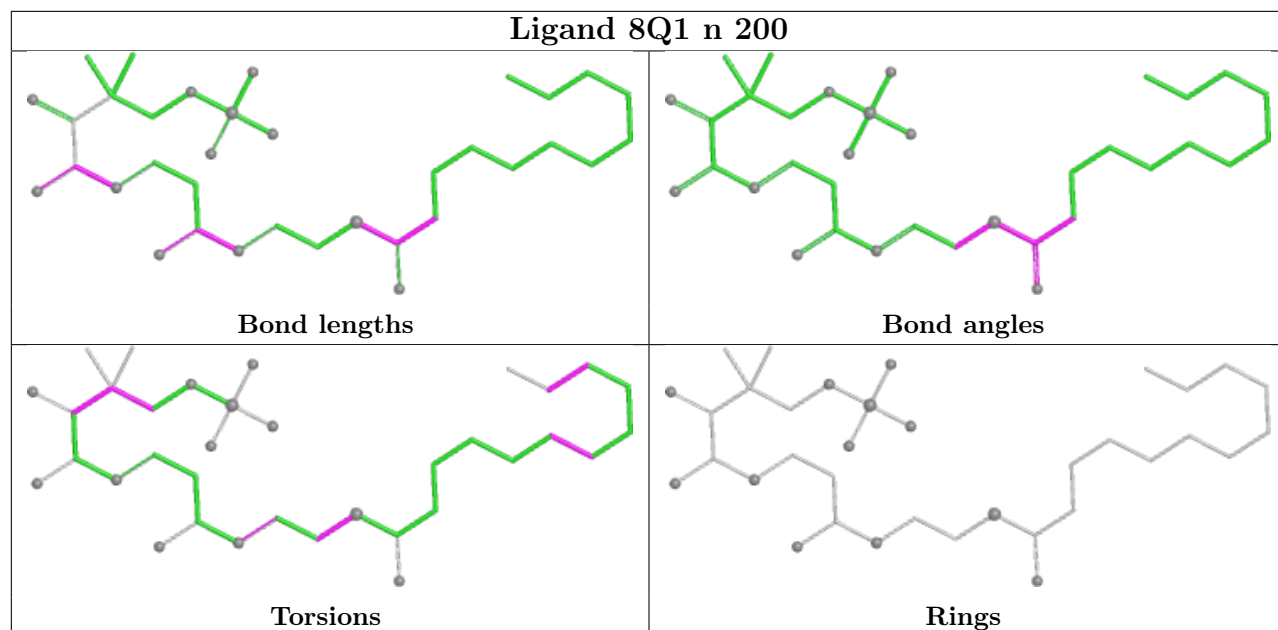
15 monomers are involved in 45 short contacts:

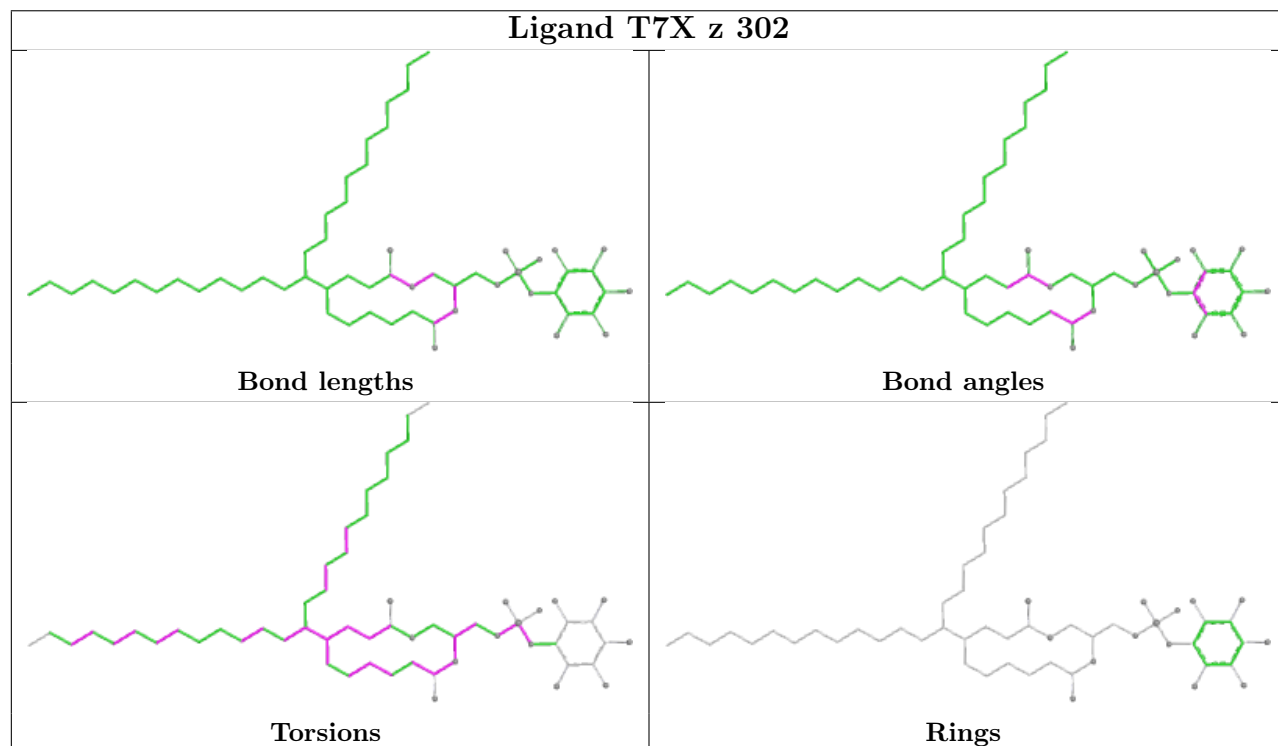
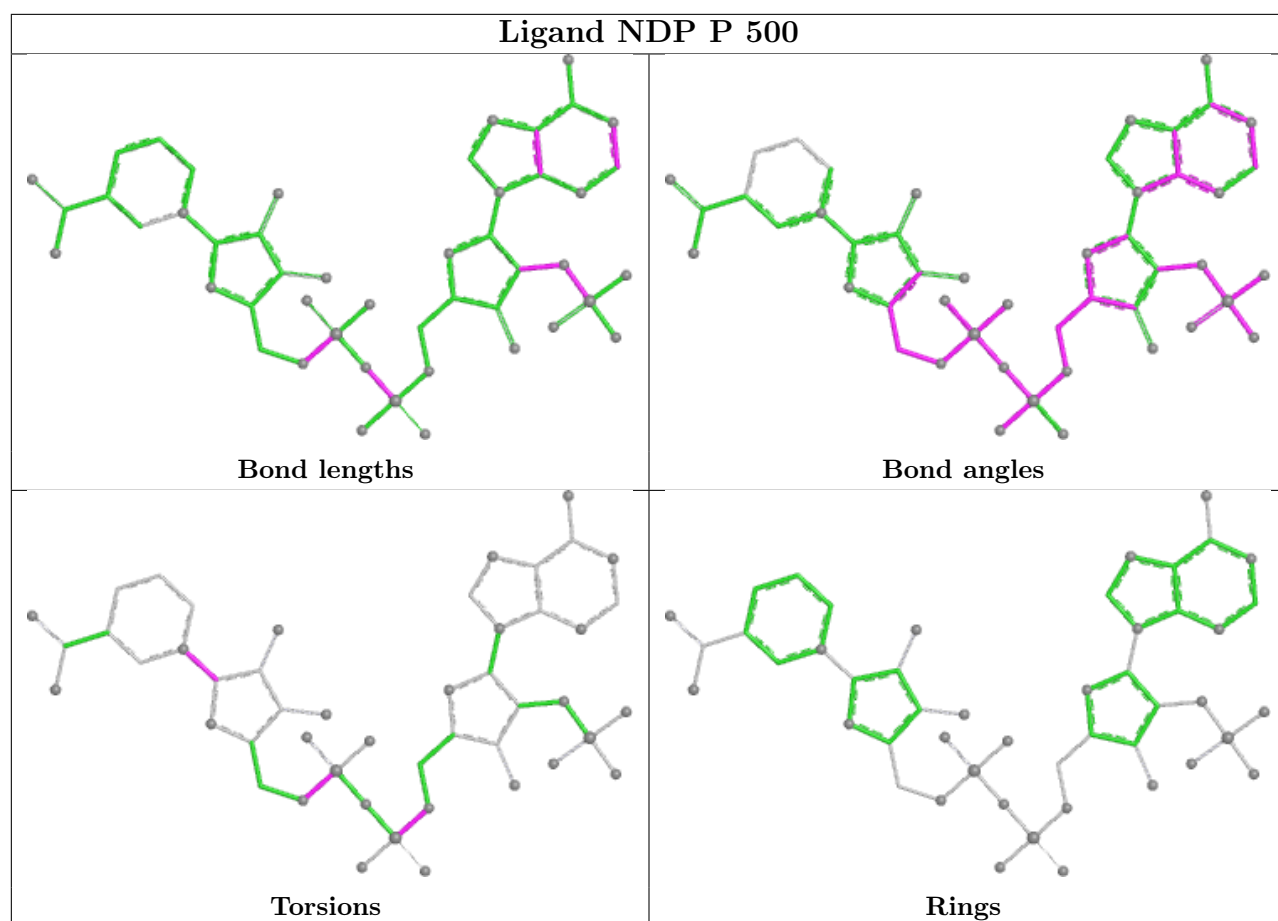
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	I	301	SF4	1	0
57	y	302	PGT	1	0
51	I	303	PTY	7	0
48	E	500	FES	2	0
58	z	301	PSF	1	0
50	H	500	UQ9	5	0
52	f	201	PC7	3	0
52	M	501	PC7	6	0
51	N	501	PTY	4	0
49	F	500	FMN	2	0
47	B	500	SF4	2	0
51	M	502	PTY	3	0
53	M	503	LMN	6	0
56	W	200	8Q1	1	0
47	F	501	SF4	2	0

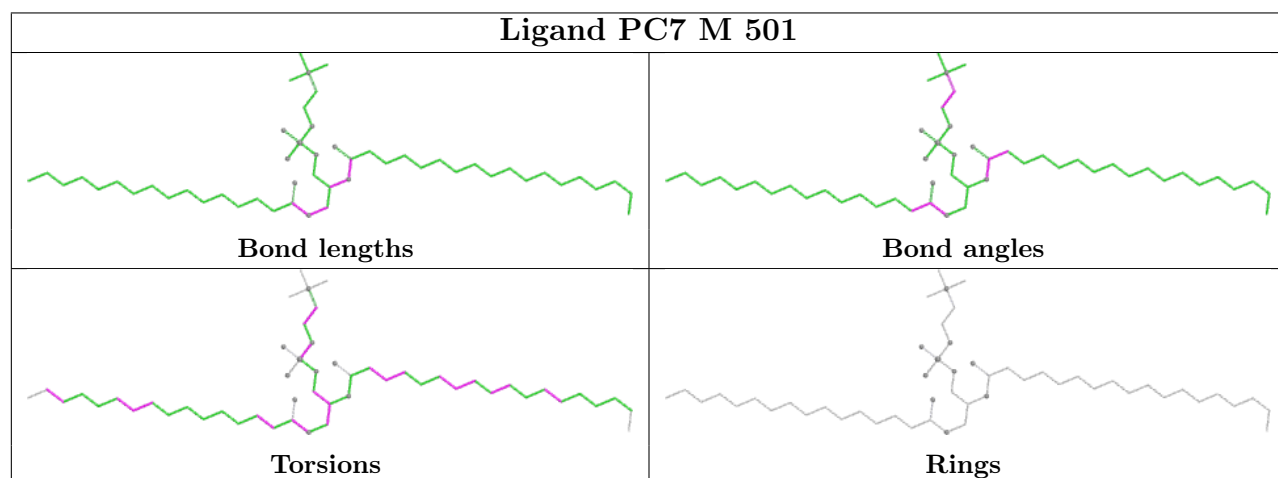
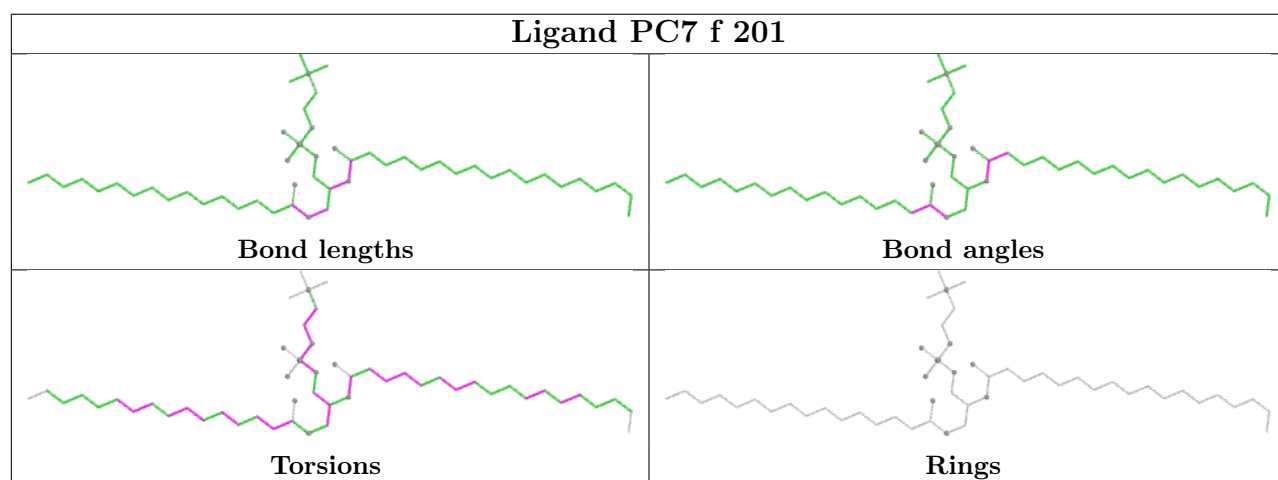
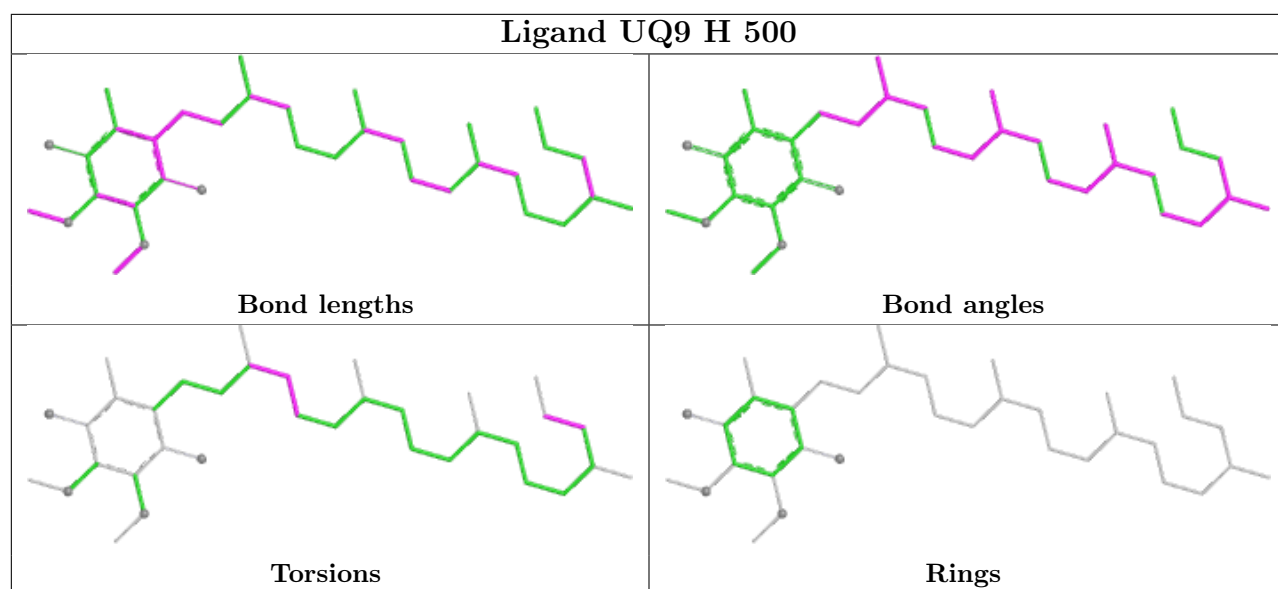
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

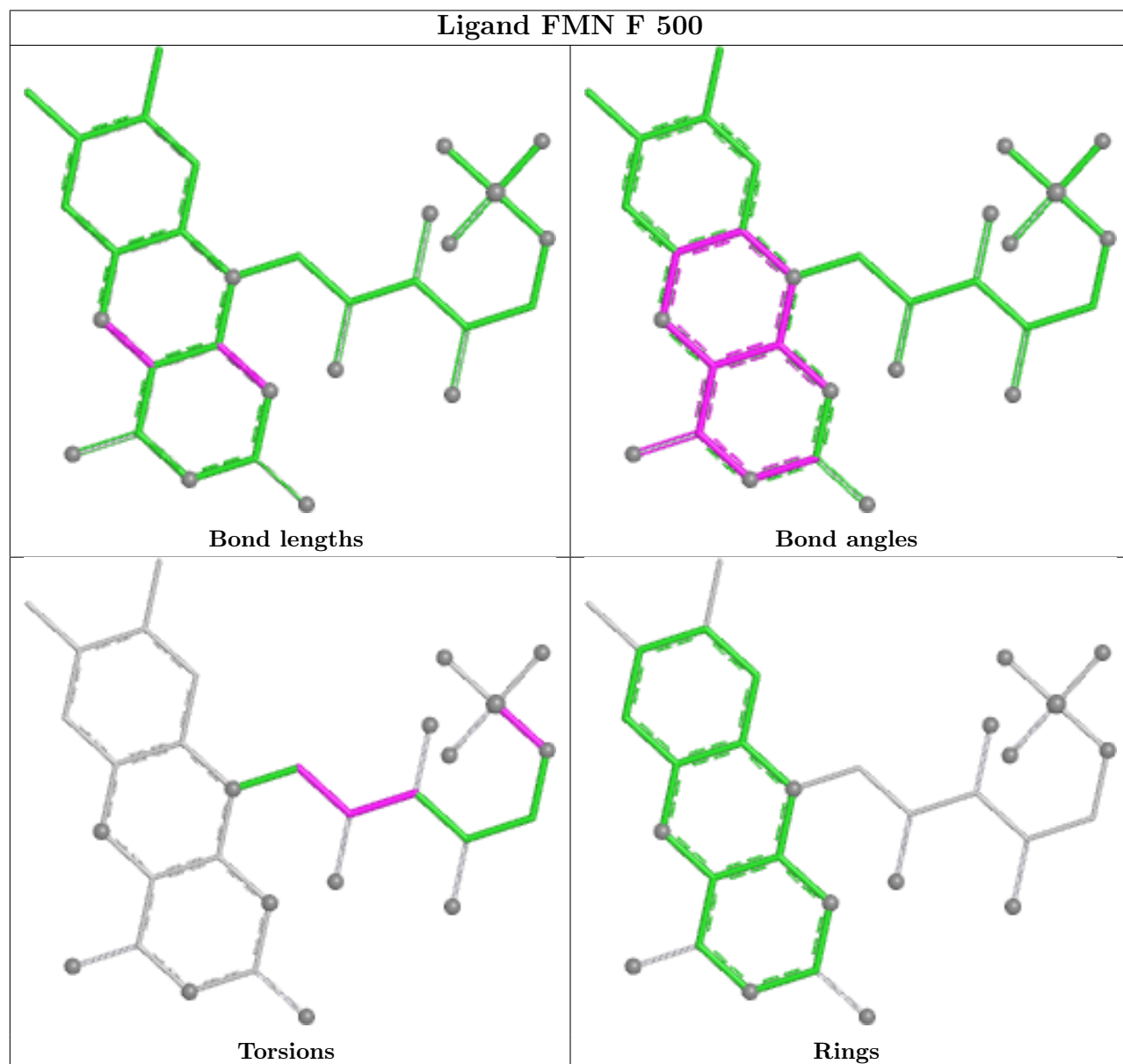
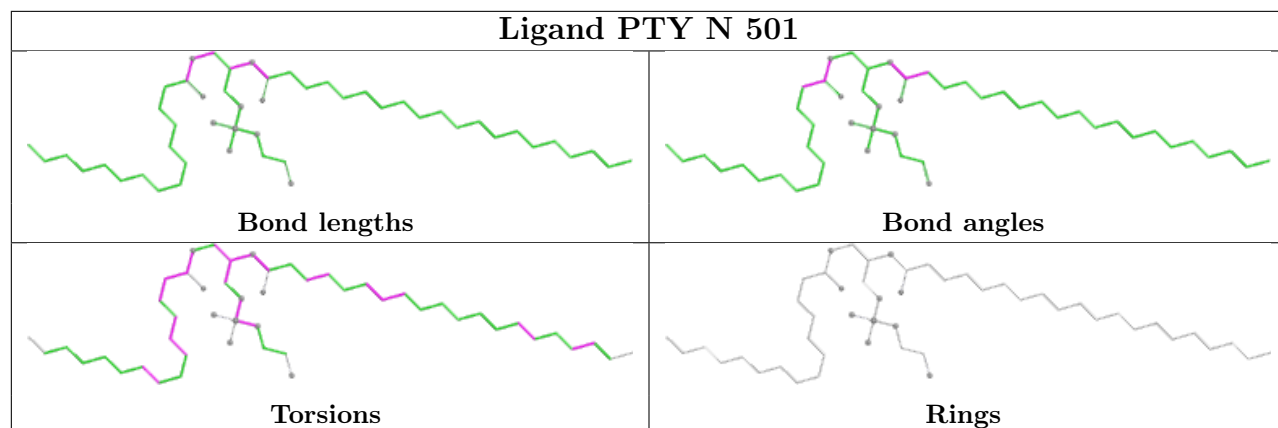
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified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

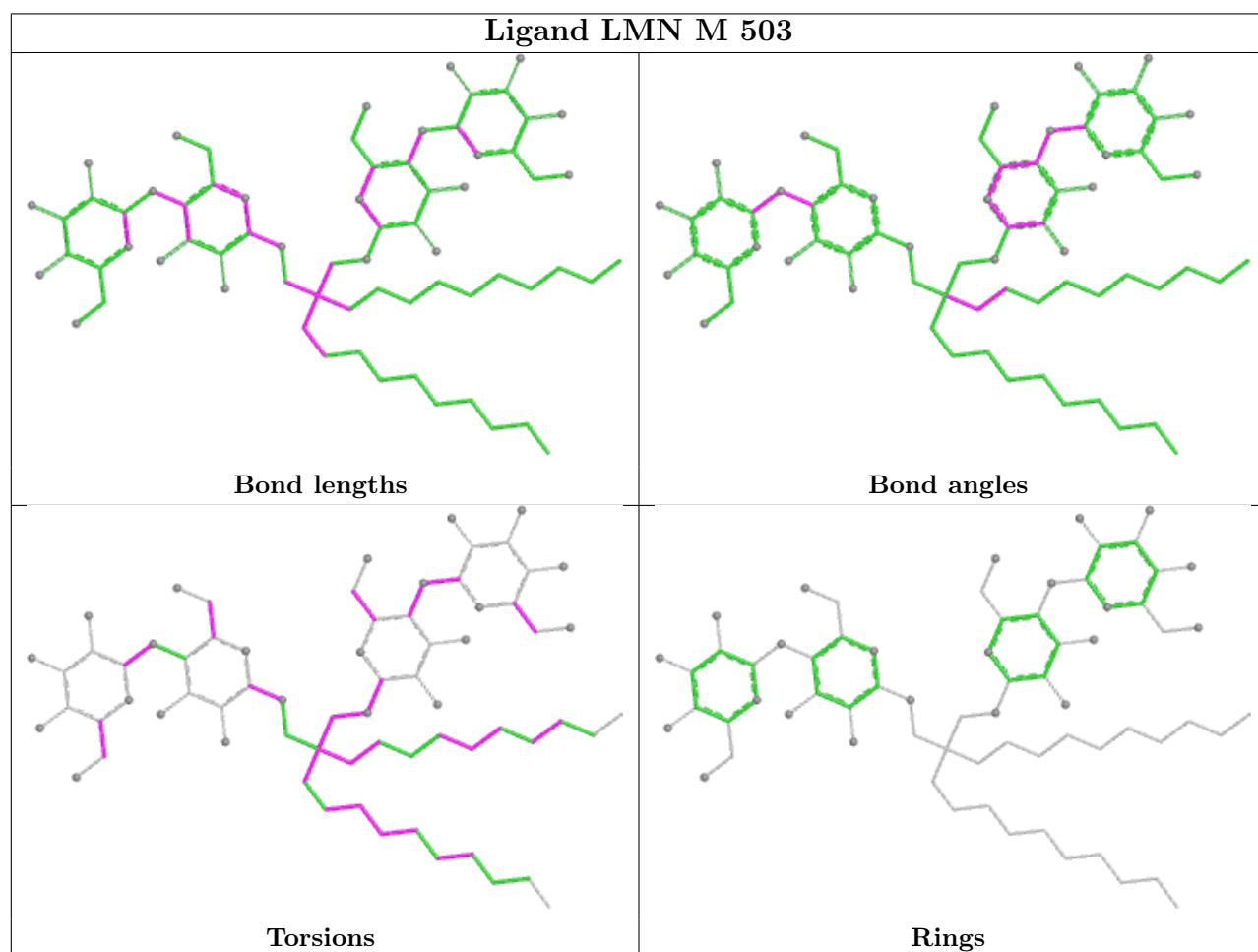
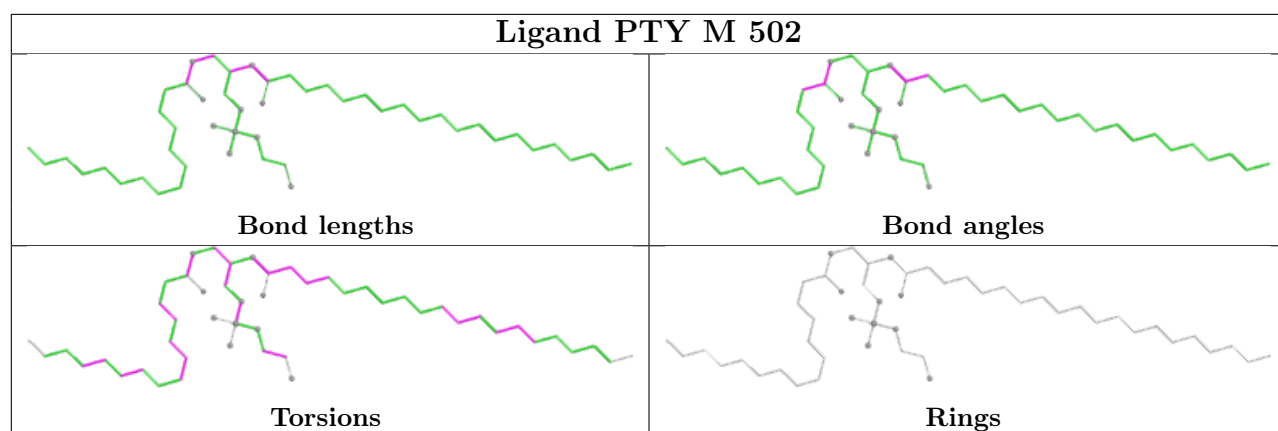


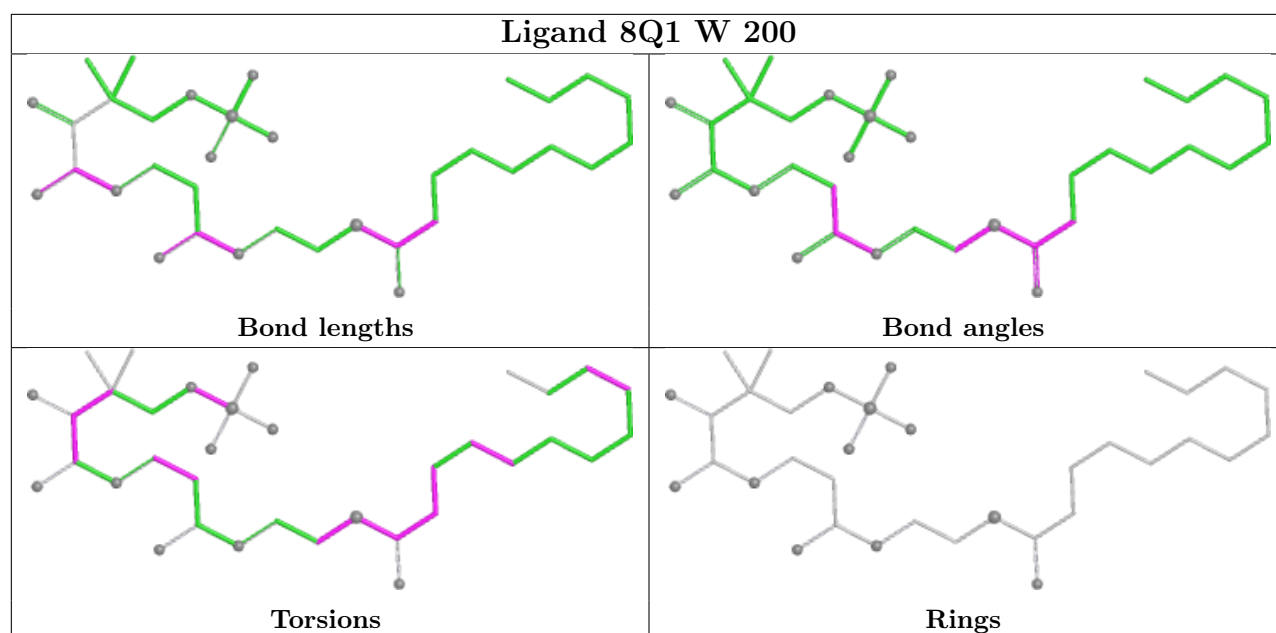












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

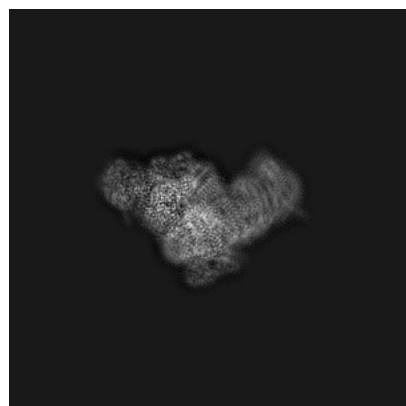
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11875. These allow visual inspection of the internal detail of the map and identification of artifacts.

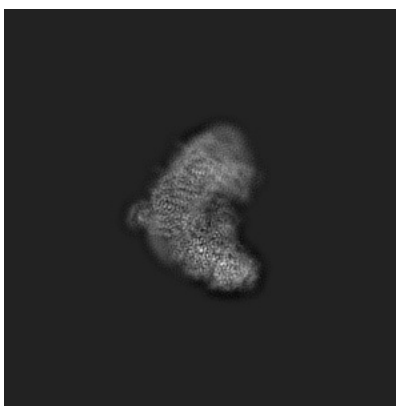
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

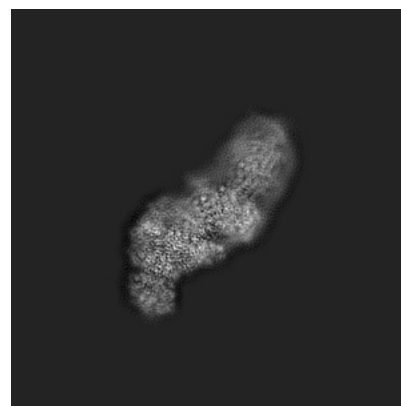
6.1.1 Primary map



X

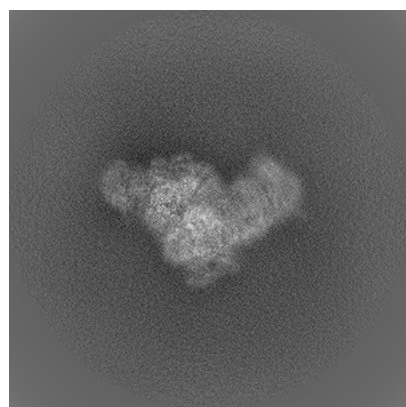


Y

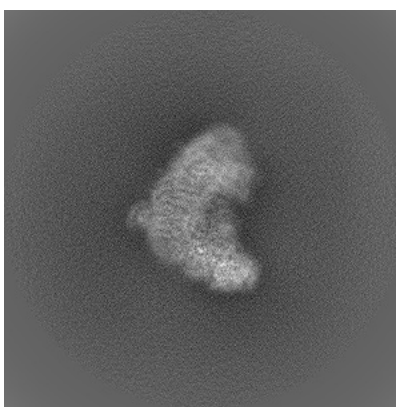


Z

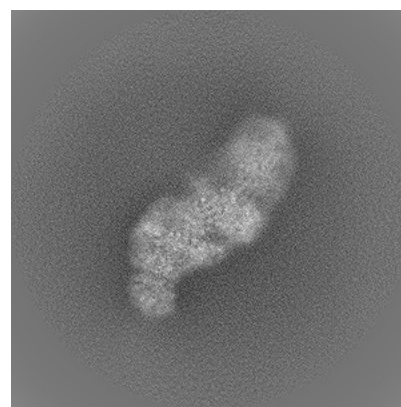
6.1.2 Raw map



X



Y

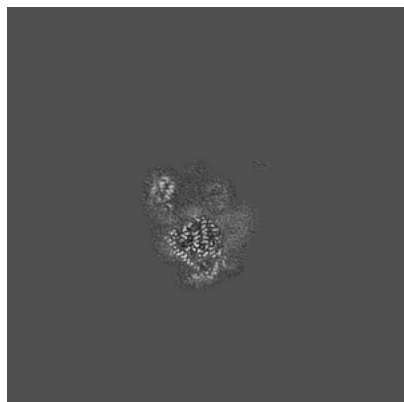


Z

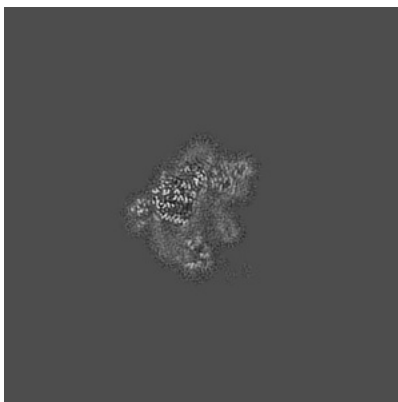
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 300

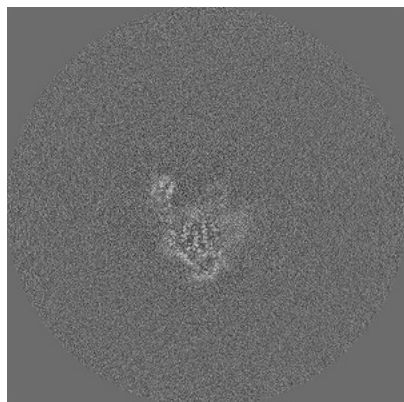


Y Index: 300

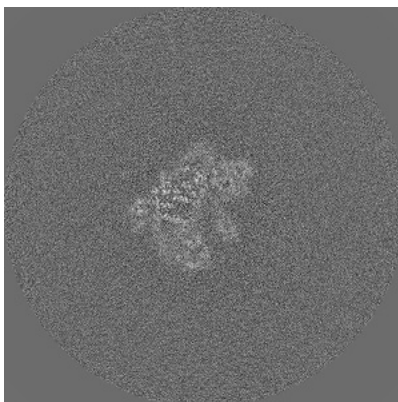


Z Index: 300

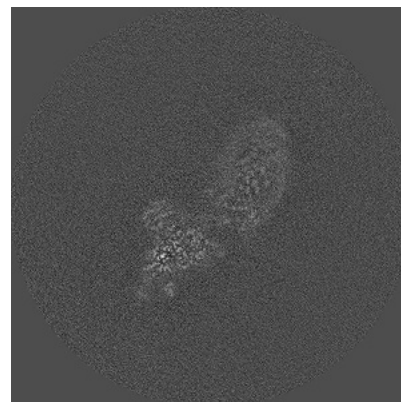
6.2.2 Raw map



X Index: 300



Y Index: 300

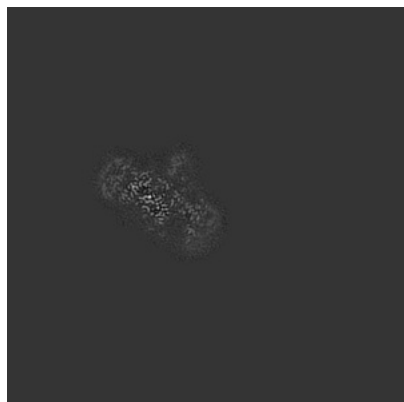


Z Index: 300

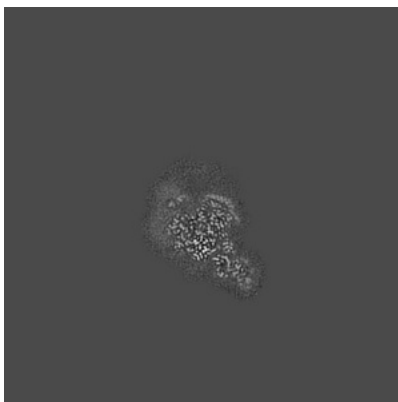
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 224

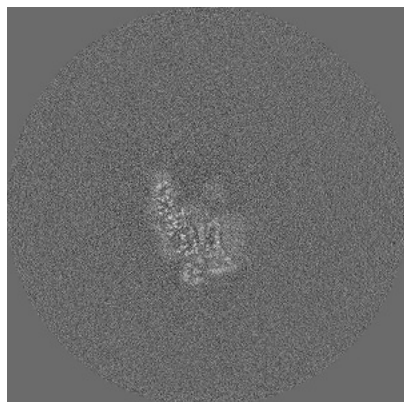


Y Index: 240

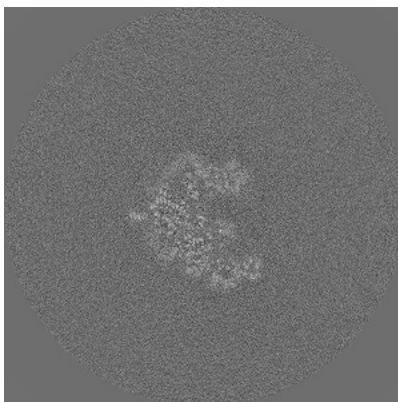


Z Index: 299

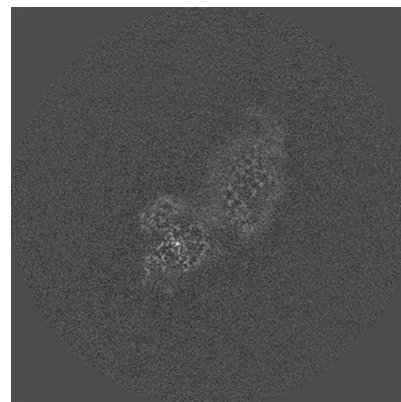
6.3.2 Raw map



X Index: 287



Y Index: 268

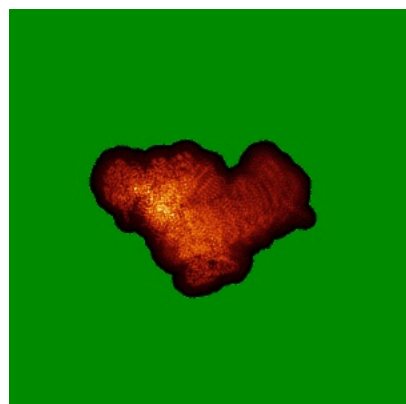


Z Index: 291

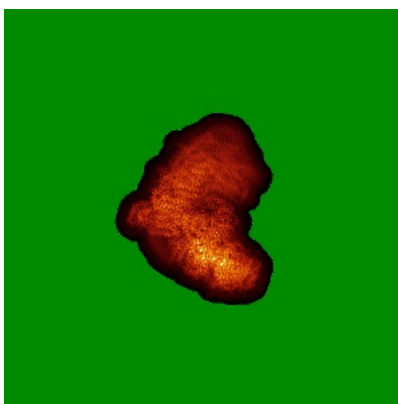
The images above show the largest variance slices of the map in three orthogonal directions.

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

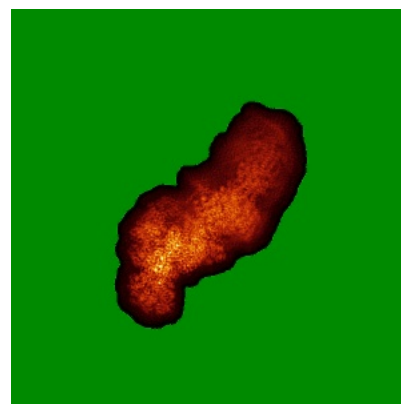
6.4.1 Primary map



X

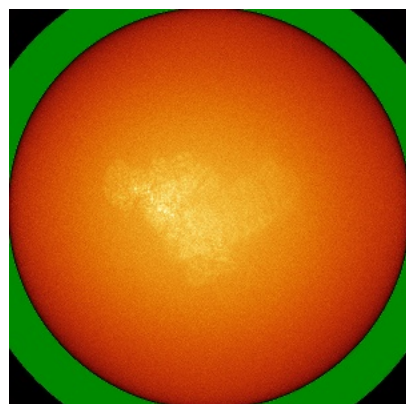


Y

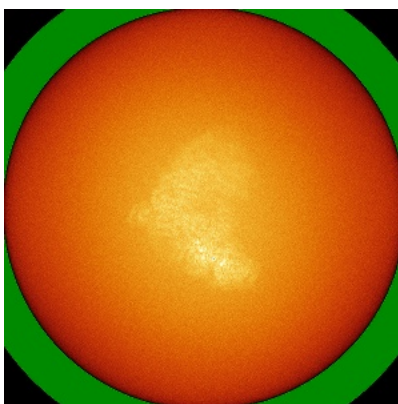


Z

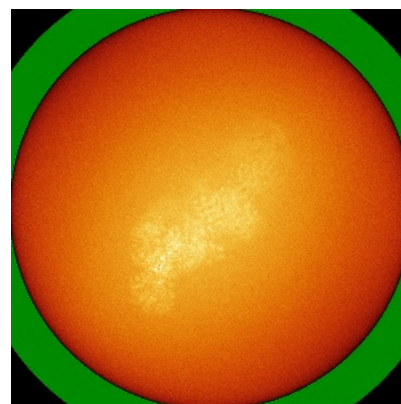
6.4.2 Raw map



X



Y

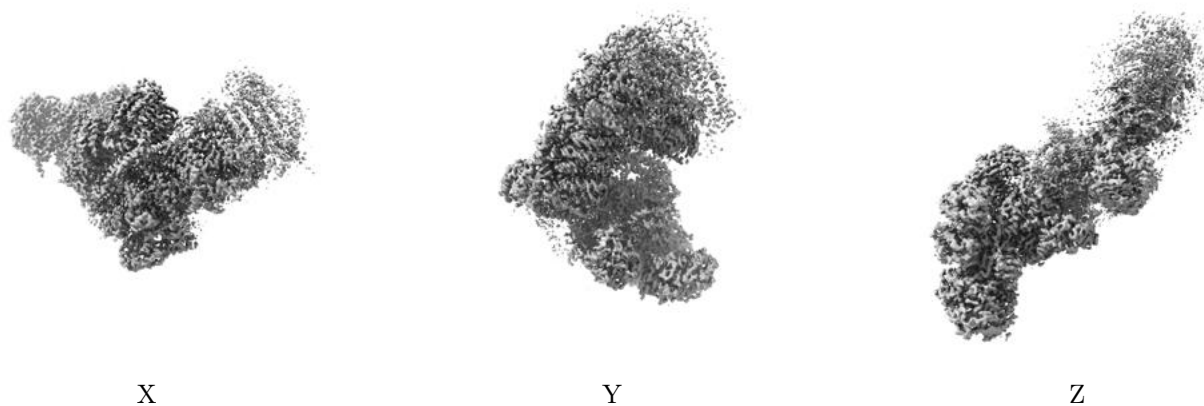


Z

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.

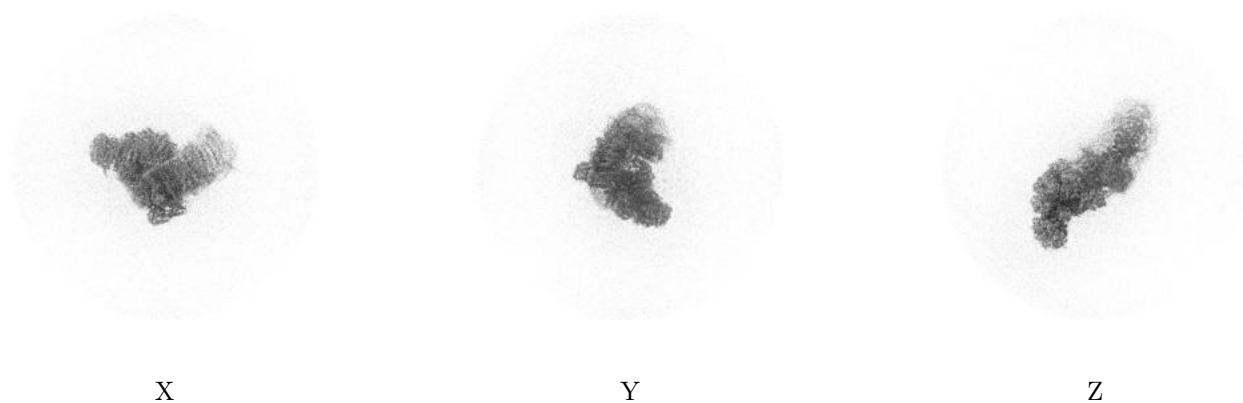
6.5 Orthogonal surface views [i](#)

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.

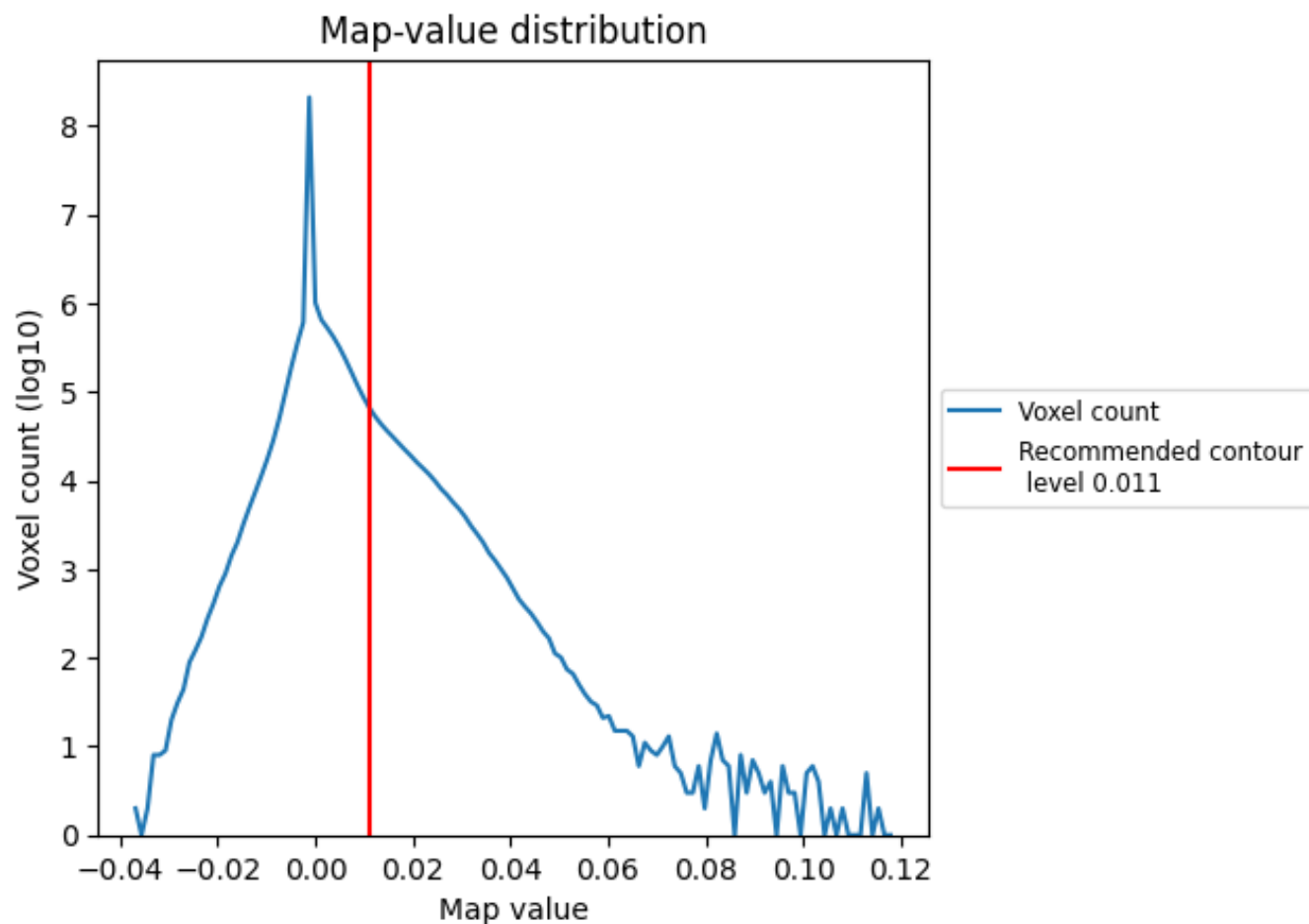
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

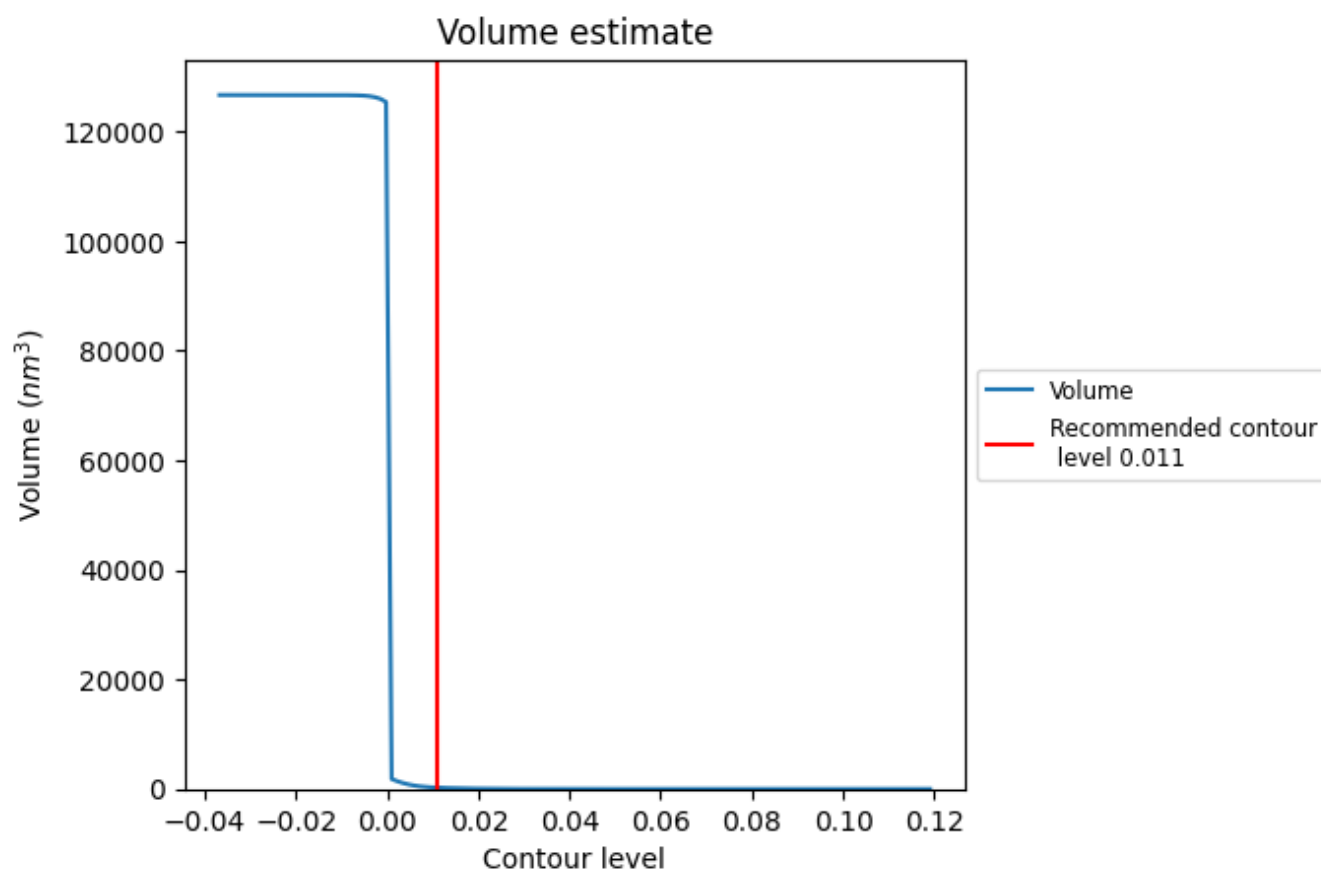
This section contains the results of statistical analysis of the map.

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.

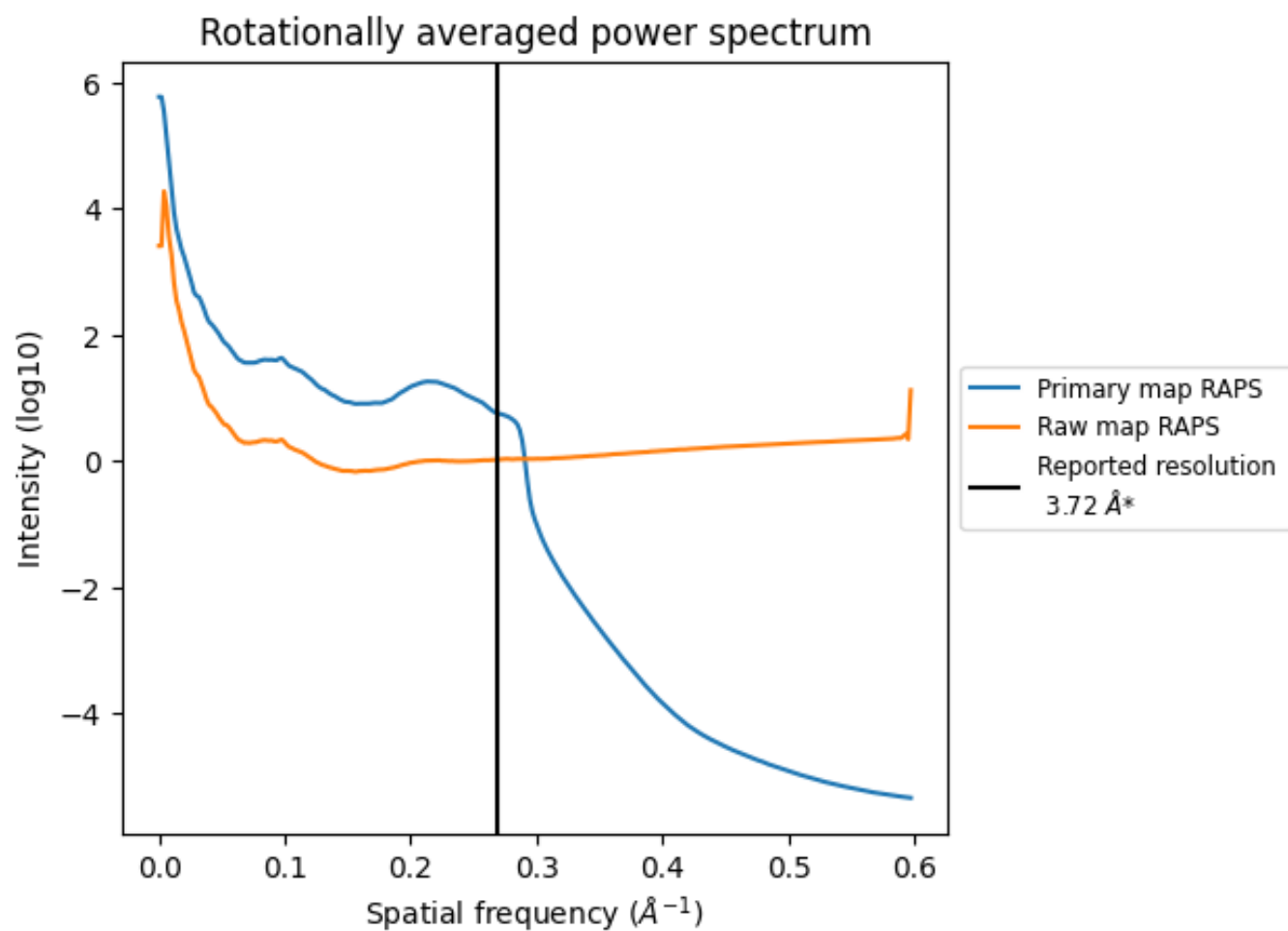
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm^3 ; this corresponds to an approximate mass of 211 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 ⓘ

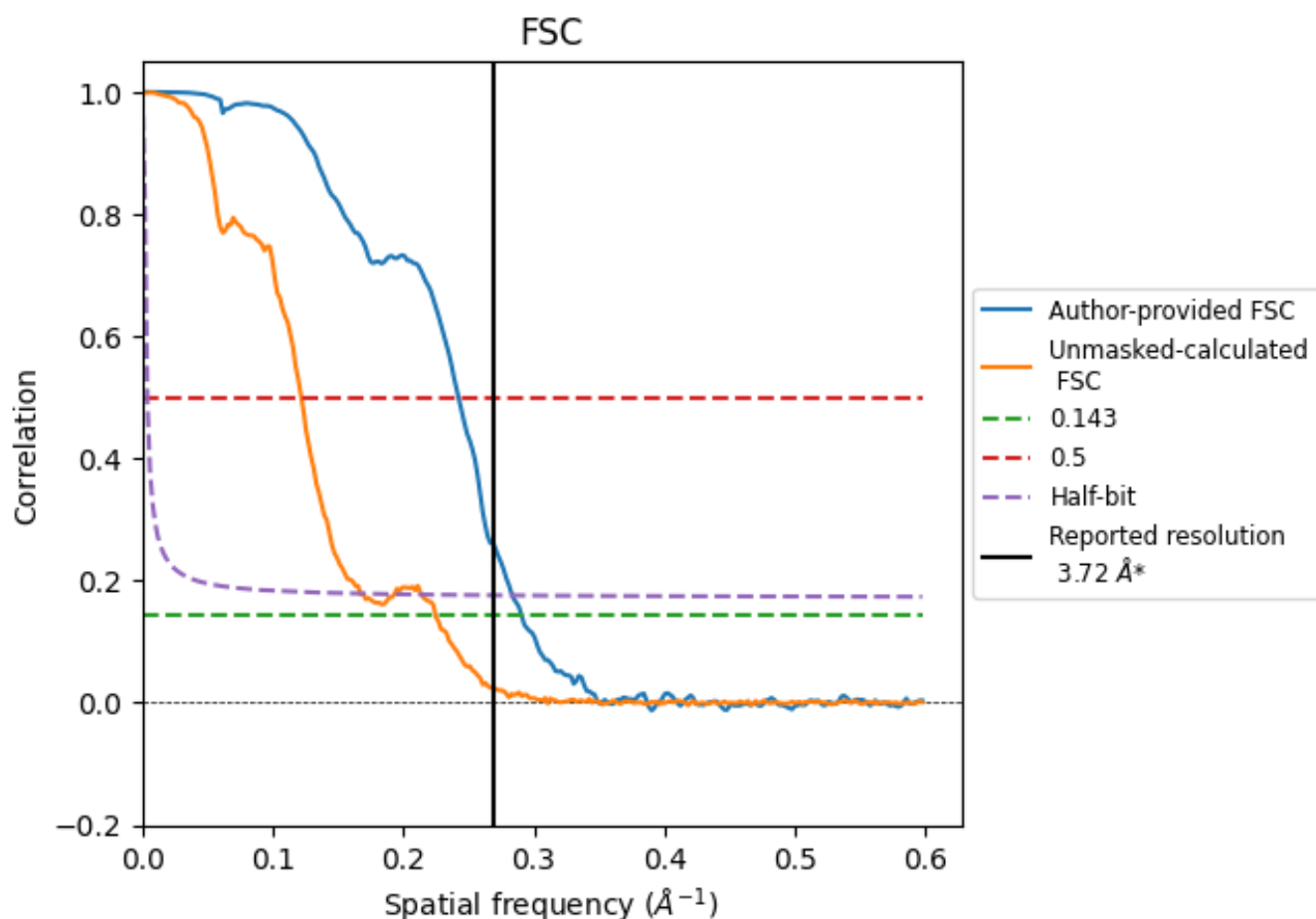


*Reported resolution corresponds to spatial frequency of 0.269 $\text{\AA}^{-1}$

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 0.269 Å⁻¹

8.2 Resolution estimates [i](#)

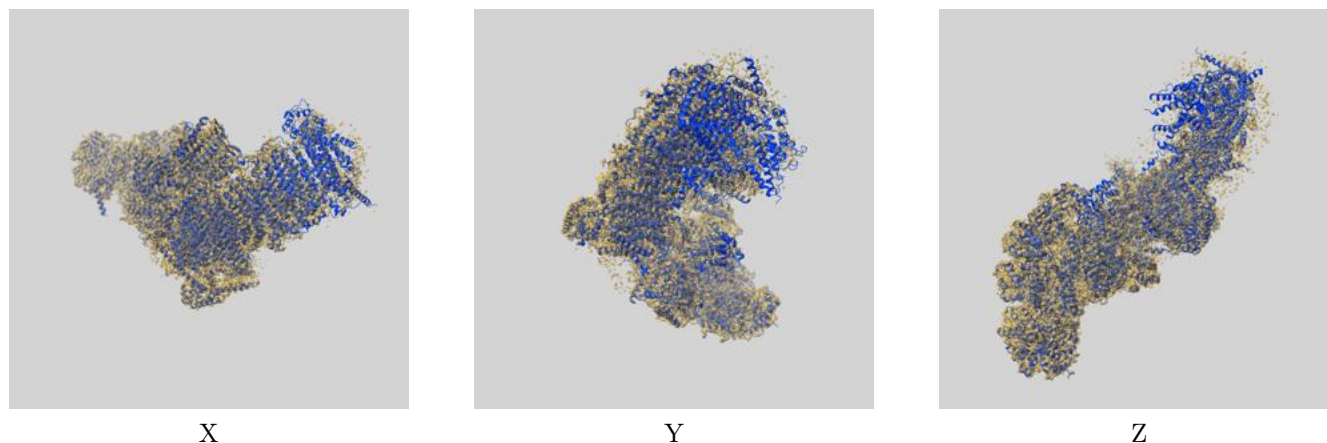
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.72	-	-
Author-provided FSC curve	3.44	4.13	3.53
Unmasked-calculated*	4.45	8.20	5.98

*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 4.45 differs from the reported value 3.72 by more than 10 %

9 Map-model fit [i](#)

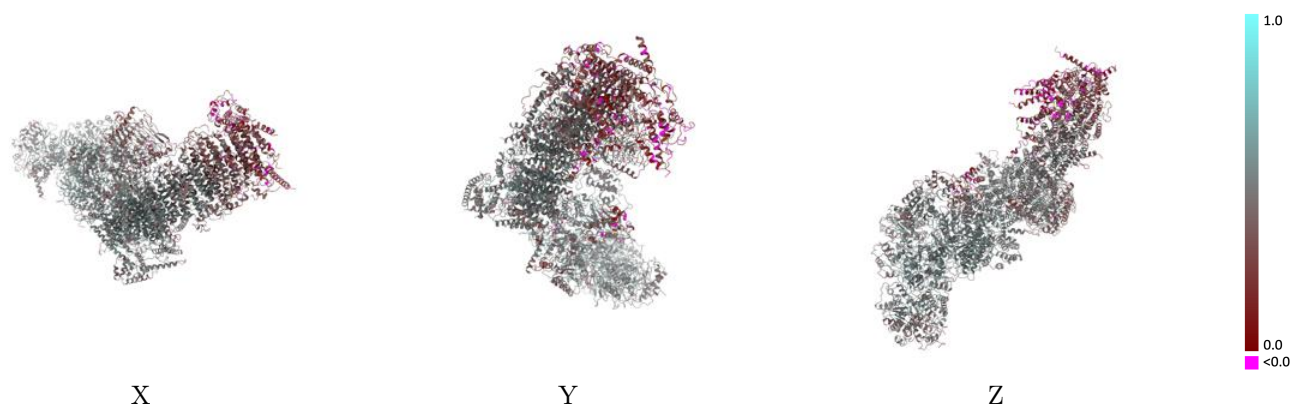
This section contains information regarding the fit between EMDB map EMD-11875 and PDB model 7AR7. Per-residue inclusion information can be found in section [3](#) on page [20](#).

9.1 Map-model overlay [i](#)



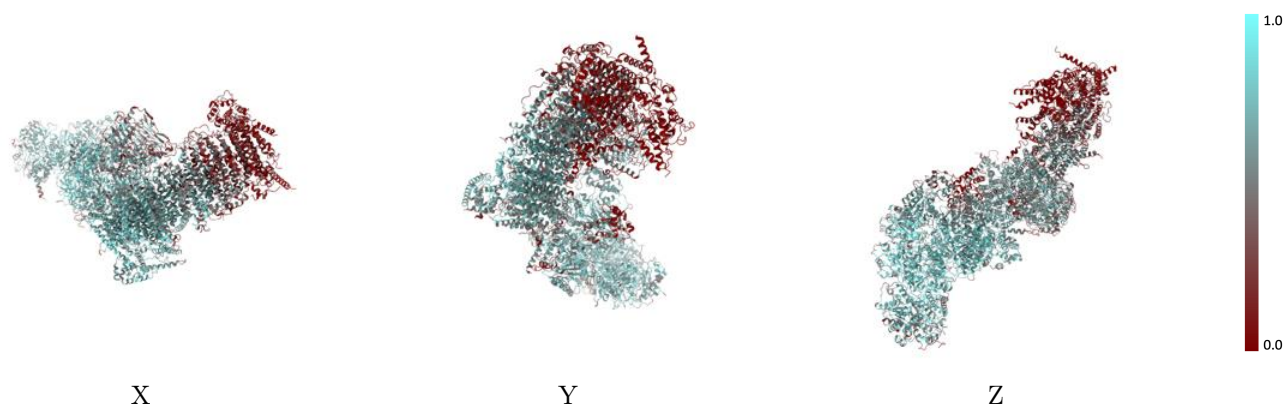
The images above show the 3D surface view of the map at the recommended contour level 0.011 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



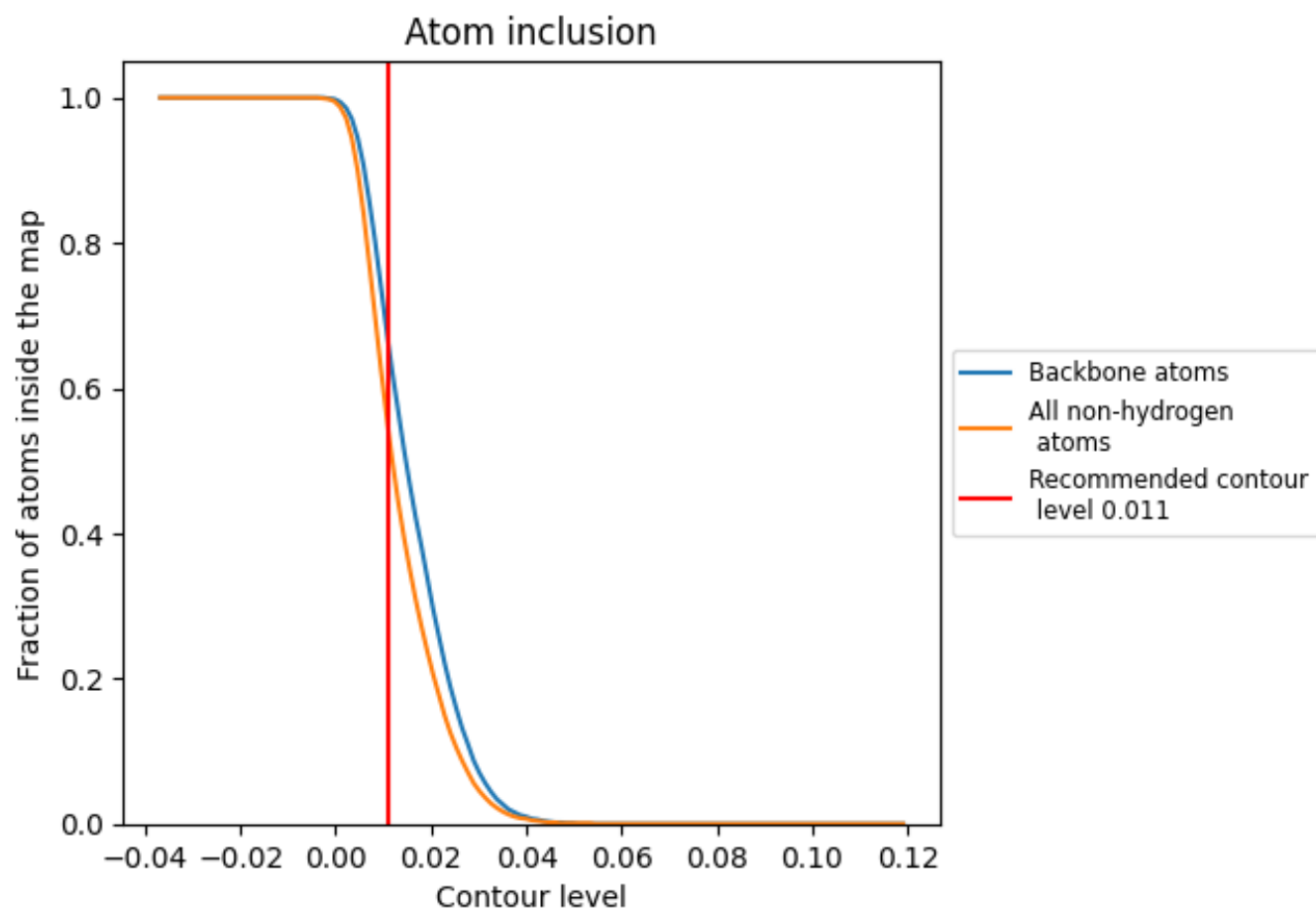
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 55% 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	 0.5450	 0.4380
A	 0.6350	 0.4980
B	 0.7590	 0.5290
C	 0.7650	 0.5350
D	 0.7750	 0.5320
E	 0.6190	 0.4410
F	 0.6440	 0.4680
G	 0.7300	 0.5110
H	 0.6610	 0.4930
I	 0.7860	 0.5380
J	 0.6460	 0.5010
K	 0.5980	 0.4920
L	 0.1770	 0.2760
M	 0.5100	 0.4500
N	 0.6410	 0.4990
P	 0.5620	 0.4460
Q	 0.6910	 0.5240
R	 0.7120	 0.5120
S	 0.6470	 0.4530
T	 0.0170	 0.1250
U	 0.0770	 0.2080
V	 0.6600	 0.4710
W	 0.4340	 0.3980
X	 0.6360	 0.4590
Z	 0.6590	 0.4850
a	 0.6560	 0.4840
b	 0.6320	 0.4870
c	 0.2450	 0.3200
d	 0.6380	 0.4850
e	 0.7020	 0.4760
f	 0.6750	 0.5020
g	 0.3900	 0.3800
i	 0.5980	 0.4490
j	 0.1090	 0.2500
k	 0.0640	 0.2160



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Chain	Atom inclusion	Q-score
l	 0.0770	 0.2590
m	 0.1760	 0.2650
n	 0.0490	 0.1900
o	 0.0980	 0.2180
p	 0.3820	 0.3740
q	 0.4030	 0.4550
r	 0.3420	 0.4450
u	 0.5130	 0.3280
v	 0.5750	 0.4650
x	 0.5150	 0.4390
y	 0.4450	 0.3960
z	 0.4980	 0.4200