



Full wwPDB EM Validation Report ⓘ

Mar 15, 2026 – 07:53 AM UTC

PDB ID : 8BA0 / pdb_00008ba0
EMDB ID : EMD-15937
Title : Drosophila melanogaster complex I in the Twisted state (Dm2)
Authors : Agip, A.N.A.; Chung, I.; Sanchez-Martinez, A.; Whitworth, A.J.; Hirst, J.
Deposited on : 2022-10-10
Resolution : 3.68 Å(reported)
Based on initial model : 6ZR2

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

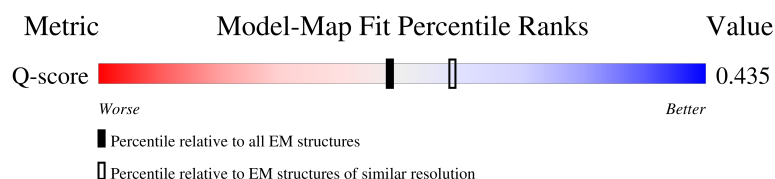
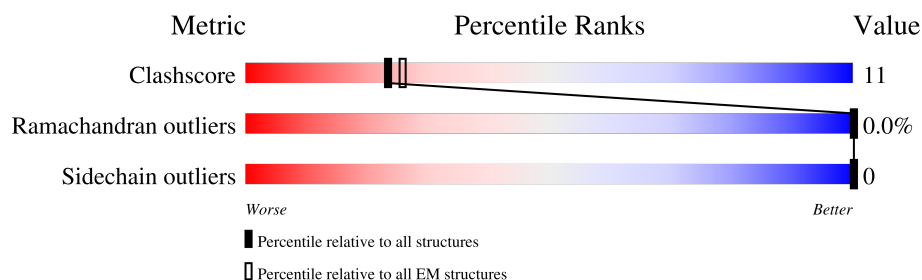
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.68 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	11376 (3.18 - 4.18)

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	117	19% 65% 35%
2	B	182	7% 72% 27%
3	C	209	9% 78% 22%
4	D	428	14% 72% 27%

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Mol	Chain	Length	Quality of chain
5	E	214	
6	F	439	
7	G	731	
8	H	315	
9	I	186	
10	J	167	
11	K	93	
12	L	577	
13	M	446	
14	N	341	
15	O	368	
16	P	377	
17	Q	130	
18	R	89	
19	T	152	
19	U	152	
20	V	118	
21	W	114	
22	X	174	
23	Y	167	
24	Z	146	
25	a	73	
26	b	66	
27	d	115	
28	e	100	

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Mol	Chain	Length	Quality of chain
29	f	56	
30	g	106	
31	h	145	
32	i	161	
33	j	59	
34	k	84	
35	l	144	
36	m	108	
37	n	134	
38	o	112	
39	p	151	
40	q	135	
41	r	103	
42	s	62	

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
43	SF4	F	502	-	-	X	-
43	SF4	G	801	-	-	X	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 65912 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	117	Total	C	N	O	S	0	0
			956	652	141	156	7		

- Molecule 2 is a protein called LD31474p.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	182	Total	C	N	O	S	0	0
			1435	920	251	250	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	209	Total	C	N	O	S	0	0
			1726	1103	303	315	5		

- Molecule 4 is a protein called Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	428	Total	C	N	O	S	0	0
			3424	2196	577	628	23		

- Molecule 5 is a protein called NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1679	1062	285	320	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	439	Total	C	N	O	S	0	0
			3367	2129	599	613	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	677	Total	C	N	O	S	0	0
			5146	3225	912	980	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	315	Total	C	N	O	S	0	0
			2571	1764	367	418	22		

- Molecule 9 is a protein called NADH dehydrogenase (ubiquinone) 23 kDa subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	186	Total	C	N	O	S	0	0
			1485	935	251	287	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	167	Total	C	N	O	S	0	0
			1351	917	192	227	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	93	Total	C	N	O	S	0	0
			771	526	110	123	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	577	Total	C	N	O	S	0	0
			4606	3092	680	774	60		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	446	Total	C	N	O	S	0	0
			3617	2459	533	583	42		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	341	Total	C	N	O	S	0	0
			2796	1893	411	458	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	368	Total	C	N	O	S	0	0
			3007	1927	504	560	16		

- Molecule 16 is a protein called NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	377	Total	C	N	O	S	0	0
			3032	1934	546	542	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	130	Total	C	N	O	S	0	0
			1054	659	198	193	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			716	453	130	129	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	77	Total	C	N	O	S	0	0
			615	398	94	121	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	85	Total	C	N	O	S	0	0
			684	442	103	137	2		

- Molecule 20 is a protein called NADH dehydrogenase (Ubiquinone) 13 kDa B subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	118	Total	C	N	O	S	0	0
			922	588	162	168	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	114	Total	C	N	O	S	0	0
			968	620	172	170	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	174	Total	C	N	O	S	0	0
			1383	867	240	266	10		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	167	Total	C	N	O	S	0	0
			1277	829	212	230	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Z	146	Total	C	N	O	S	0	0
			1201	787	203	209	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
25	a	73	Total	C	N	O	S	0	0
			601	386	101	108	6		

- Molecule 26 is a protein called RH45008p.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	b	66	Total	C	N	O	S	0	0
			519	327	95	96	1		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	115	Total	C	N	O	S	0	0
			907	590	159	157	1		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	100	Total	C	N	O	S	0	0
			828	523	145	149	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	56	Total	C	N	O	S	0	0
			437	283	77	74	3		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	106	Total	C	N	O	S	0	0
			870	560	140	169	1		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	145	Total	C	N	O	S	0	0
			1234	795	213	223	3		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	i	161	Total	C	N	O	S	0	0
			1302	829	242	226	5		

- Molecule 33 is a protein called GEO11417p1.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	j	59	Total	C	N	O	S	0	0
			489	319	88	81	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	k	84	Total	C	N	O	S	0	0
			671	437	117	116	1		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	l	144	Total	C	N	O	S	0	0
			1201	783	191	223	4		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	m	108	Total	C	N	O	S	0	0
			892	571	163	157	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	n	134	Total	C	N	O	S	0	0
			1152	735	218	196	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	o	112	Total	C	N	O	S	0	0
			937	596	163	169	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
39	p	151	Total	C	N	O	S	0	0
			1266	795	233	228	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
40	q	135	Total	C	N	O	S	0	0
			1130	735	189	201	5		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	r	89	Total	C	N	O	S	0	0
			724	457	136	130	1		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

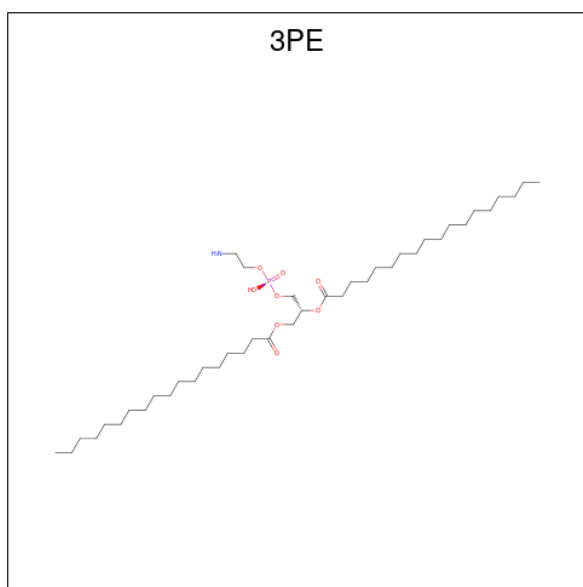
Mol	Chain	Residues	Atoms					AltConf	Trace
42	s	62	Total	C	N	O	S	0	0
			456	288	75	90	3		

- Molecule 43 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



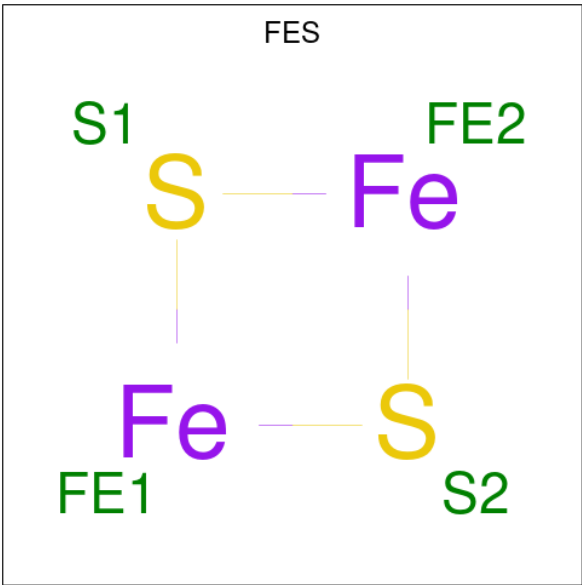
Mol	Chain	Residues	Atoms			AltConf
43	B	1	Total	Fe	S	0
			8	4	4	
43	F	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	G	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	
43	I	1	Total	Fe	S	0
			8	4	4	

- Molecule 44 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$).



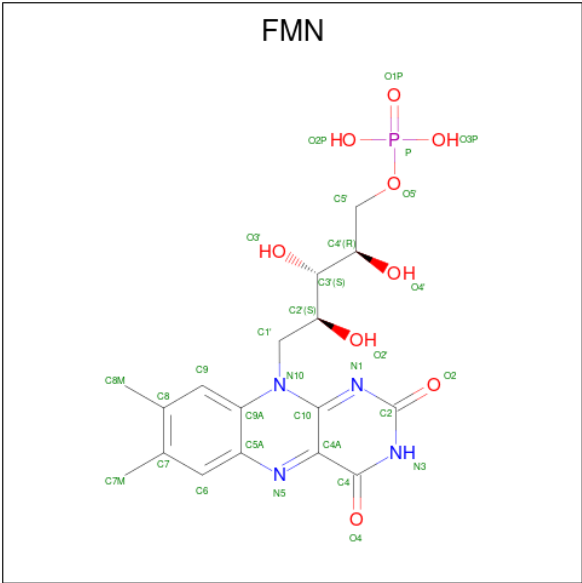
Mol	Chain	Residues	Atoms					AltConf
44	B	1	Total	C	N	O	P	0
			42	32	1	8	1	
44	B	1	Total	C	N	O	P	0
			26	16	1	8	1	
44	L	1	Total	C	N	O	P	0
			35	25	1	8	1	
44	Y	1	Total	C	N	O	P	0
			20	10	1	8	1	
44	Y	1	Total	C	N	O	P	0
			22	12	1	8	1	
44	Y	1	Total	C	N	O	P	0
			25	15	1	8	1	

- Molecule 45 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



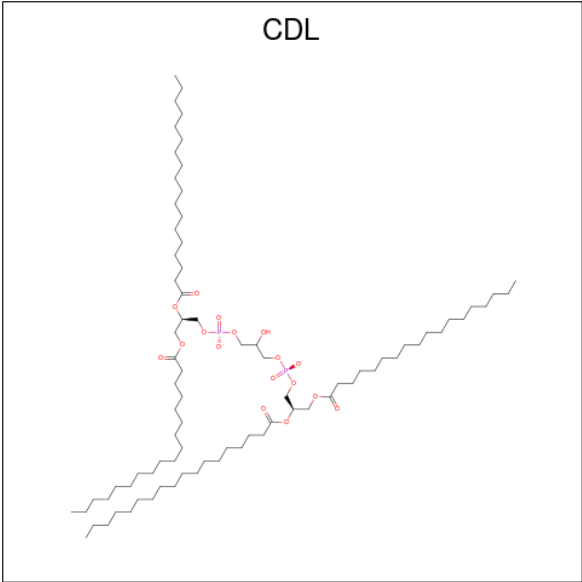
Mol	Chain	Residues	Atoms			AltConf
45	E	1	Total	Fe	S	0
			4	2	2	
45	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P).



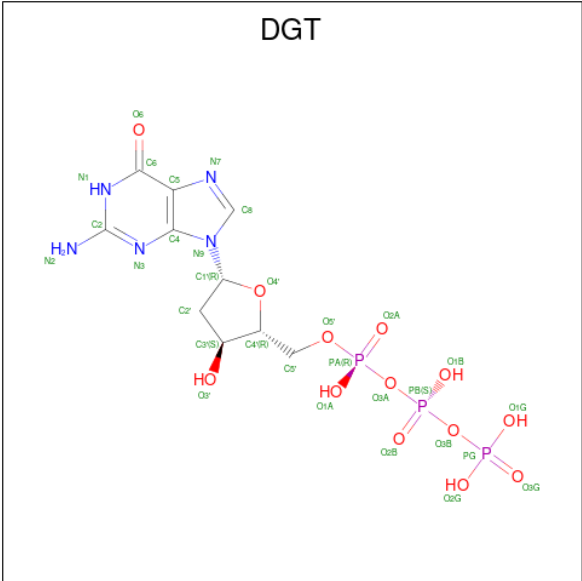
Mol	Chain	Residues	Atoms					AltConf
46	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂).



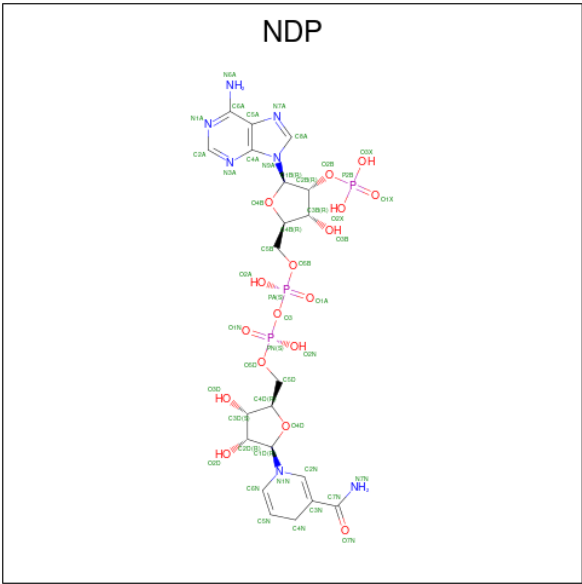
Mol	Chain	Residues	Atoms				AltConf
47	M	1	Total	C	O	P	0
			55	36	17	2	
47	P	1	Total	C	O	P	0
			41	22	17	2	

- Molecule 48 is 2'-DEOXYGUANOSINE-5'-TRIPHOSPHATE (CCD ID: DGT) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
48	O	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 49 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).

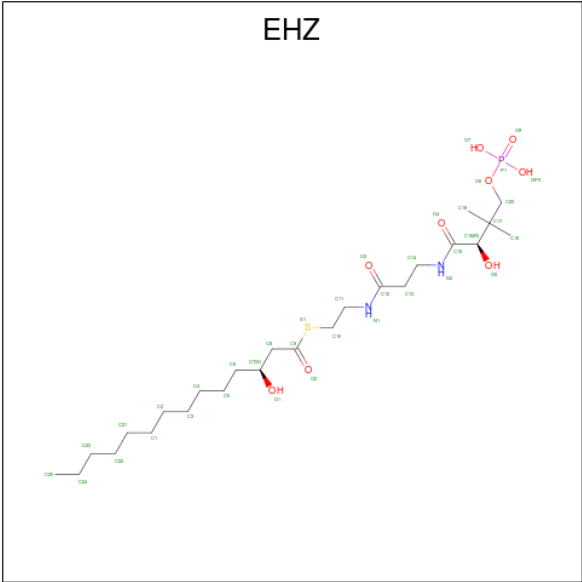


Mol	Chain	Residues	Atoms					AltConf
49	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 51 is {S}-[2-[3-[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: C₂₅H₄₉N₂O₉PS).

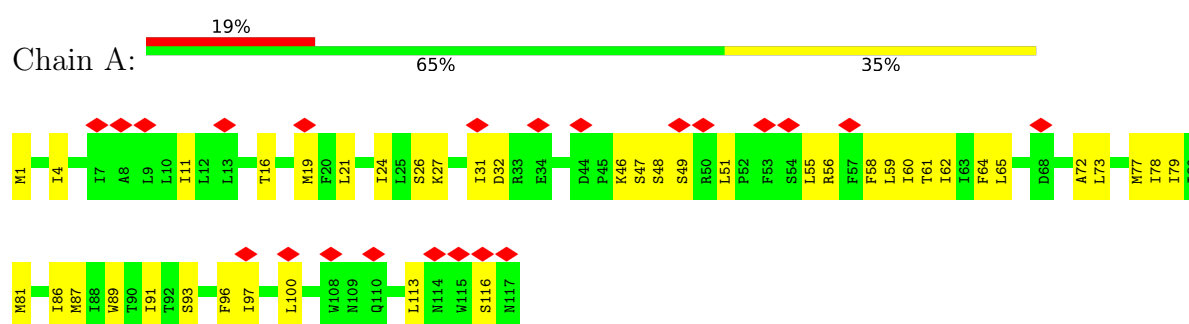


Mol	Chain	Residues	Atoms					AltConf
51	T	1	Total	C	N	O	P	S
			37	25	2	8	1	1
51	U	1	Total	C	N	O	P	S
			37	25	2	8	1	1

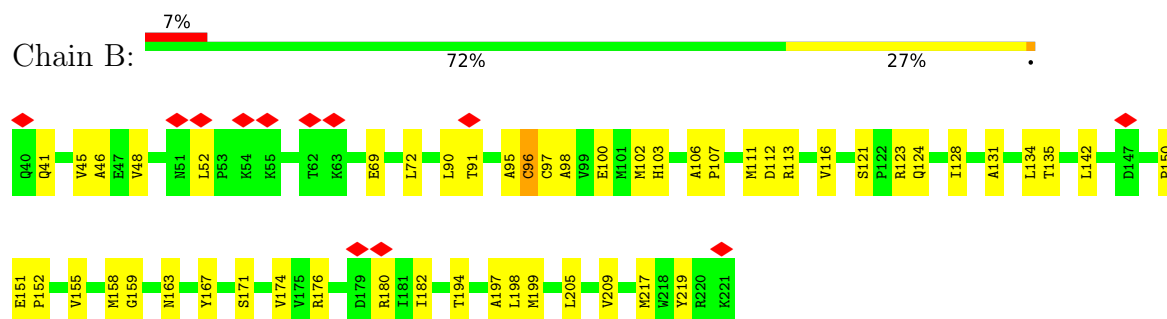
3 Residue-property plots [i](#)

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.

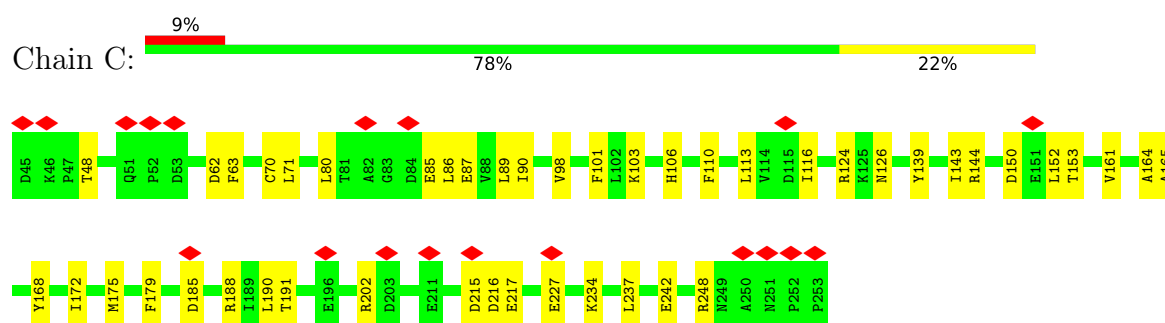
- Molecule 1: NADH-ubiquinone oxidoreductase chain 3



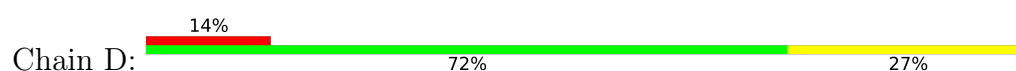
- Molecule 2: LD31474p

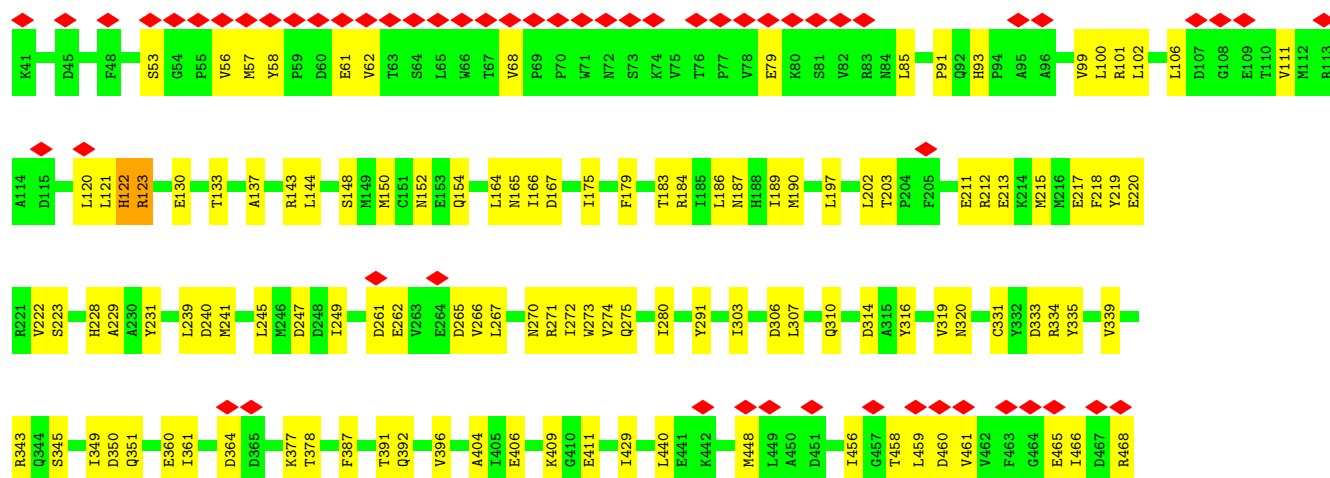


- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

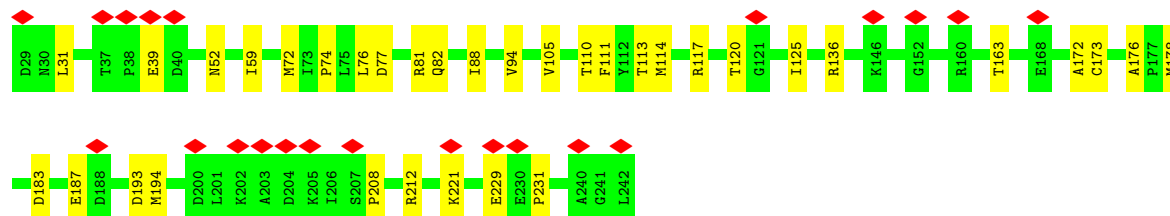
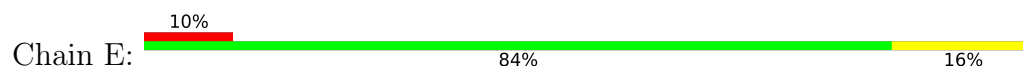


- Molecule 4: Complex I-49kD

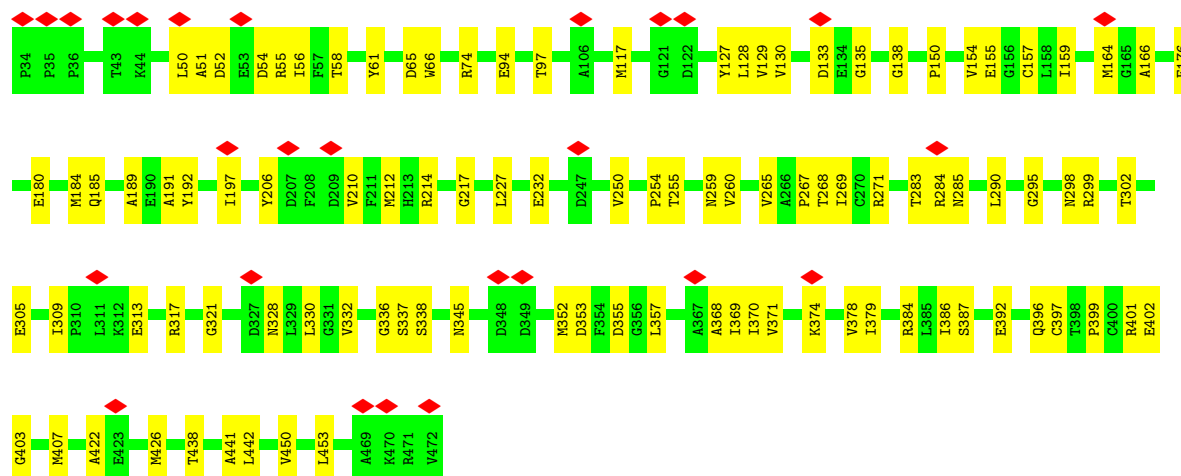
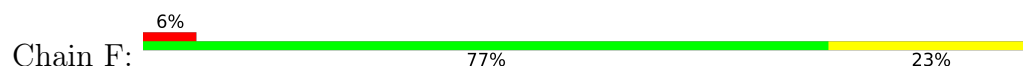




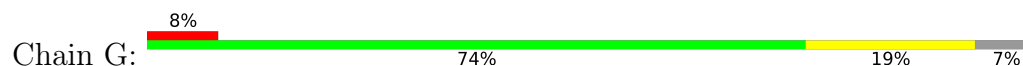
- Molecule 5: NADH dehydrogenase (Ubiquinone) 24 kDa subunit, isoform A

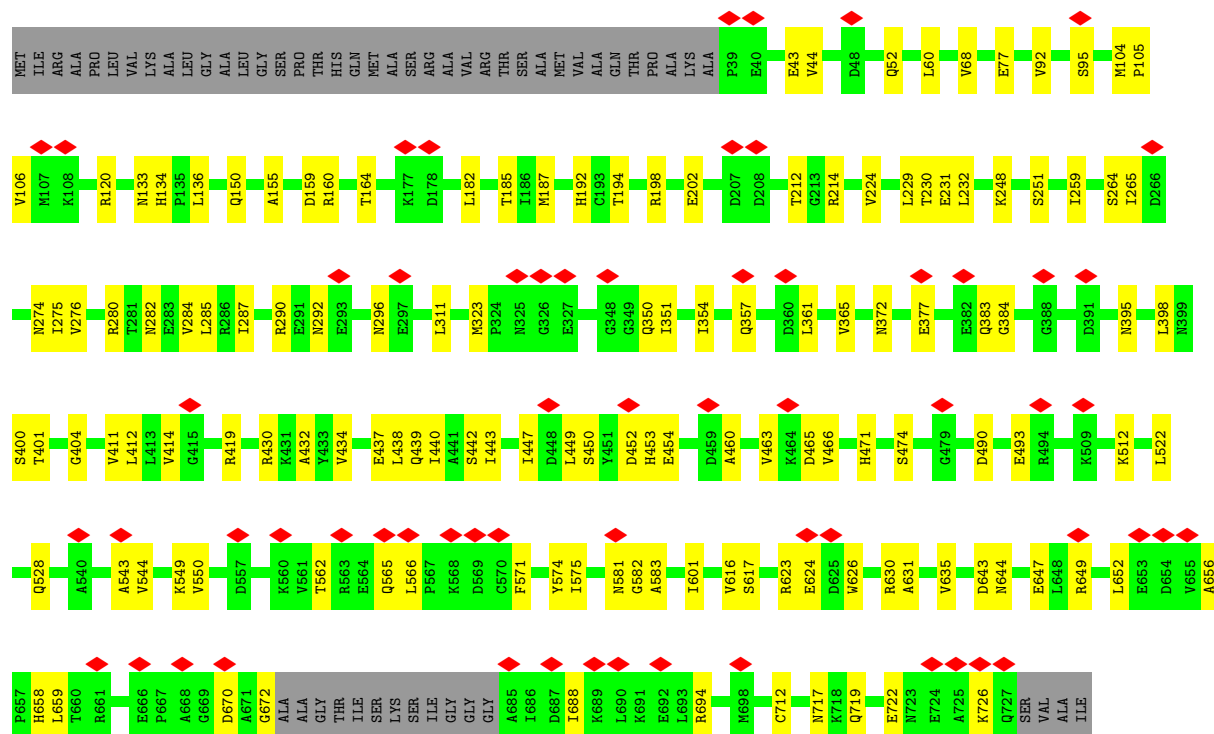


- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

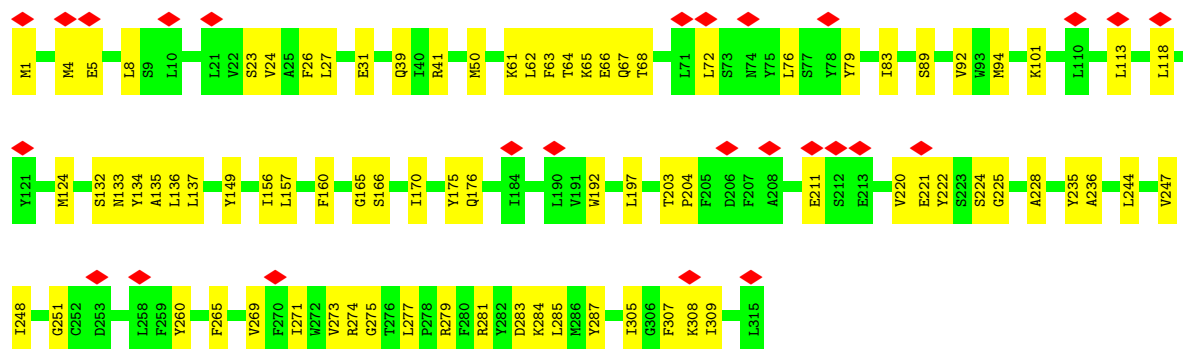
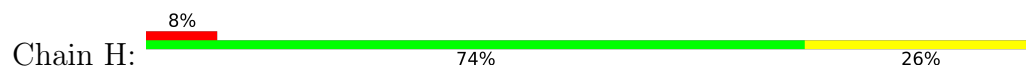


- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

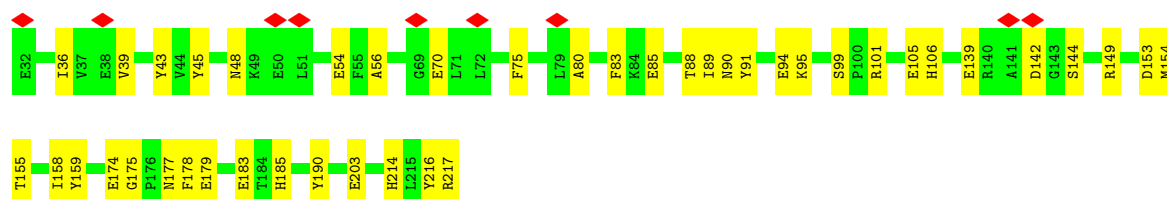
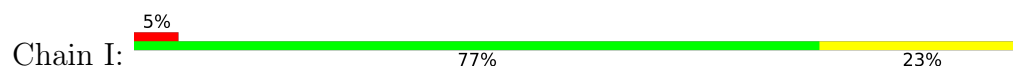




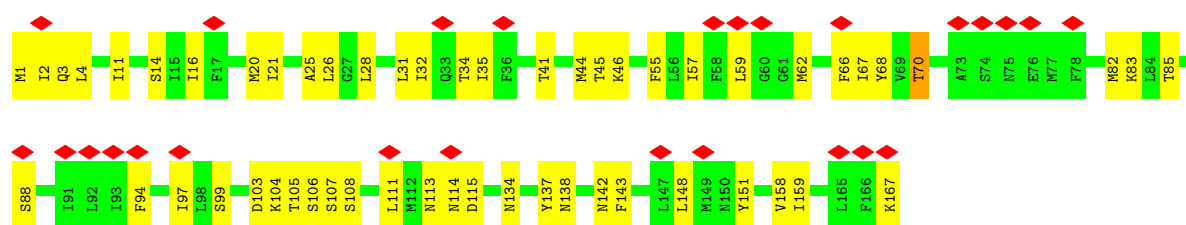
• Molecule 8: NADH-ubiquinone oxidoreductase chain 1



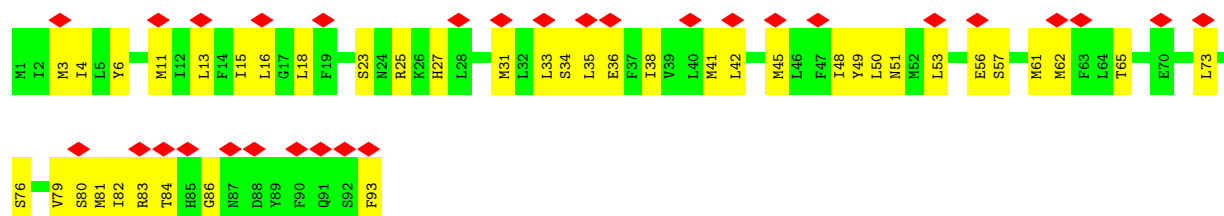
• Molecule 9: NADH dehydrogenase (ubiquinone) 23 kDa subunit



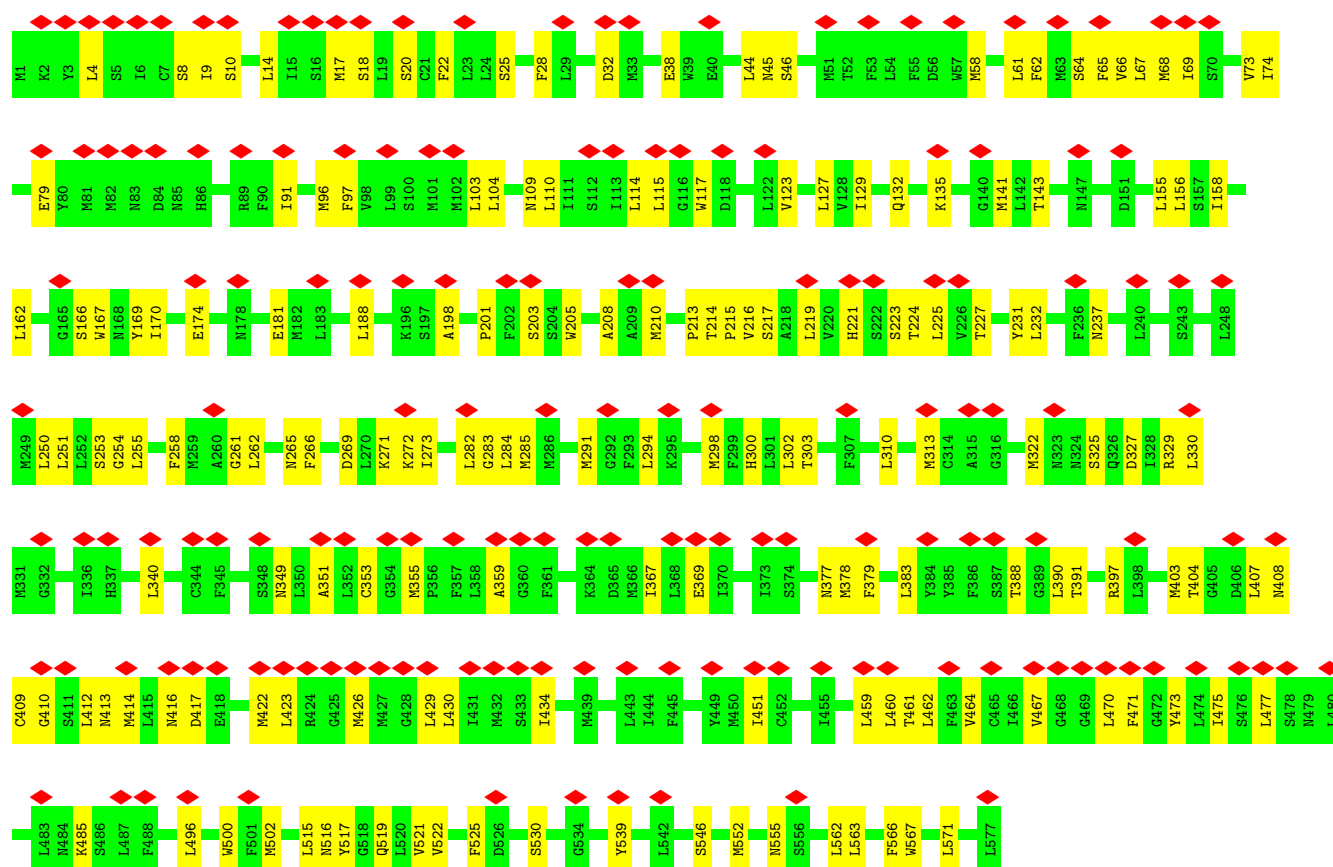
• Molecule 10: NADH-ubiquinone oxidoreductase chain 6



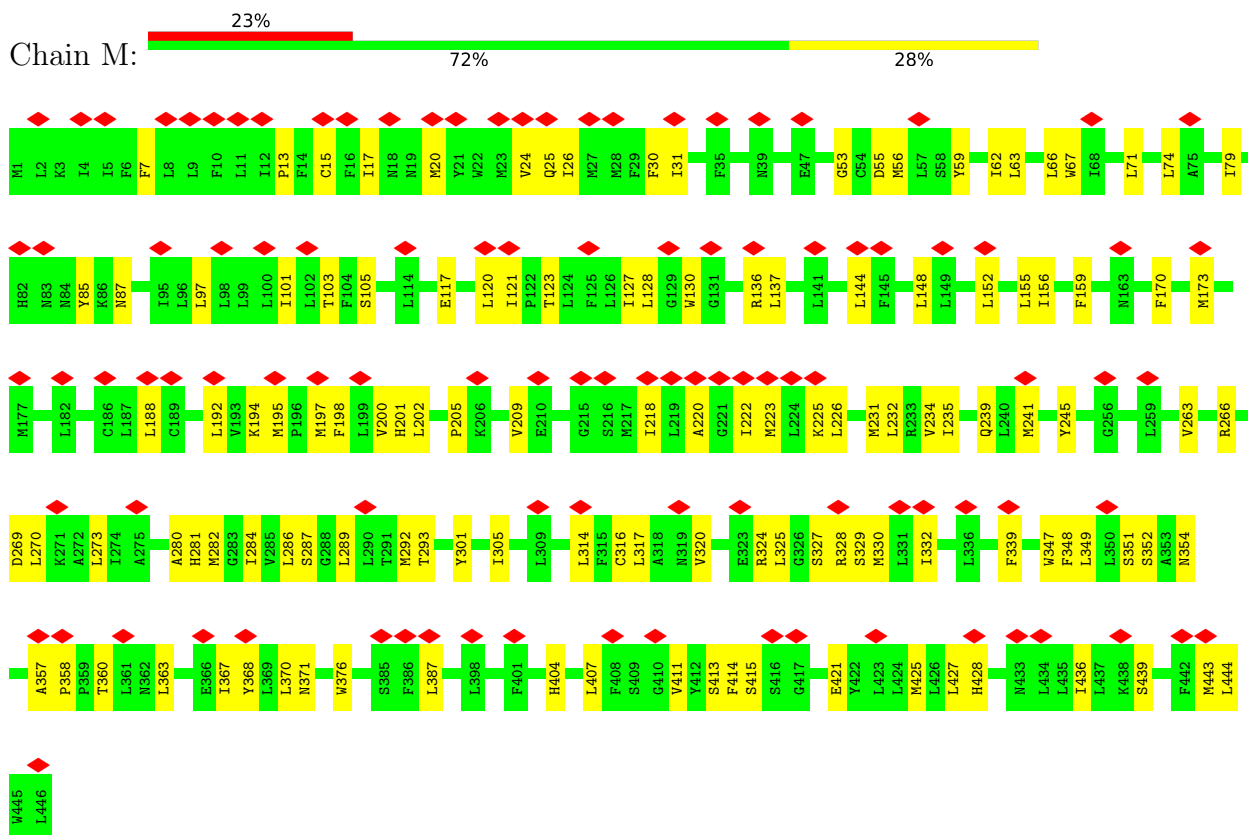
• Molecule 11: NADH-ubiquinone oxidoreductase chain 4L



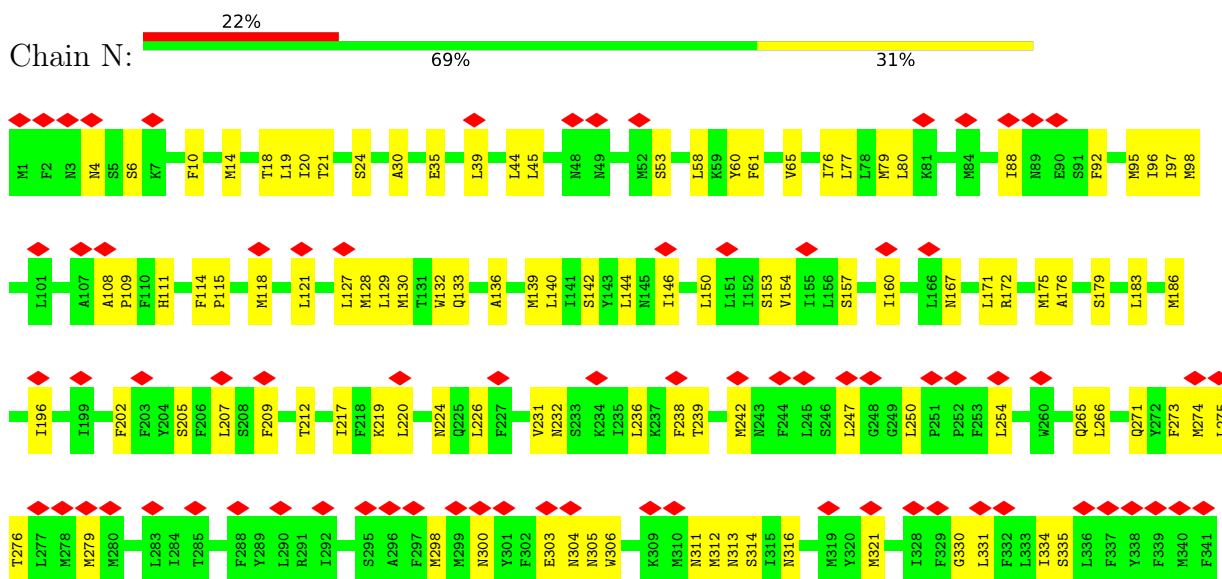
• Molecule 12: NADH-ubiquinone oxidoreductase chain 5



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

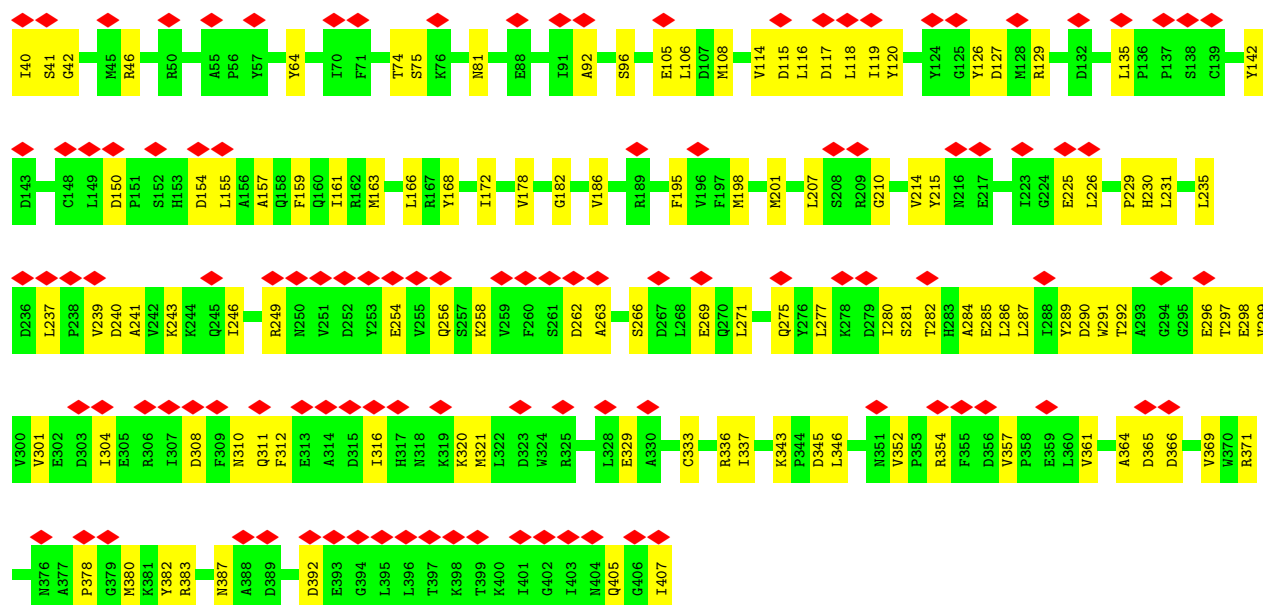


- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

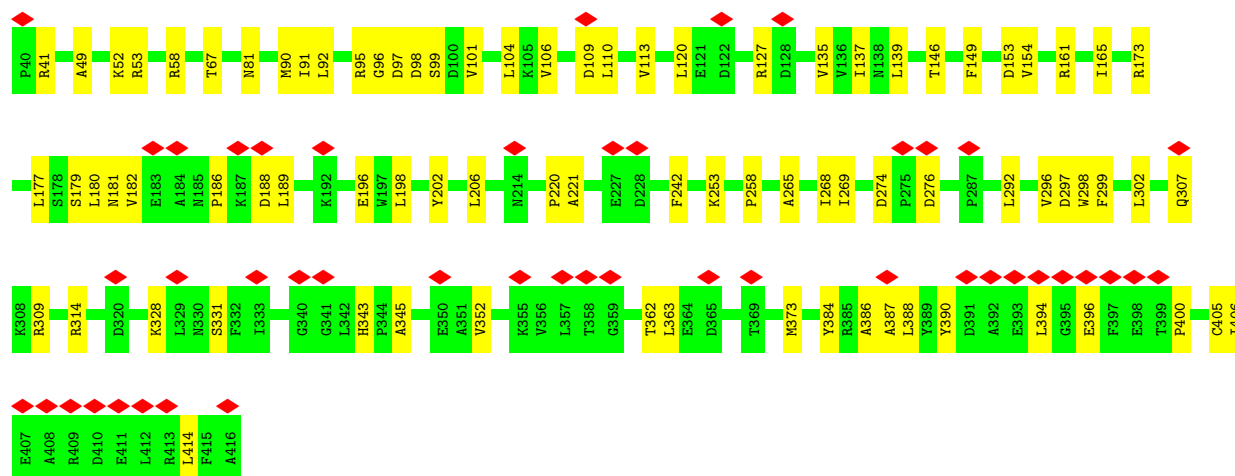
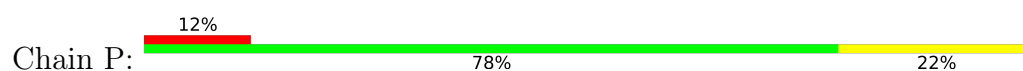


- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

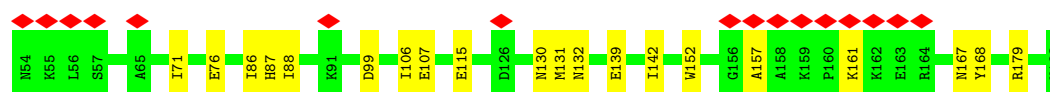
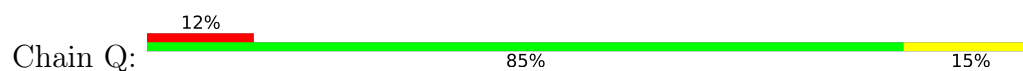




- Molecule 16: NADH dehydrogenase (Ubiquinone) 39 kDa subunit, isoform A

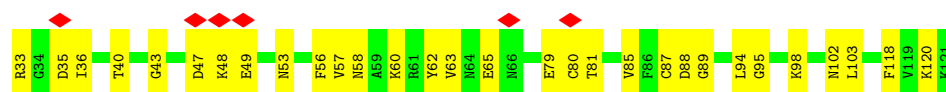


- Molecule 17: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial

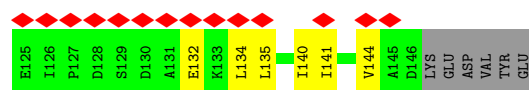
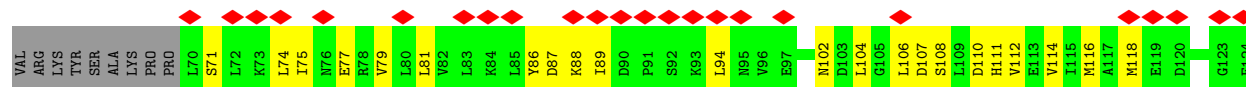
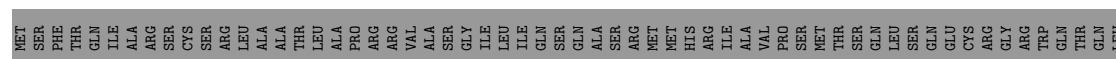
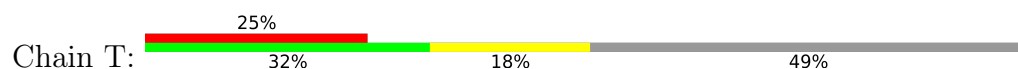


- Molecule 18: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

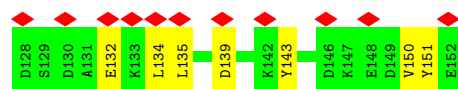
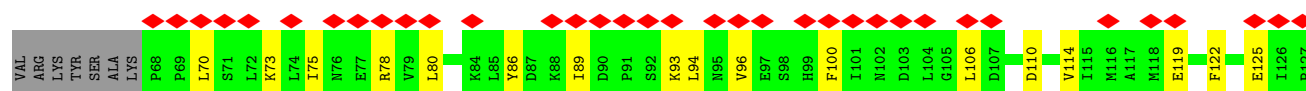
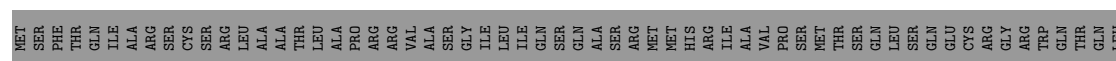




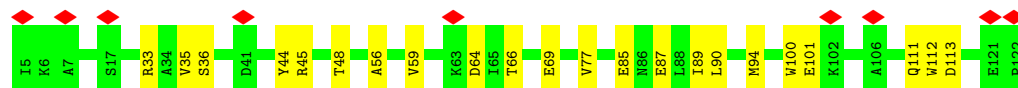
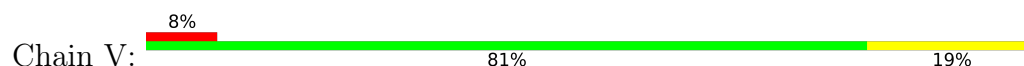
- Molecule 19: Acyl carrier protein, mitochondrial



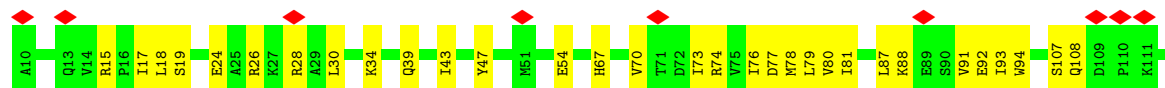
- Molecule 19: Acyl carrier protein, mitochondrial



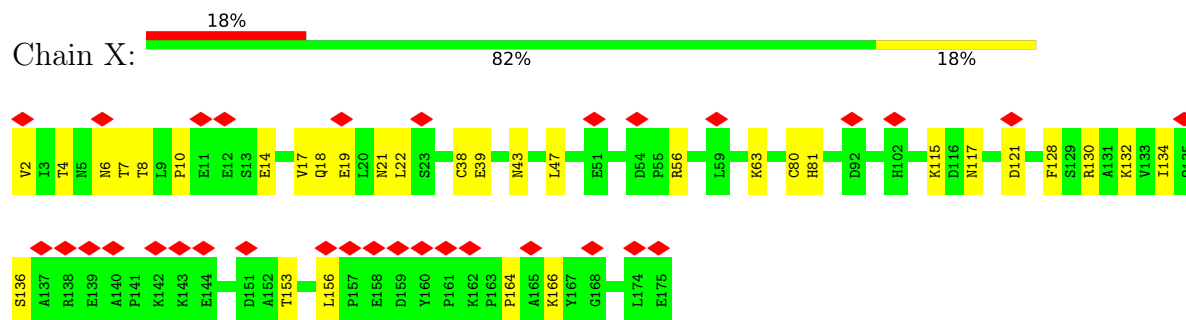
- Molecule 20: NADH dehydrogenase (Ubiquinone) 13 kDa B subunit



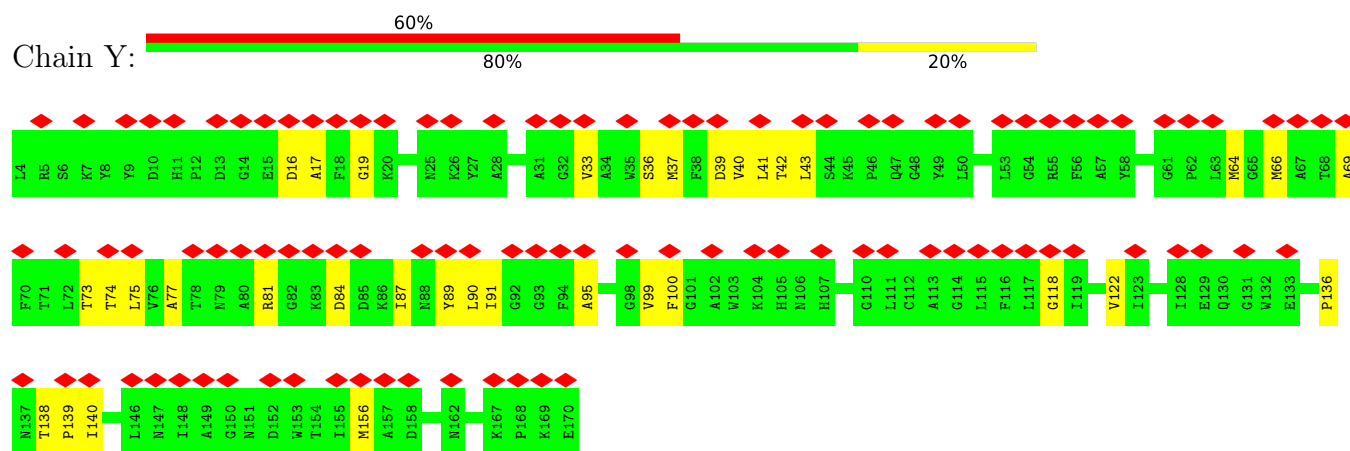
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



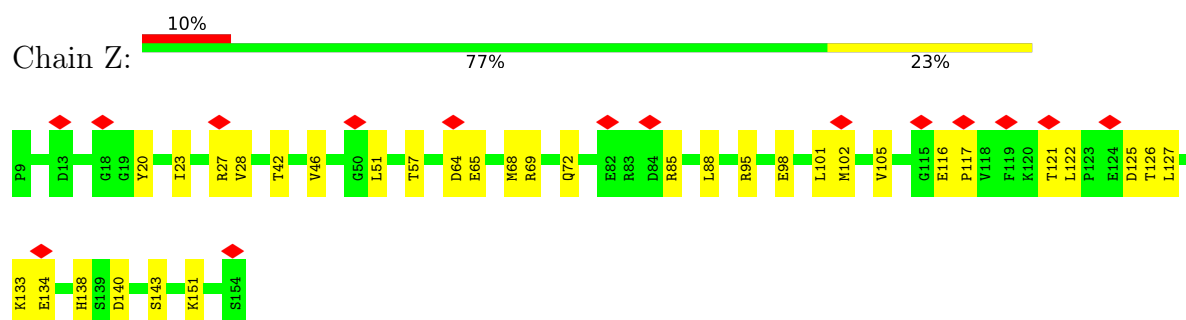
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8



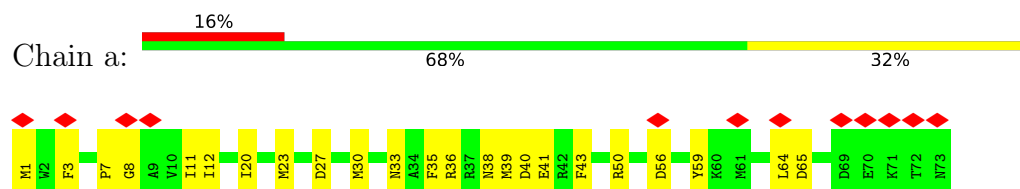
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



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



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

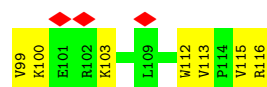
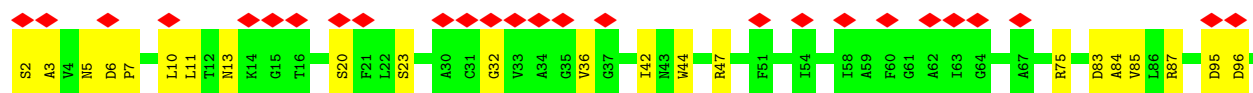
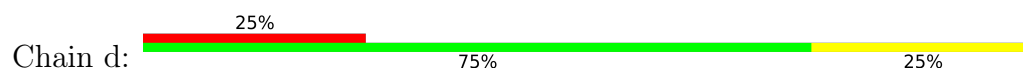


- Molecule 26: RH45008p

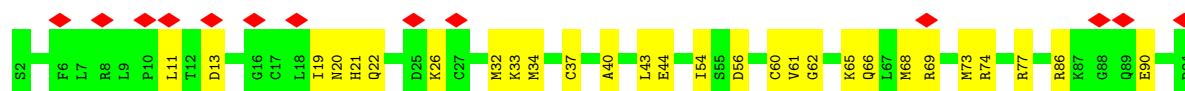




- Molecule 27: NADH dehydrogenase [ubiquinone] 1 subunit C2



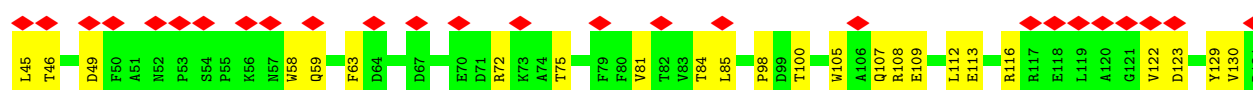
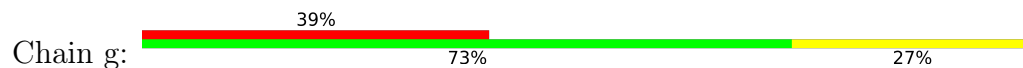
- Molecule 28: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



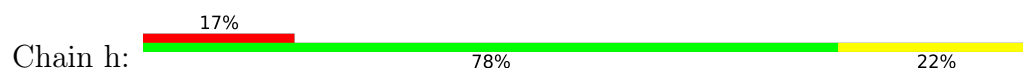
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

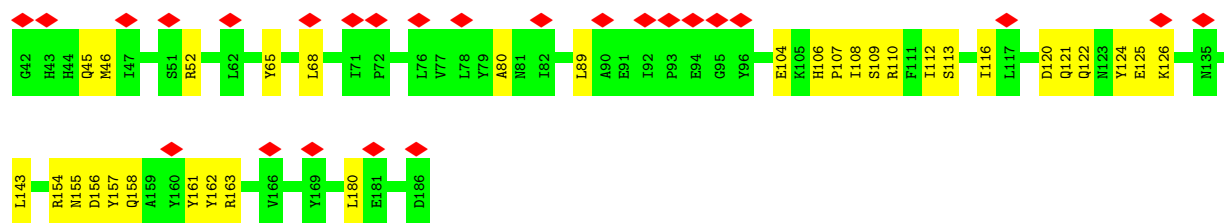


- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

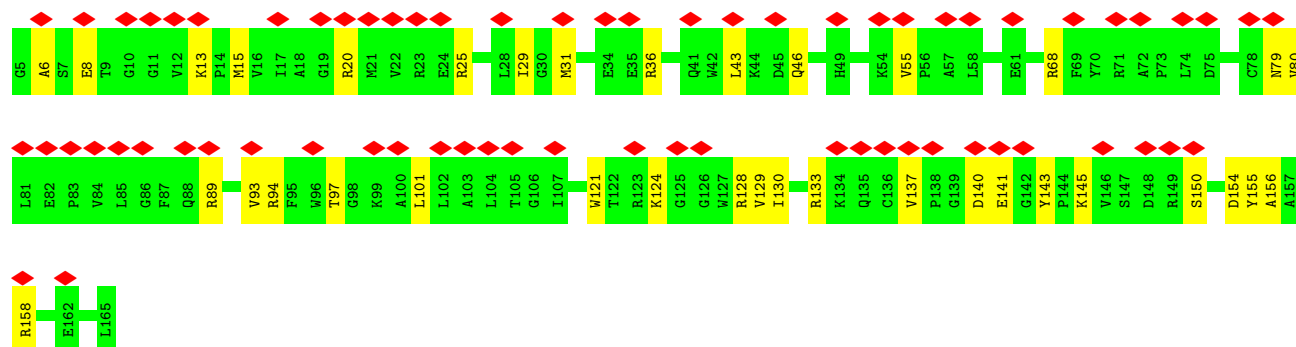
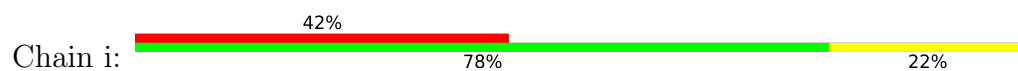


- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

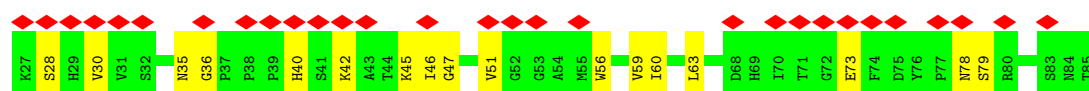




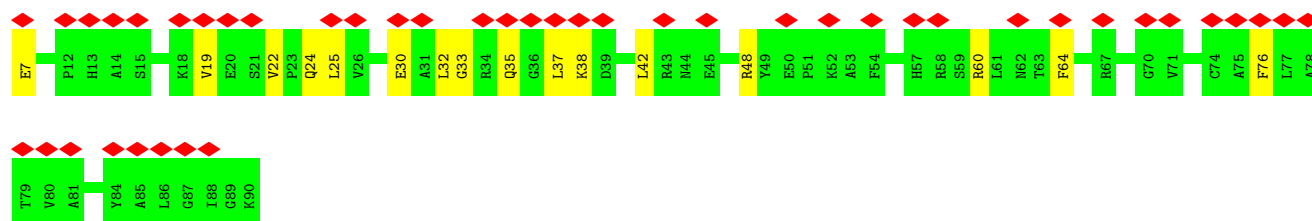
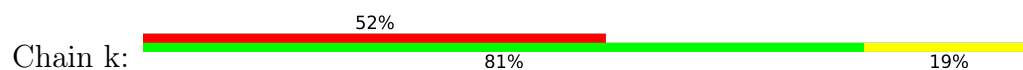
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



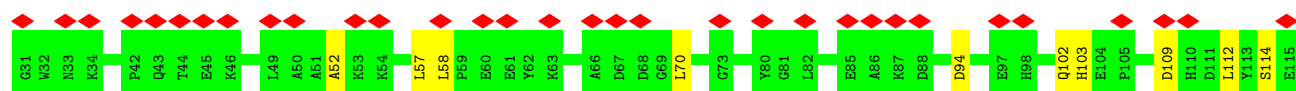
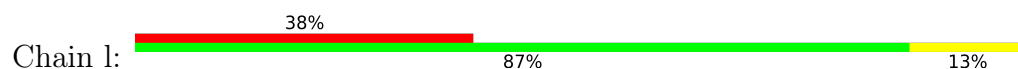
- Molecule 33: GEO11417p1

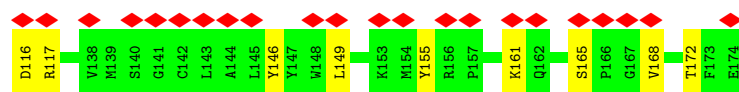


- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

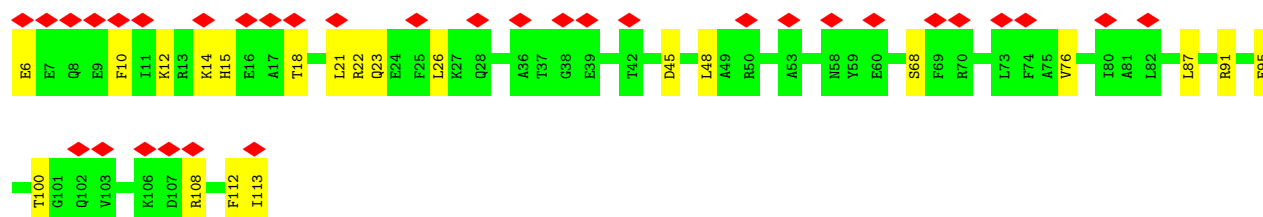
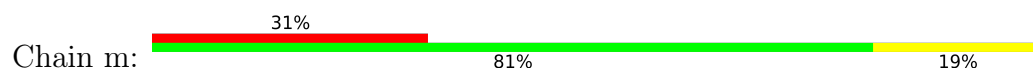


- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

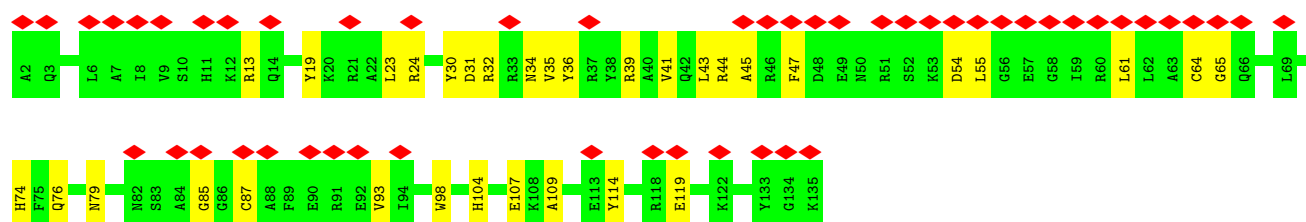
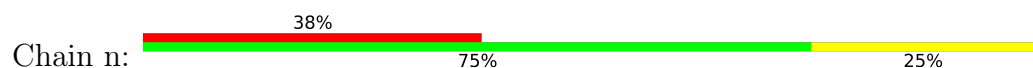




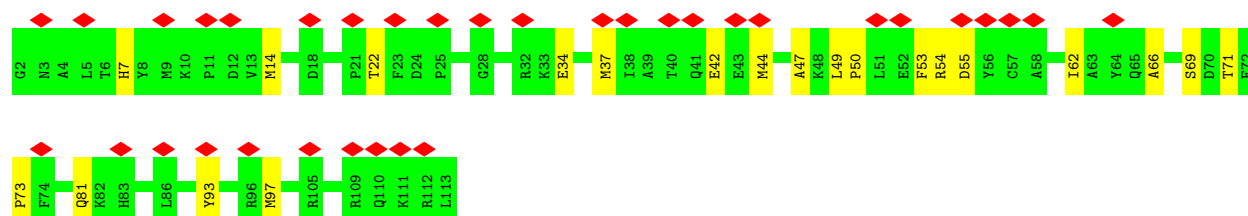
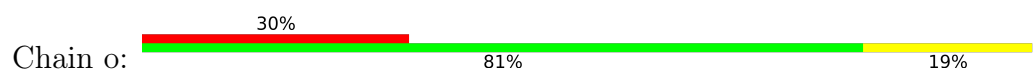
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4



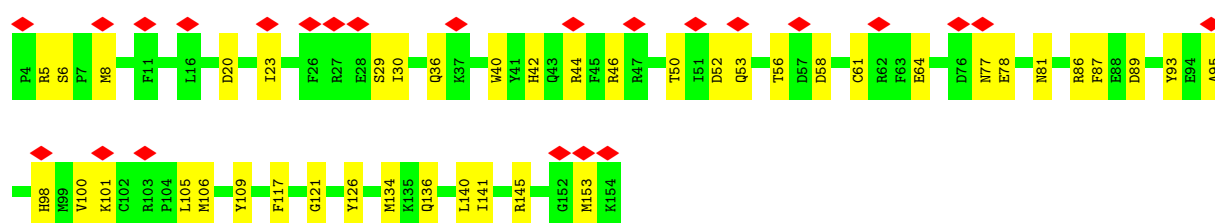
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9



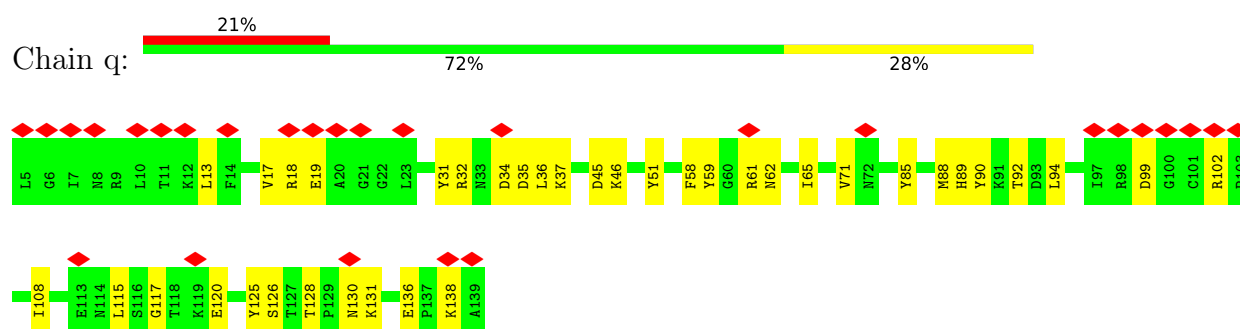
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7



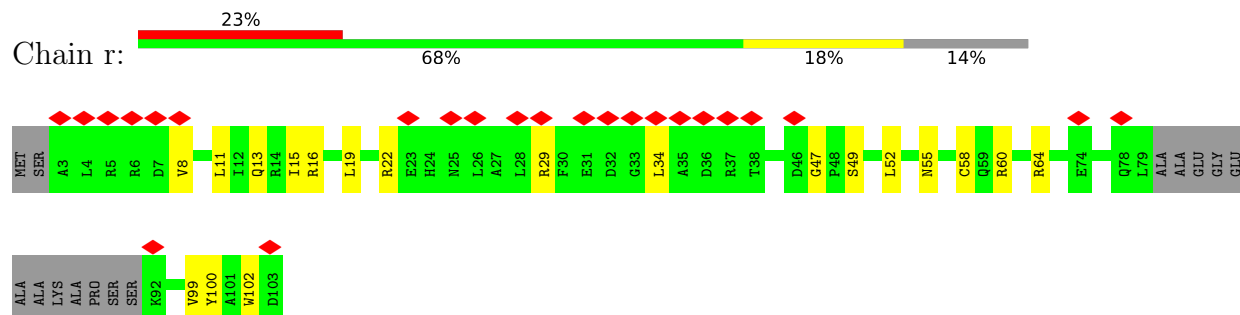
- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



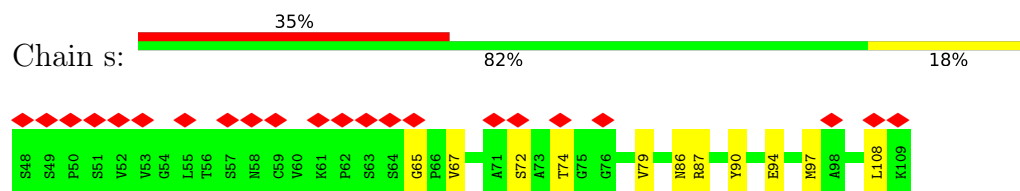
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



- Molecule 42: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	12343	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 ($e^-/\text{\AA}^2$)	41.88	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.016	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.014	Depositor
Map size (Å)	471.59998, 471.59998, 471.59998	wwPDB
Map dimensions	450, 450, 450	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 3PE, FES, DGT, 2MR, CDL, NDP, ZN, EHZ, FMN, SF4

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	0.28	0/979	0.45	0/1325
2	B	0.40	0/1473	0.54	0/1997
3	C	0.32	0/1774	0.44	0/2412
4	D	0.33	0/3495	0.45	0/4737
5	E	0.29	0/1718	0.41	0/2328
6	F	0.30	0/3447	0.45	0/4659
7	G	0.29	0/5229	0.42	0/7088
8	H	0.30	0/2651	0.43	0/3593
9	I	0.38	0/1518	0.48	0/2050
10	J	0.28	0/1377	0.53	2/1863 (0.1%)
11	K	0.31	0/792	0.51	0/1066
12	L	0.26	0/4726	0.42	0/6396
13	M	0.29	0/3723	0.41	0/5045
14	N	0.30	0/2875	0.46	0/3890
15	O	0.23	0/3082	0.43	0/4168
16	P	0.27	0/3108	0.45	0/4205
17	Q	0.30	0/1082	0.43	0/1465
18	R	0.32	0/733	0.42	0/987
19	T	0.22	0/624	0.45	0/843
19	U	0.24	0/696	0.53	0/940
20	V	0.25	0/942	0.41	0/1278
21	W	0.29	0/988	0.47	0/1329
22	X	0.24	0/1416	0.43	0/1911
23	Y	0.19	0/1314	0.35	0/1784
24	Z	0.26	0/1239	0.44	0/1682
25	a	0.29	0/614	0.49	0/827
26	b	0.25	0/528	0.46	0/714
27	d	0.22	0/935	0.42	0/1271
28	e	0.28	0/846	0.52	0/1128
29	f	0.27	0/448	0.62	0/600
30	g	0.27	0/895	0.48	0/1222
31	h	0.27	0/1269	0.45	0/1714

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	i	0.24	0/1338	0.50	0/1808
33	j	0.22	0/513	0.39	0/704
34	k	0.25	0/690	0.51	0/936
35	l	0.23	0/1250	0.41	0/1701
36	m	0.23	0/913	0.46	0/1222
37	n	0.24	0/1185	0.47	0/1597
38	o	0.20	0/960	0.47	0/1290
39	p	0.31	0/1299	0.51	0/1752
40	q	0.28	0/1169	0.39	0/1585
41	r	0.26	0/740	0.46	0/1003
42	s	0.24	0/469	0.43	0/637
All	All	0.28	0/67062	0.45	2/90752 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	J	70	THR	OG1-CB-CG2	5.85	120.99	109.30
10	J	70	THR	CA-CB-CG2	5.26	119.44	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	956	0	1030	45	0
2	B	1435	0	1446	46	0
3	C	1726	0	1673	41	0
4	D	3424	0	3396	106	0
5	E	1679	0	1657	28	0
6	F	3367	0	3350	76	0
7	G	5146	0	5189	98	0
8	H	2571	0	2628	80	0
9	I	1485	0	1422	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	J	1351	0	1461	56	0
11	K	771	0	793	36	0
12	L	4606	0	4742	144	0
13	M	3617	0	3750	96	0
14	N	2796	0	2879	93	0
15	O	3007	0	2945	90	0
16	P	3032	0	3030	66	0
17	Q	1054	0	1029	17	0
18	R	716	0	700	25	0
19	T	615	0	625	25	0
19	U	684	0	687	19	0
20	V	922	0	946	17	0
21	W	968	0	991	40	0
22	X	1383	0	1328	38	0
23	Y	1277	0	1258	24	0
24	Z	1201	0	1211	35	0
25	a	601	0	603	22	0
26	b	519	0	517	14	0
27	d	907	0	896	26	0
28	e	828	0	809	31	0
29	f	437	0	448	14	0
30	g	870	0	822	31	0
31	h	1234	0	1198	33	0
32	i	1302	0	1295	30	0
33	j	489	0	455	13	0
34	k	671	0	671	16	0
35	l	1201	0	1107	19	0
36	m	892	0	885	20	0
37	n	1152	0	1124	29	0
38	o	937	0	920	22	0
39	p	1266	0	1217	38	0
40	q	1130	0	1085	32	0
41	r	724	0	727	22	0
42	s	456	0	440	9	0
43	B	8	0	0	0	0
43	F	8	0	0	2	0
43	G	16	0	0	2	0
43	I	16	0	0	0	0
44	B	68	0	84	2	0
44	L	35	0	44	3	0
44	Y	67	0	56	0	0
45	E	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	G	4	0	0	0	0
46	F	31	0	19	1	0
47	M	55	0	54	1	0
47	P	41	0	26	0	0
48	O	31	0	12	4	0
49	P	48	0	26	2	0
50	R	1	0	0	0	0
51	T	37	0	0	1	0
51	U	37	0	0	1	0
All	All	65912	0	65706	1452	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 11.

All (1452) 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)
4:D:203:THR:OG1	8:H:275:GLY:O	1.82	0.97
11:K:81:MET:HE1	14:N:58:LEU:HD23	1.50	0.93
13:M:121:ILE:HD11	14:N:250:LEU:HD23	1.52	0.91
19:T:112:VAL:HG21	21:W:30:LEU:HD12	1.55	0.89
5:E:111:PHE:O	7:G:214:ARG:NH2	2.04	0.89
4:D:164:LEU:HD21	4:D:396:VAL:HG22	1.55	0.87
12:L:198:ALA:O	12:L:203:SER:OG	1.93	0.87
10:J:44:MET:O	11:K:51:ASN:ND2	2.08	0.86
4:D:272:ILE:HD12	8:H:277:LEU:HD12	1.58	0.86
19:U:119:GLU:OE2	37:n:24:ARG:NH1	2.07	0.86
1:A:46:LYS:NZ	21:W:92:GLU:OE2	2.08	0.85
13:M:188:LEU:HD12	13:M:231:MET:HE1	1.59	0.85
3:C:234:LYS:NZ	17:Q:130:ASN:O	2.09	0.84
34:k:19:VAL:HG13	34:k:42:LEU:HD22	1.58	0.83
7:G:411:VAL:HG23	7:G:438:LEU:HD11	1.58	0.82
2:B:112:ASP:OD1	8:H:41:ARG:NH2	2.12	0.82
12:L:219:LEU:O	12:L:224:THR:OG1	1.96	0.82
12:L:525:PHE:O	12:L:530:SER:OG	1.96	0.82
6:F:232:GLU:OE2	17:Q:179:ARG:NH2	2.13	0.82
12:L:284:LEU:HD21	12:L:367:ILE:HG21	1.61	0.82
12:L:413:ASN:ND2	33:j:35:ASN:O	2.12	0.82
18:R:81:THR:O	18:R:120:LYS:NZ	2.13	0.82
15:O:254:GLU:OE2	48:O:501:DGT:O3'	1.95	0.82
1:A:26:SER:OG	8:H:63:PHE:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:128:PHE:O	22:X:132:LYS:NZ	2.14	0.81
32:i:156:ALA:N	39:p:89:ASP:OD2	2.13	0.81
6:F:313:GLU:OE2	6:F:317:ARG:NH2	2.13	0.81
5:E:77:ASP:OD2	6:F:214:ARG:NH2	2.11	0.81
13:M:376:TRP:O	36:m:91:ARG:NH2	2.14	0.81
3:C:242:GLU:N	17:Q:99:ASP:OD2	2.13	0.81
21:W:15:ARG:O	21:W:74:ARG:NH1	2.13	0.81
12:L:210:MET:O	12:L:271:LYS:NZ	2.12	0.80
1:A:113:LEU:HD22	8:H:287:TYR:HE2	1.46	0.80
5:E:136:ARG:NH2	6:F:295:GLY:O	2.14	0.80
22:X:19:GLU:OE2	22:X:21:ASN:ND2	2.14	0.80
3:C:103:LYS:NZ	3:C:161:VAL:O	2.13	0.80
7:G:401:THR:O	7:G:404:GLY:N	2.15	0.80
13:M:270:LEU:HD23	13:M:330:MET:HE1	1.61	0.80
35:l:114:SER:OG	35:l:116:ASP:OD1	1.98	0.80
7:G:512:LYS:NZ	7:G:670:ASP:OD1	2.15	0.80
14:N:271:GLN:NE2	23:Y:136:PRO:O	2.15	0.80
38:o:69:SER:O	39:p:6:SER:OG	2.00	0.79
10:J:105:THR:OG1	28:e:74:ARG:NH2	2.15	0.79
7:G:365:VAL:HG21	7:G:652:LEU:HD11	1.65	0.79
4:D:217:GLU:OE1	41:r:29:ARG:NH1	2.17	0.78
9:I:94:GLU:OE2	40:q:37:LYS:NZ	2.16	0.78
4:D:247:ASP:OD1	24:Z:20:TYR:OH	2.00	0.78
7:G:437:GLU:OE2	7:G:439:GLN:NE2	2.15	0.78
7:G:284:VAL:HG23	7:G:616:VAL:HG21	1.65	0.78
15:O:40:ILE:N	15:O:81:ASN:OD1	2.16	0.78
6:F:155:GLU:OE2	6:F:271:ARG:NH1	2.17	0.78
7:G:155:ALA:O	41:r:64:ARG:NH1	2.16	0.78
13:M:209:VAL:O	13:M:328:ARG:NH2	2.17	0.78
14:N:121:LEU:O	14:N:172:ARG:NH2	2.17	0.78
27:d:11:LEU:HD11	31:h:143:LEU:HD22	1.65	0.78
14:N:153:SER:O	14:N:157:SER:OG	2.01	0.77
10:J:103:ASP:O	10:J:107:SER:OG	2.03	0.77
4:D:364:ASP:O	7:G:160:ARG:NH1	2.18	0.77
12:L:407:LEU:O	34:k:48:ARG:NH2	2.18	0.77
4:D:265:ASP:OD2	41:r:22:ARG:NH1	2.18	0.77
1:A:51:LEU:HD13	8:H:136:LEU:HD22	1.65	0.76
3:C:215:ASP:OD1	3:C:217:GLU:N	2.18	0.76
42:s:72:SER:OG	42:s:74:THR:O	2.04	0.76
19:T:79:VAL:HA	19:T:118:MET:HE1	1.68	0.76
36:m:100:THR:HG23	39:p:153:MET:HE1	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
44:L:601:3PE:N	35:l:117:ARG:O	2.19	0.76
15:O:298:GLU:N	15:O:298:GLU:OE1	2.19	0.76
31:h:124:TYR:OH	39:p:64:GLU:OE1	2.02	0.76
35:l:94:ASP:OD2	35:l:102:GLN:N	2.19	0.75
15:O:281:SER:O	15:O:320:LYS:NZ	2.20	0.75
4:D:183:THR:OG1	4:D:219:TYR:OH	2.05	0.75
8:H:8:LEU:HD21	25:a:30:MET:HE3	1.67	0.75
10:J:113:ASN:OD1	10:J:114:ASN:N	2.19	0.75
38:o:42:GLU:N	38:o:42:GLU:OE1	2.20	0.75
3:C:90:ILE:HG21	3:C:98:VAL:HG21	1.68	0.75
13:M:53:GLY:O	13:M:105:SER:OG	2.03	0.75
17:Q:87:HIS:NE2	17:Q:107:GLU:OE1	2.20	0.75
36:m:22:ARG:NH2	36:m:23:GLN:OE1	2.20	0.74
6:F:52:ASP:OD1	6:F:55:ARG:NH2	2.20	0.74
7:G:150:GLN:NE2	43:G:801:SF4:S3	2.61	0.74
22:X:115:LYS:NZ	22:X:121:ASP:OD1	2.20	0.74
7:G:383:GLN:O	7:G:528:GLN:NE2	2.21	0.74
7:G:430:ARG:NH2	7:G:450:SER:O	2.20	0.74
2:B:121:SER:OG	2:B:124:GLN:OE1	2.01	0.74
12:L:322:MET:SD	12:L:325:SER:OG	2.46	0.74
29:f:44:GLY:O	39:p:46:ARG:NH2	2.21	0.74
10:J:151:TYR:OH	14:N:35:GLU:OE1	2.04	0.73
18:R:33:ARG:NH1	18:R:56:PHE:O	2.21	0.73
11:K:31:MET:O	11:K:34:SER:OG	2.06	0.73
15:O:96:SER:OG	48:O:501:DGT:O1G	2.07	0.73
25:a:33:ASN:ND2	25:a:35:PHE:O	2.21	0.73
13:M:357:ALA:O	13:M:360:THR:OG1	2.03	0.73
2:B:113:ARG:NH1	9:I:90:ASN:OD1	2.21	0.73
15:O:383:ARG:NH1	15:O:405:GLN:OE1	2.22	0.73
18:R:80:CYS:SG	18:R:81:THR:N	2.62	0.73
14:N:331:LEU:O	14:N:334:ILE:HG23	1.89	0.73
22:X:130:ARG:NH1	26:b:75:GLU:O	2.21	0.73
12:L:17:MET:O	12:L:20:SER:OG	2.06	0.73
4:D:148:SER:O	4:D:152:ASN:ND2	2.22	0.72
14:N:207:LEU:HD21	14:N:247:LEU:HD22	1.69	0.72
35:l:161:LYS:NZ	38:o:55:ASP:OD1	2.21	0.72
6:F:283:THR:HG22	6:F:284:ARG:H	1.54	0.72
7:G:419:ARG:NH2	7:G:450:SER:OG	2.22	0.72
9:I:139:GLU:N	9:I:139:GLU:OE2	2.22	0.72
13:M:439:SER:O	13:M:443:MET:N	2.22	0.72
22:X:166:LYS:NZ	27:d:10:LEU:O	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:249:ARG:NH2	15:O:254:GLU:OE1	2.23	0.72
2:B:151:GLU:N	8:H:66:GLU:OE2	2.23	0.72
4:D:306:ASP:O	4:D:310:GLN:NE2	2.22	0.72
7:G:134:HIS:NE2	43:G:801:SF4:FE3	1.56	0.72
8:H:113:LEU:HD21	8:H:157:LEU:HD12	1.72	0.72
9:I:83:PHE:O	41:r:16:ARG:NH2	2.23	0.72
13:M:324:ARG:NH2	13:M:415:SER:O	2.21	0.72
3:C:86:LEU:HD23	3:C:143:ILE:HD13	1.72	0.72
15:O:387:ASN:N	15:O:392:ASP:OD2	2.23	0.72
22:X:4:THR:O	24:Z:95:ARG:NH2	2.23	0.72
38:o:49:LEU:O	38:o:54:ARG:NE	2.23	0.71
2:B:150:PRO:O	8:H:65:LYS:NZ	2.22	0.71
51:T:201:EHZ:O7	21:W:26:ARG:NH2	2.23	0.71
15:O:142:TYR:OH	15:O:150:ASP:O	2.07	0.71
31:h:46:MET:HE1	37:n:114:TYR:CE1	2.26	0.71
6:F:65:ASP:O	6:F:74:ARG:NH2	2.23	0.71
31:h:106:HIS:O	31:h:109:SER:OG	2.07	0.71
3:C:175:MET:HE3	3:C:190:LEU:HD12	1.72	0.71
13:M:198:PHE:O	13:M:201:HIS:ND1	2.24	0.71
10:J:151:TYR:CE2	14:N:39:LEU:HD22	2.26	0.70
8:H:101:LYS:O	25:a:36:ARG:NH2	2.24	0.70
7:G:623:ARG:NH1	21:W:119:PHE:O	2.24	0.70
37:n:79:ASN:ND2	37:n:85:GLY:O	2.24	0.70
12:L:224:THR:HG22	12:L:225:LEU:H	1.57	0.70
42:s:86:ASN:OD1	42:s:87:ARG:N	2.25	0.70
2:B:102:MET:HE1	4:D:190:MET:HE1	1.73	0.70
9:I:88:THR:O	40:q:61:ARG:NH2	2.24	0.69
15:O:230:HIS:HA	15:O:321:MET:HE1	1.72	0.69
32:i:121:TRP:N	32:i:158:ARG:O	2.25	0.69
7:G:92:VAL:O	7:G:95:SER:OG	2.10	0.69
12:L:355:MET:HE1	33:j:59:VAL:HG21	1.74	0.69
17:Q:76:GLU:N	17:Q:76:GLU:OE1	2.24	0.69
9:I:70:GLU:OE1	9:I:70:GLU:N	2.23	0.69
2:B:155:VAL:HG11	2:B:182:ILE:CD1	2.22	0.69
13:M:324:ARG:NH1	13:M:421:GLU:OE2	2.25	0.69
27:d:20:SER:OG	27:d:23:SER:N	2.26	0.69
6:F:396:GLN:O	6:F:401:ARG:NH1	2.26	0.69
14:N:207:LEU:HD21	14:N:247:LEU:CD2	2.22	0.68
19:T:111:HIS:HE1	19:T:134:LEU:HD11	1.59	0.68
13:M:71:LEU:HD13	13:M:428:HIS:CD2	2.29	0.68
24:Z:98:GLU:OE2	28:e:69:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:U:132:GLU:OE2	37:n:13:ARG:NH2	2.26	0.68
2:B:134:LEU:HD11	2:B:142:LEU:HD22	1.74	0.68
12:L:404:THR:O	34:k:60:ARG:NH1	2.27	0.68
26:b:51:ASN:ND2	26:b:70:LYS:O	2.27	0.68
4:D:197:LEU:HD11	4:D:202:LEU:HD23	1.76	0.68
12:L:265:ASN:O	12:L:397:ARG:NE	2.27	0.68
4:D:331:CYS:HB3	4:D:458:THR:HG21	1.75	0.68
7:G:44:VAL:HG11	7:G:106:VAL:CG1	2.24	0.68
15:O:114:VAL:HG11	15:O:163:MET:HE3	1.75	0.68
10:J:134:ASN:OD1	10:J:138:ASN:ND2	2.27	0.68
24:Z:116:GLU:N	24:Z:116:GLU:OE2	2.26	0.68
7:G:384:GLY:N	7:G:493:GLU:OE1	2.28	0.67
28:e:32:MET:HA	28:e:32:MET:HE2	1.74	0.67
7:G:465:ASP:OD1	7:G:466:VAL:N	2.27	0.67
14:N:266:LEU:HD22	14:N:275:LEU:HG	1.76	0.67
11:K:6:TYR:OH	24:Z:133:LYS:NZ	2.27	0.67
11:K:81:MET:CE	14:N:58:LEU:HD23	2.25	0.67
5:E:221:LYS:O	6:F:299:ARG:NH2	2.28	0.67
8:H:224:SER:OG	8:H:225:GLY:N	2.27	0.67
18:R:49:GLU:OE2	18:R:49:GLU:N	2.27	0.67
2:B:123:ARG:NH2	8:H:68:THR:OG1	2.27	0.67
10:J:115:ASP:OD2	24:Z:151:LYS:N	2.27	0.67
15:O:308:ASP:O	15:O:311:GLN:NE2	2.27	0.67
10:J:44:MET:HB2	10:J:111:LEU:HD12	1.78	0.66
12:L:379:PHE:CE2	35:l:149:LEU:HD12	2.30	0.66
13:M:376:TRP:HZ3	36:m:87:LEU:HD21	1.60	0.66
35:l:155:TYR:OH	38:o:14:MET:SD	2.49	0.66
28:e:34:MET:HE2	28:e:54:ILE:HA	1.78	0.66
17:Q:88:ILE:HD12	17:Q:157:ALA:CB	2.25	0.66
1:A:113:LEU:HD22	8:H:287:TYR:CE2	2.29	0.66
12:L:388:THR:O	12:L:391:THR:OG1	2.13	0.66
14:N:239:THR:HA	14:N:242:MET:HE2	1.77	0.66
15:O:106:LEU:HD21	15:O:301:VAL:HG13	1.77	0.66
20:V:33:ARG:O	20:V:36:SER:OG	2.10	0.66
13:M:349:LEU:O	13:M:352:SER:OG	2.07	0.66
16:P:253:LYS:NZ	16:P:414:LEU:O	2.28	0.66
2:B:171:SER:O	2:B:176:ARG:NH1	2.28	0.66
6:F:379:ILE:HD13	6:F:453:LEU:HD11	1.76	0.66
4:D:231:TYR:OH	4:D:239:LEU:O	2.13	0.66
7:G:412:LEU:HD21	7:G:443:ILE:CD1	2.25	0.66
9:I:155:THR:HG21	9:I:185:HIS:CD2	2.31	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:Y:87:ILE:HD12	23:Y:90:LEU:HD23	1.77	0.66
10:J:151:TYR:HE2	14:N:39:LEU:HD22	1.59	0.65
2:B:128:ILE:HG23	2:B:155:VAL:HG13	1.78	0.65
12:L:4:LEU:HD21	12:L:8:SER:OG	1.96	0.65
14:N:139:MET:O	14:N:142:SER:OG	2.13	0.65
14:N:273:PHE:O	14:N:276:THR:OG1	2.13	0.65
12:L:22:PHE:O	12:L:25:SER:OG	2.08	0.65
12:L:369:GLU:HB3	12:L:451:ILE:HG21	1.78	0.65
14:N:88:ILE:HD11	28:e:54:ILE:HD13	1.77	0.65
28:e:43:LEU:HD23	31:h:163:ARG:CD	2.26	0.65
33:j:73:GLU:OE1	33:j:73:GLU:N	2.29	0.65
2:B:124:GLN:NE2	8:H:222:TYR:O	2.29	0.65
14:N:4:ASN:OD1	14:N:6:SER:N	2.29	0.65
22:X:56:ARG:NH1	24:Z:125:ASP:O	2.29	0.65
23:Y:77:ALA:O	23:Y:81:ARG:N	2.29	0.65
22:X:4:THR:OG1	22:X:6:ASN:OD1	2.13	0.65
22:X:39:GLU:N	22:X:39:GLU:OE1	2.30	0.65
8:H:211:GLU:O	8:H:279:ARG:NH2	2.29	0.65
19:U:110:ASP:OD1	37:n:44:ARG:NH1	2.29	0.65
41:r:8:VAL:O	41:r:13:GLN:NE2	2.29	0.65
21:W:107:SER:OG	21:W:108:GLN:OE1	2.15	0.65
6:F:422:ALA:HB3	41:r:52:LEU:HD23	1.78	0.65
3:C:227:GLU:OE1	16:P:58:ARG:N	2.31	0.64
4:D:222:VAL:O	9:I:101:ARG:NH2	2.30	0.64
6:F:180:GLU:N	6:F:180:GLU:OE1	2.30	0.64
12:L:143:THR:HG22	12:L:205:TRP:HB2	1.78	0.64
4:D:271:ARG:NH2	9:I:70:GLU:OE2	2.31	0.64
7:G:274:ASN:O	7:G:296:ASN:ND2	2.30	0.64
12:L:378:MET:HB2	35:l:149:LEU:HD13	1.80	0.64
15:O:240:ASP:OD1	15:O:241:ALA:N	2.30	0.64
15:O:168:TYR:HD1	15:O:226:LEU:HD11	1.61	0.64
2:B:41:GLN:NE2	40:q:115:LEU:HD11	2.13	0.64
10:J:104:LYS:HG3	10:J:105:THR:HG23	1.79	0.64
15:O:382:TYR:O	27:d:47:ARG:NH1	2.30	0.64
18:R:62:TYR:O	40:q:125:TYR:OH	2.11	0.64
7:G:43:GLU:OE2	7:G:52:GLN:NE2	2.31	0.64
9:I:101:ARG:NH1	9:I:216:TYR:OH	2.30	0.64
30:g:46:THR:N	30:g:49:ASP:OD2	2.30	0.64
24:Z:64:ASP:OD1	24:Z:65:GLU:N	2.31	0.64
6:F:285:ASN:ND2	6:F:353:ASP:OD2	2.31	0.63
12:L:224:THR:HG22	12:L:225:LEU:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:20:ASN:OD1	28:e:22:GLN:N	2.31	0.63
40:q:45:ASP:OD1	40:q:46:LYS:N	2.31	0.63
2:B:155:VAL:HG11	2:B:182:ILE:HD11	1.80	0.63
12:L:303:THR:CG2	12:L:359:ALA:HB1	2.28	0.63
29:f:33:MET:HE3	31:h:126:LYS:N	2.13	0.63
12:L:174:GLU:OE1	12:L:174:GLU:N	2.31	0.63
13:M:232:LEU:O	39:p:126:TYR:OH	2.07	0.63
18:R:65:GLU:N	18:R:65:GLU:OE1	2.31	0.63
44:B:302:3PE:N	40:q:34:ASP:OD1	2.31	0.63
27:d:96:ASP:OD1	31:h:154:ARG:NH1	2.30	0.63
22:X:153:THR:HG23	31:h:158:GLN:HE21	1.64	0.63
39:p:42:HIS:O	39:p:44:ARG:NH2	2.32	0.63
8:H:72:LEU:HD11	16:P:386:ALA:HB2	1.81	0.63
12:L:61:LEU:O	12:L:64:SER:OG	2.11	0.63
33:j:60:ILE:HG22	34:k:76:PHE:CE2	2.34	0.63
2:B:95:ALA:O	2:B:98:ALA:N	2.30	0.63
6:F:250:VAL:HG22	6:F:255:THR:HG21	1.80	0.63
15:O:321:MET:HE3	15:O:321:MET:HA	1.80	0.63
10:J:148:LEU:HD13	11:K:65:THR:HG21	1.79	0.63
19:T:107:ASP:OD1	19:T:108:SER:N	2.32	0.63
19:U:93:LYS:NZ	19:U:94:LEU:O	2.31	0.63
30:g:45:LEU:HD22	30:g:49:ASP:HB3	1.81	0.63
5:E:183:ASP:OD1	42:s:87:ARG:NH1	2.32	0.62
12:L:169:TYR:CE1	12:L:170:ILE:HG23	2.34	0.62
12:L:253:SER:OG	12:L:283:GLY:O	2.17	0.62
1:A:1:MET:O	1:A:4:ILE:N	2.31	0.62
10:J:103:ASP:OD2	10:J:106:SER:OG	2.17	0.62
35:l:58:LEU:HD12	36:m:10:PHE:CE1	2.34	0.62
3:C:124:ARG:NH1	20:V:113:ASP:O	2.32	0.62
4:D:100:LEU:HD21	4:D:102:LEU:HD21	1.80	0.62
6:F:166:ALA:O	6:F:206:TYR:OH	2.16	0.62
15:O:135:LEU:HD12	15:O:366:ASP:CG	2.25	0.62
28:e:86:ARG:NH1	28:e:90:GLU:O	2.32	0.62
12:L:135:LYS:NZ	37:n:87:CYS:O	2.32	0.62
32:i:150:SER:N	32:i:154:ASP:OD2	2.33	0.62
27:d:85:VAL:HG23	31:h:157:TYR:CE2	2.34	0.62
8:H:5:GLU:OE2	25:a:36:ARG:NE	2.33	0.62
12:L:517:TYR:O	12:L:521:VAL:HG23	1.99	0.62
32:i:8:GLU:OE1	32:i:8:GLU:N	2.33	0.62
4:D:58:TYR:HH	12:L:539:TYR:HH	1.46	0.62
16:P:307:GLN:OE1	16:P:307:GLN:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:186:LEU:HD23	4:D:215:MET:HE3	1.81	0.62
12:L:18:SER:HB3	12:L:67:LEU:HD22	1.82	0.62
14:N:18:THR:O	14:N:21:THR:OG1	2.14	0.62
12:L:65:PHE:CD1	12:L:302:LEU:HD13	2.34	0.62
18:R:87:CYS:SG	18:R:89:GLY:N	2.73	0.62
1:A:16:THR:HG22	8:H:83:ILE:HD13	1.82	0.61
6:F:128:LEU:HD13	6:F:164:MET:SD	2.40	0.61
6:F:130:VAL:HG21	6:F:157:CYS:SG	2.40	0.61
14:N:118:MET:HG3	14:N:176:ALA:HB2	1.82	0.61
15:O:41:SER:O	15:O:46:ARG:NH2	2.33	0.61
15:O:225:GLU:N	15:O:225:GLU:OE1	2.33	0.61
15:O:256:GLN:O	15:O:258:LYS:NZ	2.29	0.61
8:H:39:GLN:OE1	8:H:41:ARG:NH1	2.32	0.61
22:X:80:CYS:SG	22:X:117:ASN:ND2	2.73	0.61
28:e:43:LEU:HD23	31:h:163:ARG:HD3	1.81	0.61
34:k:25:LEU:HD23	34:k:42:LEU:HD21	1.82	0.61
6:F:336:GLY:N	6:F:368:ALA:O	2.33	0.61
30:g:59:GLN:O	30:g:72:ARG:NH1	2.33	0.61
31:h:89:LEU:HD12	39:p:40:TRP:O	2.00	0.61
40:q:130:ASN:OD1	40:q:131:LYS:N	2.32	0.61
38:o:47:ALA:CB	38:o:62:ILE:HD13	2.31	0.61
16:P:49:ALA:O	16:P:53:ARG:NH2	2.33	0.61
19:U:80:LEU:HD21	19:U:96:VAL:HG23	1.81	0.61
23:Y:33:VAL:HG12	23:Y:37:MET:CE	2.31	0.61
8:H:50:MET:HE2	8:H:50:MET:H	1.66	0.61
7:G:259:ILE:HD12	7:G:285:LEU:HD12	1.83	0.61
7:G:581:ASN:OD1	7:G:582:GLY:N	2.33	0.61
10:J:34:THR:HG21	10:J:59:LEU:HB2	1.82	0.61
16:P:67:THR:HG22	16:P:91:ILE:HB	1.82	0.61
16:P:120:LEU:O	16:P:161:ARG:NH1	2.34	0.61
7:G:644:ASN:ND2	7:G:647:GLU:OE2	2.34	0.61
26:b:47:LYS:O	26:b:72:ARG:NH1	2.33	0.61
6:F:422:ALA:CB	41:r:52:LEU:HD23	2.31	0.60
7:G:361:LEU:CD2	7:G:659:LEU:HD21	2.31	0.60
9:I:80:ALA:HB2	41:r:19:LEU:HB2	1.83	0.60
27:d:5:ASN:N	27:d:100:LYS:O	2.35	0.60
27:d:6:ASP:HA	27:d:99:VAL:HG23	1.83	0.60
30:g:129:TYR:N	39:p:136:GLN:OE1	2.33	0.60
33:j:35:ASN:OD1	33:j:36:GLY:N	2.33	0.60
3:C:242:GLU:OE1	3:C:248:ARG:NH2	2.34	0.60
15:O:75:SER:N	15:O:329:GLU:OE2	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:O:92:ALA:N	48:O:501:DGT:O1A	2.32	0.60
13:M:339:PHE:CE1	13:M:407:LEU:HD22	2.36	0.60
16:P:196:GLU:N	16:P:196:GLU:OE1	2.35	0.60
39:p:36:GLN:N	39:p:36:GLN:OE1	2.34	0.60
28:e:44:GLU:OE1	28:e:44:GLU:N	2.34	0.60
40:q:92:THR:HG21	40:q:102:ARG:NH1	2.17	0.60
7:G:471:HIS:O	7:G:474:SER:OG	2.10	0.60
4:D:320:ASN:O	4:D:351:GLN:NE2	2.35	0.60
9:I:185:HIS:ND1	16:P:110:LEU:HD11	2.17	0.60
10:J:159:ILE:HD12	11:K:76:SER:OG	2.01	0.60
11:K:11:MET:CE	14:N:77:LEU:HD11	2.32	0.60
13:M:15:CYS:O	13:M:87:ASN:ND2	2.33	0.60
16:P:302:LEU:HD23	16:P:400:PRO:HG3	1.83	0.60
2:B:158:MET:SD	2:B:198:LEU:HD22	2.41	0.60
12:L:516:ASN:ND2	35:l:112:LEU:HD21	2.17	0.60
16:P:258:PRO:HD2	16:P:373:MET:HE1	1.84	0.60
7:G:412:LEU:HD21	7:G:443:ILE:HD12	1.84	0.59
31:h:104:GLU:OE2	31:h:113:SER:OG	2.20	0.59
8:H:176:GLN:NE2	8:H:248:ILE:O	2.34	0.59
13:M:317:LEU:HD23	13:M:425:MET:CE	2.32	0.59
37:n:34:ASN:OD1	37:n:35:VAL:N	2.34	0.59
4:D:345:SER:O	4:D:349:ILE:HD12	2.02	0.59
4:D:429:ILE:O	4:D:468:ARG:NH1	2.35	0.59
13:M:188:LEU:HD12	13:M:231:MET:CE	2.31	0.59
23:Y:33:VAL:HG12	23:Y:37:MET:HE2	1.84	0.59
15:O:297:THR:O	15:O:301:VAL:HG23	2.02	0.59
13:M:367:ILE:O	13:M:371:ASN:ND2	2.36	0.59
22:X:47:LEU:HD22	22:X:134:ILE:HD11	1.84	0.59
14:N:130:MET:HE2	14:N:175:MET:HG3	1.85	0.59
15:O:287:LEU:HD21	15:O:289:TYR:CD2	2.37	0.59
9:I:105:GLU:O	9:I:175:GLY:N	2.35	0.59
15:O:198:MET:HE2	15:O:215:TYR:CD1	2.37	0.59
19:T:110:ASP:O	19:T:114:VAL:HG23	2.02	0.59
22:X:47:LEU:CD2	22:X:134:ILE:HD11	2.32	0.59
12:L:416:ASN:OD1	12:L:417:ASP:N	2.35	0.59
34:k:42:LEU:HD23	34:k:42:LEU:O	2.03	0.59
7:G:350:GLN:O	7:G:549:LYS:N	2.32	0.59
16:P:179:SER:O	16:P:182:VAL:HG23	2.03	0.59
2:B:217:MET:HE1	16:P:96:GLY:C	2.28	0.59
13:M:284:ILE:O	13:M:287:SER:OG	2.19	0.59
1:A:113:LEU:HD23	1:A:113:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:237:ASN:ND2	12:L:294:LEU:HD11	2.18	0.58
12:L:563:LEU:HD21	23:Y:41:LEU:HD12	1.85	0.58
14:N:335:SER:O	27:d:75:ARG:NH2	2.36	0.58
15:O:262:ASP:OD1	15:O:263:ALA:N	2.36	0.58
39:p:50:THR:OG1	39:p:52:ASP:OD1	2.13	0.58
11:K:35:LEU:HA	11:K:38:ILE:HD12	1.85	0.58
16:P:173:ARG:NH2	16:P:274:ASP:O	2.36	0.58
19:T:116:MET:HE1	21:W:34:LYS:HA	1.85	0.58
27:d:103:LYS:O	39:p:56:THR:N	2.36	0.58
29:f:38:ASP:OD1	29:f:55:SER:OG	2.21	0.58
30:g:45:LEU:HB2	37:n:119:GLU:OE2	2.03	0.58
40:q:136:GLU:OE1	40:q:138:LYS:N	2.36	0.58
6:F:197:ILE:HD11	6:F:210:VAL:HG23	1.85	0.58
7:G:276:VAL:HG23	7:G:290:ARG:HB2	1.85	0.58
8:H:50:MET:HE2	8:H:50:MET:N	2.18	0.58
22:X:8:THR:OG1	24:Z:125:ASP:OD1	2.16	0.58
23:Y:156:MET:HE1	28:e:13:ASP:HA	1.86	0.58
33:j:56:TRP:O	33:j:60:ILE:HD12	2.04	0.58
5:E:72:MET:SD	5:E:105:VAL:HG22	2.43	0.58
9:I:155:THR:HG21	9:I:185:HIS:NE2	2.18	0.58
13:M:55:ASP:OD1	13:M:56:MET:N	2.36	0.58
13:M:192:LEU:HD22	13:M:286:LEU:HD11	1.86	0.58
22:X:153:THR:HG22	28:e:40:ALA:O	2.04	0.58
5:E:31:LEU:O	5:E:117:ARG:NH1	2.34	0.58
6:F:352:MET:SD	6:F:357:LEU:HD11	2.44	0.58
7:G:136:LEU:HD12	18:R:98:LYS:O	2.04	0.58
13:M:358:PRO:HB3	13:M:363:LEU:HD23	1.86	0.58
28:e:65:LYS:HA	28:e:68:MET:HE2	1.86	0.58
30:g:108:ARG:NH1	32:i:121:TRP:O	2.28	0.58
18:R:36:ILE:HD11	18:R:53:ASN:OD1	2.04	0.58
23:Y:73:THR:HG21	23:Y:95:ALA:CB	2.34	0.58
7:G:284:VAL:HG23	7:G:616:VAL:CG2	2.32	0.58
12:L:266:PHE:CD1	12:L:496:LEU:HD22	2.39	0.58
19:T:94:LEU:O	19:T:94:LEU:HD23	2.04	0.58
38:o:93:TYR:HE2	38:o:97:MET:HE3	1.67	0.58
4:D:461:VAL:HG13	4:D:466:ILE:HD11	1.86	0.58
12:L:231:TYR:HE1	12:L:298:MET:HE1	1.69	0.58
18:R:79:GLU:OE1	18:R:79:GLU:N	2.37	0.58
30:g:137:LEU:HD21	39:p:140:LEU:HB3	1.86	0.58
11:K:80:SER:O	11:K:84:THR:HG23	2.04	0.57
13:M:413:SER:HG	37:n:98:TRP:CG	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:64:ASP:CG	20:V:66:THR:HG1	2.12	0.57
36:m:6:GLU:N	36:m:6:GLU:OE1	2.37	0.57
4:D:239:LEU:HD11	9:I:217:ARG:HA	1.85	0.57
20:V:44:TYR:CD2	20:V:94:MET:HE2	2.39	0.57
1:A:58:PHE:CE1	11:K:79:VAL:HG21	2.39	0.57
2:B:103:HIS:ND1	4:D:213:GLU:OE2	2.37	0.57
14:N:19:LEU:HD22	28:e:11:LEU:HD23	1.85	0.57
16:P:202:TYR:HE1	16:P:206:LEU:HD11	1.69	0.57
29:f:43:TYR:OH	31:h:120:ASP:OD2	2.20	0.57
2:B:69:GLU:N	2:B:69:GLU:OE1	2.36	0.57
8:H:5:GLU:OE1	25:a:59:TYR:OH	2.21	0.57
15:O:296:GLU:HB2	15:O:299:VAL:HG22	1.85	0.57
19:T:112:VAL:HG21	21:W:30:LEU:CD1	2.33	0.57
31:h:155:ASN:ND2	31:h:161:TYR:O	2.37	0.57
6:F:369:ILE:HG22	6:F:371:VAL:HG23	1.85	0.57
15:O:277:LEU:HD22	15:O:286:LEU:HD22	1.85	0.57
16:P:146:THR:OG1	16:P:149:PHE:N	2.38	0.57
7:G:550:VAL:HG13	7:G:571:PHE:HD2	1.69	0.57
3:C:71:LEU:HD21	3:C:101:PHE:CD2	2.40	0.57
9:I:80:ALA:HB2	41:r:19:LEU:CB	2.35	0.57
15:O:117:ASP:O	15:O:120:TYR:N	2.37	0.57
20:V:64:ASP:OD1	20:V:66:THR:OG1	2.22	0.57
7:G:365:VAL:HG21	7:G:652:LEU:CD1	2.34	0.57
10:J:11:ILE:O	10:J:14:SER:OG	2.16	0.57
13:M:301:TYR:CE1	13:M:305:ILE:HD11	2.40	0.57
15:O:198:MET:HE2	15:O:215:TYR:HD1	1.70	0.57
3:C:217:GLU:OE1	16:P:81:ASN:ND2	2.37	0.57
7:G:185:THR:HG23	7:G:187:MET:HE2	1.87	0.57
12:L:409:CYS:SG	12:L:410:GLY:N	2.78	0.57
14:N:24:SER:OG	14:N:30:ALA:N	2.38	0.57
25:a:8:GLY:O	25:a:12:ILE:HD12	2.05	0.57
12:L:412:LEU:HD11	19:U:78:ARG:HH22	1.69	0.57
10:J:31:LEU:O	10:J:35:ILE:HD12	2.05	0.56
23:Y:69:ALA:HB2	23:Y:99:VAL:HG21	1.87	0.56
23:Y:118:GLY:O	23:Y:122:VAL:HG23	2.05	0.56
5:E:88:ILE:CD1	7:G:224:VAL:HG11	2.34	0.56
12:L:269:ASP:O	12:L:273:ILE:HD12	2.05	0.56
15:O:157:ALA:O	15:O:161:ILE:HD12	2.04	0.56
2:B:135:THR:HG21	4:D:121:LEU:O	2.05	0.56
4:D:154:GLN:NE2	4:D:314:ASP:OD2	2.38	0.56
4:D:262:GLU:O	4:D:266:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:77:GLU:OE2	17:Q:161:LYS:NZ	2.39	0.56
10:J:4:LEU:HD22	10:J:99:SER:HB2	1.86	0.56
14:N:150:LEU:O	14:N:154:VAL:HG23	2.05	0.56
14:N:311:ASN:OD1	14:N:312:MET:N	2.38	0.56
15:O:277:LEU:HD22	15:O:286:LEU:CD2	2.35	0.56
19:T:77:GLU:O	19:T:81:LEU:HD23	2.05	0.56
4:D:150:MET:HE1	4:D:229:ALA:HB3	1.87	0.56
10:J:111:LEU:HD13	11:K:51:ASN:CG	2.31	0.56
12:L:103:LEU:HD23	12:L:115:LEU:HD22	1.87	0.56
6:F:127:TYR:HB2	6:F:255:THR:HG22	1.88	0.56
7:G:383:GLN:NE2	7:G:384:GLY:O	2.39	0.56
7:G:414:VAL:O	7:G:414:VAL:HG13	2.05	0.56
7:G:694:ARG:NH1	7:G:717:ASN:OD1	2.38	0.56
37:n:54:ASP:OD1	37:n:55:LEU:N	2.37	0.56
1:A:51:LEU:HG	4:D:85:LEU:HD22	1.87	0.56
6:F:129:VAL:HG11	6:F:227:LEU:HD22	1.87	0.56
14:N:98:MET:HG3	14:N:144:LEU:HD13	1.88	0.56
15:O:243:LYS:HA	15:O:246:ILE:HG22	1.87	0.56
19:T:134:LEU:C	19:T:135:LEU:HD12	2.31	0.56
23:Y:138:THR:OG1	23:Y:140:ILE:O	2.23	0.56
32:i:94:ARG:O	32:i:97:THR:OG1	2.23	0.56
7:G:282:ASN:OD1	7:G:617:SER:N	2.38	0.56
8:H:76:LEU:O	8:H:79:TYR:N	2.39	0.56
12:L:166:SER:OG	12:L:167:TRP:N	2.39	0.56
32:i:133:ARG:NH1	39:p:93:TYR:O	2.39	0.56
15:O:239:VAL:HG21	15:O:266:SER:HB3	1.87	0.56
17:Q:167:ASN:OD1	17:Q:168:TYR:N	2.39	0.56
18:R:60:LYS:NZ	40:q:120:GLU:OE2	2.35	0.56
22:X:153:THR:OG1	31:h:156:ASP:O	2.14	0.56
28:e:26:LYS:NZ	28:e:60:CYS:SG	2.67	0.56
4:D:184:ARG:NH1	4:D:406:GLU:O	2.38	0.55
19:U:100:PHE:O	19:U:106:LEU:N	2.37	0.55
39:p:87:PHE:HA	39:p:105:LEU:HD22	1.88	0.55
4:D:378:THR:O	7:G:136:LEU:HD11	2.05	0.55
3:C:168:TYR:O	3:C:172:ILE:HD12	2.06	0.55
7:G:351:ILE:HD12	7:G:550:VAL:HB	1.87	0.55
13:M:137:LEU:HD21	14:N:298:MET:HE2	1.89	0.55
13:M:293:THR:HB	36:m:113:ILE:HD13	1.89	0.55
39:p:117:PHE:O	39:p:121:GLY:N	2.39	0.55
3:C:215:ASP:OD1	3:C:216:ASP:N	2.39	0.55
8:H:124:MET:HE2	10:J:67:ILE:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:316:CYS:O	13:M:320:VAL:HG23	2.05	0.55
4:D:265:ASP:OD1	24:Z:27:ARG:NH1	2.37	0.55
6:F:442:LEU:HD23	43:F:502:SF4:S1	2.46	0.55
12:L:567:TRP:CH2	12:L:571:LEU:HD21	2.42	0.55
13:M:327:SER:HB3	13:M:332:ILE:HG21	1.89	0.55
9:I:85:GLU:OE1	9:I:85:GLU:N	2.40	0.55
12:L:340:LEU:HD22	12:L:423:LEU:HD13	1.87	0.55
19:T:140:ILE:O	19:T:144:VAL:HG23	2.07	0.55
3:C:113:LEU:HD21	3:C:116:ILE:HD11	1.89	0.55
12:L:250:LEU:HD22	12:L:291:MET:HE3	1.87	0.55
6:F:191:ALA:HB1	6:F:197:ILE:HG22	1.89	0.55
7:G:631:ALA:O	7:G:635:VAL:HG23	2.07	0.55
8:H:260:TYR:OH	25:a:20:ILE:HD13	2.07	0.55
9:I:54:GLU:OE1	9:I:56:ALA:N	2.37	0.55
10:J:1:MET:HE1	10:J:3:GLN:HB2	1.89	0.55
12:L:467:VAL:HA	12:L:470:LEU:HD12	1.88	0.55
14:N:118:MET:HE1	14:N:130:MET:SD	2.47	0.55
21:W:78:MET:HE3	21:W:78:MET:HA	1.88	0.55
35:l:102:GLN:HB3	36:m:21:LEU:HD13	1.88	0.55
13:M:329:SER:HB2	13:M:332:ILE:HG22	1.89	0.55
24:Z:134:GLU:OE2	28:e:69:ARG:NH1	2.40	0.55
7:G:275:ILE:HG23	7:G:287:ILE:HG23	1.87	0.55
15:O:168:TYR:CD1	15:O:226:LEU:HD11	2.42	0.55
34:k:37:LEU:HD13	37:n:41:VAL:HG12	1.88	0.55
1:A:89:TRP:CZ3	8:H:309:ILE:HD11	2.42	0.54
7:G:438:LEU:HD23	7:G:440:ILE:HD11	1.88	0.54
7:G:562:THR:O	7:G:565:GLN:N	2.39	0.54
12:L:104:LEU:HD13	12:L:117:TRP:N	2.22	0.54
12:L:217:SER:O	12:L:221:HIS:ND1	2.39	0.54
15:O:154:ASP:OD2	15:O:155:LEU:N	2.40	0.54
3:C:248:ARG:CZ	7:G:68:VAL:HG22	2.38	0.54
13:M:103:THR:HG21	13:M:226:LEU:HD11	1.87	0.54
38:o:81:GLN:OE1	38:o:81:GLN:N	2.39	0.54
1:A:51:LEU:CD1	8:H:136:LEU:HD22	2.34	0.54
7:G:354:ILE:HD11	7:G:543:ALA:HB3	1.89	0.54
14:N:92:PHE:HA	14:N:95:MET:HE2	1.89	0.54
14:N:108:ALA:HB3	14:N:109:PRO:HD3	1.90	0.54
14:N:236:LEU:HD21	27:d:44:TRP:NE1	2.22	0.54
15:O:201:MET:HB3	15:O:207:LEU:HD23	1.90	0.54
37:n:74:HIS:ND1	37:n:76:GLN:O	2.41	0.54
2:B:41:GLN:HE21	40:q:115:LEU:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:162:LEU:HD23	12:L:162:LEU:O	2.07	0.54
14:N:171:LEU:HD21	14:N:226:LEU:HD21	1.89	0.54
7:G:248:LYS:O	7:G:251:SER:OG	2.23	0.54
14:N:45:LEU:O	14:N:53:SER:OG	2.23	0.54
3:C:70:CYS:C	3:C:71:LEU:HD22	2.32	0.54
12:L:349:ASN:O	12:L:353:CYS:N	2.38	0.54
22:X:8:THR:O	22:X:56:ARG:NH2	2.39	0.54
3:C:152:LEU:O	21:W:17:ILE:HD11	2.07	0.54
10:J:82:MET:SD	10:J:83:LYS:NZ	2.69	0.54
20:V:35:VAL:O	20:V:45:ARG:NH2	2.41	0.54
12:L:414:MET:HE3	12:L:414:MET:O	2.07	0.54
12:L:515:LEU:HB2	35:l:112:LEU:HD13	1.88	0.54
12:L:519:GLN:OE1	13:M:266:ARG:NH1	2.40	0.54
13:M:67:TRP:CZ2	13:M:427:LEU:HD22	2.43	0.54
14:N:202:PHE:O	14:N:205:SER:OG	2.18	0.54
15:O:126:TYR:OH	15:O:378:PRO:O	2.16	0.54
38:o:53:PHE:O	38:o:55:ASP:N	2.41	0.54
3:C:237:LEU:HD12	4:D:392:GLN:HA	1.89	0.54
9:I:36:ILE:HG22	9:I:48:ASN:HA	1.89	0.54
21:W:76:ILE:O	21:W:80:VAL:HG23	2.08	0.54
21:W:87:LEU:O	21:W:91:VAL:HG23	2.07	0.54
3:C:179:PHE:HD2	21:W:78:MET:HE1	1.73	0.54
15:O:290:ASP:OD1	15:O:291:TRP:N	2.40	0.54
16:P:101:VAL:HG23	16:P:104:LEU:HD12	1.89	0.54
31:h:112:ILE:HA	31:h:116:ILE:HD12	1.90	0.54
4:D:53:SER:HG	14:N:224:ASN:CG	2.09	0.53
4:D:267:LEU:HD21	4:D:273:TRP:CE2	2.43	0.53
8:H:24:VAL:HG11	8:H:236:ALA:HA	1.89	0.53
8:H:124:MET:CE	10:J:67:ILE:HG22	2.39	0.53
12:L:38:GLU:O	32:i:128:ARG:N	2.41	0.53
13:M:281:HIS:NE2	13:M:354:ASN:OD1	2.41	0.53
16:P:58:ARG:NH1	16:P:109:ASP:OD1	2.40	0.53
1:A:19:MET:HE3	8:H:83:ILE:HD11	1.89	0.53
4:D:99:VAL:O	4:D:120:LEU:HD12	2.07	0.53
6:F:298:ASN:ND2	6:F:321:GLY:O	2.41	0.53
8:H:283:ASP:OD1	8:H:284:LYS:N	2.41	0.53
15:O:74:THR:N	15:O:329:GLU:OE2	2.39	0.53
22:X:164:PRO:O	27:d:13:ASN:ND2	2.41	0.53
31:h:120:ASP:OD1	31:h:121:GLN:N	2.42	0.53
15:O:108:MET:HE2	15:O:186:VAL:HG21	1.88	0.53
15:O:115:ASP:OD1	15:O:118:LEU:HD23	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:36:MET:HA	26:b:39:ILE:HD12	1.90	0.53
12:L:69:ILE:O	12:L:73:VAL:HG23	2.08	0.53
12:L:224:THR:N	12:L:227:THR:OG1	2.41	0.53
12:L:117:TRP:CZ3	12:L:232:LEU:HD22	2.44	0.53
15:O:172:ILE:CD1	15:O:346:LEU:HD13	2.39	0.53
37:n:30:TYR:OH	37:n:39:ARG:NH1	2.42	0.53
8:H:23:SER:O	8:H:27:LEU:N	2.38	0.53
12:L:407:LEU:O	12:L:409:CYS:N	2.40	0.53
13:M:363:LEU:O	13:M:367:ILE:HD12	2.08	0.53
34:k:37:LEU:CD1	37:n:45:ALA:HB2	2.38	0.53
4:D:211:GLU:N	4:D:211:GLU:OE1	2.41	0.53
5:E:52:ASN:ND2	5:E:82:GLN:OE1	2.42	0.53
9:I:183:GLU:OE1	40:q:117:GLY:N	2.42	0.53
12:L:74:ILE:CD1	12:L:91:ILE:HD12	2.39	0.53
13:M:128:LEU:O	13:M:136:ARG:NH1	2.36	0.53
13:M:205:PRO:O	13:M:209:VAL:HG23	2.09	0.53
14:N:313:ASN:OD1	14:N:314:SER:N	2.41	0.53
20:V:85:GLU:O	20:V:89:ILE:HD12	2.09	0.53
32:i:79:ASN:OD1	32:i:80:VAL:N	2.41	0.53
6:F:192:TYR:CD1	6:F:197:ILE:HG23	2.44	0.53
13:M:195:MET:SD	13:M:282:MET:HE3	2.49	0.53
13:M:280:ALA:O	13:M:284:ILE:HD12	2.09	0.53
14:N:231:VAL:O	15:O:371:ARG:NH2	2.42	0.53
22:X:136:SER:OG	26:b:62:ARG:NH2	2.42	0.53
33:j:47:GLY:O	33:j:51:VAL:HG23	2.09	0.53
13:M:284:ILE:HD11	13:M:387:LEU:HD21	1.91	0.53
25:a:7:PRO:O	25:a:11:ILE:HD12	2.09	0.53
31:h:125:GLU:OE1	31:h:125:GLU:N	2.42	0.53
1:A:51:LEU:HD22	8:H:136:LEU:HD22	1.90	0.52
5:E:77:ASP:OD1	5:E:81:ARG:NH1	2.41	0.52
11:K:93:PHE:CE1	14:N:58:LEU:HD21	2.45	0.52
12:L:169:TYR:CD1	12:L:170:ILE:HG23	2.44	0.52
1:A:27:LYS:NZ	2:B:151:GLU:OE1	2.28	0.52
3:C:89:LEU:HD22	20:V:112:TRP:CZ3	2.44	0.52
4:D:241:MET:HE3	4:D:245:LEU:HD22	1.92	0.52
7:G:575:ILE:HG22	7:G:575:ILE:O	2.10	0.52
15:O:42:GLY:HA2	15:O:106:LEU:HD13	1.90	0.52
40:q:115:LEU:HD12	40:q:120:GLU:HB2	1.91	0.52
21:W:39:GLN:O	21:W:43:ILE:HD12	2.08	0.52
12:L:155:LEU:HD21	13:M:370:LEU:CD1	2.40	0.52
16:P:180:LEU:N	16:P:220:PRO:O	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:b:51:ASN:O	26:b:72:ARG:NE	2.43	0.52
30:g:107:GLN:HG3	39:p:78:GLU:OE2	2.08	0.52
2:B:102:MET:CE	4:D:190:MET:HE1	2.39	0.52
5:E:39:GLU:N	5:E:39:GLU:OE1	2.42	0.52
7:G:372:ASN:ND2	7:G:377:GLU:OE1	2.42	0.52
7:G:400:SER:O	7:G:401:THR:OG1	2.26	0.52
12:L:66:VAL:HG22	12:L:223:SER:CB	2.39	0.52
12:L:516:ASN:CG	35:l:112:LEU:HD21	2.34	0.52
12:L:231:TYR:CE1	12:L:298:MET:HE1	2.44	0.52
12:L:525:PHE:CE2	36:m:76:VAL:HG22	2.45	0.52
13:M:222:ILE:HB	13:M:223:MET:HE2	1.92	0.52
14:N:304:ASN:ND2	15:O:352:VAL:O	2.43	0.52
39:p:78:GLU:O	39:p:81:ASN:N	2.43	0.52
12:L:291:MET:HE2	12:L:291:MET:HA	1.92	0.52
14:N:128:MET:HE3	14:N:132:TRP:CB	2.40	0.52
16:P:274:ASP:OD1	16:P:276:ASP:N	2.38	0.52
18:R:57:VAL:HG23	18:R:58:ASN:OD1	2.10	0.52
19:U:134:LEU:HD21	19:U:143:TYR:HB2	1.90	0.52
22:X:56:ARG:NH1	24:Z:125:ASP:OD2	2.43	0.52
24:Z:101:LEU:HD21	28:e:77:ARG:HB2	1.92	0.52
3:C:188:ARG:NH2	3:C:191:THR:OG1	2.40	0.52
4:D:175:ILE:HD12	4:D:361:ILE:HD11	1.90	0.52
6:F:189:ALA:HA	42:s:97:MET:HE1	1.92	0.52
8:H:67:GLN:OE1	8:H:225:GLY:N	2.39	0.52
10:J:20:MET:SD	10:J:25:ALA:HB1	2.50	0.52
13:M:123:THR:O	13:M:127:ILE:HD12	2.10	0.52
35:l:52:ALA:O	35:l:57:LEU:N	2.43	0.52
40:q:35:ASP:OD2	40:q:36:LEU:N	2.42	0.52
4:D:465:GLU:HG3	4:D:466:ILE:HD13	1.91	0.52
8:H:8:LEU:HD13	25:a:27:ASP:OD1	2.10	0.52
10:J:4:LEU:HD22	10:J:99:SER:CB	2.39	0.52
10:J:111:LEU:HD11	11:K:48:ILE:HG13	1.91	0.52
40:q:19:GLU:OE1	40:q:19:GLU:N	2.42	0.52
3:C:179:PHE:CD2	21:W:78:MET:HE1	2.45	0.52
12:L:522:VAL:HG11	13:M:263:VAL:HG13	1.92	0.52
35:l:102:GLN:HG2	35:l:103:HIS:H	1.74	0.52
1:A:56:ARG:O	1:A:59:LEU:N	2.42	0.51
2:B:217:MET:HE1	16:P:96:GLY:HA2	1.92	0.51
7:G:442:SER:N	7:G:454:GLU:O	2.43	0.51
1:A:73:LEU:O	10:J:137:TYR:OH	2.25	0.51
8:H:165:GLY:O	8:H:166:SER:OG	2.18	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:79:ILE:HD12	13:M:130:TRP:CD1	2.45	0.51
14:N:274:MET:HA	14:N:274:MET:HE2	1.92	0.51
21:W:54:GLU:N	21:W:54:GLU:OE1	2.42	0.51
1:A:47:SER:O	1:A:49:SER:N	2.43	0.51
2:B:96:CYS:SG	4:D:228:HIS:CE1	3.03	0.51
5:E:76:LEU:HD23	5:E:94:VAL:HG21	1.91	0.51
8:H:175:TYR:O	24:Z:57:THR:HG21	2.10	0.51
16:P:153:ASP:OD1	16:P:154:VAL:N	2.44	0.51
18:R:47:ASP:OD1	18:R:48:LYS:N	2.43	0.51
18:R:103:LEU:HD21	18:R:118:PHE:HB3	1.93	0.51
19:T:75:ILE:O	19:T:79:VAL:HG23	2.11	0.51
39:p:29:SER:O	39:p:30:ILE:HD13	2.10	0.51
40:q:13:LEU:O	40:q:17:VAL:HG12	2.09	0.51
6:F:328:ASN:OD1	6:F:374:LYS:N	2.38	0.51
24:Z:138:HIS:NE2	28:e:73:MET:HE2	2.26	0.51
38:o:7:HIS:ND1	38:o:14:MET:SD	2.73	0.51
6:F:399:PRO:O	6:F:403:GLY:N	2.38	0.51
10:J:167:LYS:O	11:K:83:ARG:NH2	2.44	0.51
12:L:330:LEU:HD13	12:L:408:ASN:O	2.09	0.51
12:L:414:MET:HE1	33:j:28:SER:HB2	1.92	0.51
30:g:146:THR:HG22	30:g:146:THR:O	2.11	0.51
4:D:101:ARG:CB	4:D:120:LEU:HD11	2.41	0.51
4:D:270:ASN:O	4:D:274:VAL:HG23	2.10	0.51
14:N:254:LEU:HD22	14:N:330:GLY:HA3	1.93	0.51
22:X:10:PRO:HG2	24:Z:88:LEU:HD13	1.93	0.51
39:p:58:ASP:O	39:p:61:CYS:N	2.44	0.51
15:O:74:THR:HG1	15:O:333:CYS:HG	1.51	0.51
19:U:125:GLU:OE2	37:n:24:ARG:NH1	2.43	0.51
22:X:2:VAL:N	24:Z:134:GLU:OE2	2.44	0.51
24:Z:72:GLN:NE2	25:a:43:PHE:CD2	2.78	0.51
4:D:267:LEU:HD21	4:D:273:TRP:CD2	2.46	0.51
19:T:104:LEU:HD23	19:T:106:LEU:HD12	1.93	0.51
19:U:151:TYR:OH	32:i:43:LEU:HD22	2.11	0.51
40:q:88:MET:HE3	40:q:88:MET:O	2.09	0.51
7:G:430:ARG:O	7:G:434:VAL:HG23	2.10	0.51
8:H:170:ILE:HD12	8:H:170:ILE:H	1.75	0.51
8:H:277:LEU:HD21	9:I:75:PHE:HE1	1.76	0.51
14:N:14:MET:CE	14:N:128:MET:HE2	2.41	0.51
19:T:71:SER:O	19:T:74:LEU:N	2.43	0.51
29:f:28:LYS:HE3	29:f:28:LYS:HA	1.93	0.51
11:K:27:HIS:ND1	16:P:390:TYR:OH	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:120:LEU:HD12	49:P:501:NDP:N6A	2.25	0.51
32:i:140:ASP:OD1	39:p:5:ARG:NH1	2.41	0.51
1:A:78:ILE:HG23	1:A:79:ILE:CD1	2.41	0.50
4:D:79:GLU:OE1	4:D:79:GLU:N	2.41	0.50
4:D:101:ARG:HB2	4:D:120:LEU:HD11	1.92	0.50
4:D:150:MET:HE1	4:D:229:ALA:CB	2.41	0.50
8:H:26:PHE:CZ	25:a:11:ILE:HD13	2.46	0.50
10:J:148:LEU:HD11	11:K:62:MET:SD	2.51	0.50
12:L:44:LEU:HB3	13:M:444:LEU:HD21	1.93	0.50
12:L:519:GLN:NE2	35:l:109:ASP:OD1	2.43	0.50
13:M:317:LEU:HD23	13:M:425:MET:HE1	1.92	0.50
27:d:116:ARG:NH2	36:m:95:GLU:OE2	2.44	0.50
32:i:137:VAL:HG13	38:o:66:ALA:HA	1.93	0.50
34:k:37:LEU:HD22	37:n:41:VAL:CG1	2.41	0.50
3:C:71:LEU:HD21	3:C:101:PHE:CE2	2.46	0.50
9:I:179:GLU:OE1	9:I:179:GLU:N	2.41	0.50
15:O:310:ASN:OD1	15:O:311:GLN:N	2.45	0.50
3:C:150:ASP:OD1	3:C:153:THR:N	2.42	0.50
6:F:353:ASP:N	6:F:353:ASP:OD1	2.44	0.50
8:H:72:LEU:HD13	16:P:384:TYR:HA	1.94	0.50
14:N:76:ILE:O	14:N:80:LEU:N	2.44	0.50
19:U:73:LYS:NZ	34:k:7:GLU:OE2	2.44	0.50
21:W:47:TYR:CZ	21:W:93:ILE:HG23	2.45	0.50
30:g:58:TRP:CZ2	32:i:6:ALA:HB2	2.46	0.50
8:H:149:TYR:HE2	8:H:285:LEU:HD21	1.76	0.50
12:L:310:LEU:HB2	12:L:429:LEU:HD22	1.92	0.50
12:L:475:ILE:HD11	12:L:485:LYS:HE3	1.93	0.50
23:Y:36:SER:O	23:Y:40:VAL:HG13	2.11	0.50
6:F:332:VAL:HG12	6:F:371:VAL:HG22	1.93	0.50
7:G:202:GLU:O	7:G:430:ARG:NE	2.42	0.50
7:G:259:ILE:CD1	7:G:285:LEU:HD12	2.42	0.50
7:G:460:ALA:O	7:G:463:VAL:HG12	2.11	0.50
12:L:141:MET:HE1	44:L:601:3PE:O21	2.12	0.50
15:O:407:ILE:HD12	15:O:407:ILE:H	1.77	0.50
25:a:38:ASN:OD1	25:a:39:MET:N	2.45	0.50
34:k:37:LEU:HD11	37:n:45:ALA:HB2	1.92	0.50
38:o:47:ALA:HB1	38:o:62:ILE:HD13	1.93	0.50
1:A:21:LEU:O	1:A:24:ILE:HG22	2.11	0.50
6:F:386:ILE:HD11	6:F:450:VAL:HG13	1.93	0.50
7:G:120:ARG:NH1	41:r:58:CYS:O	2.44	0.50
9:I:149:ARG:NH1	40:q:126:SER:OG	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:255:LEU:HD11	12:L:500:TRP:CH2	2.46	0.50
12:L:262:LEU:HB3	12:L:496:LEU:HD21	1.93	0.50
19:T:118:MET:HE3	19:T:140:ILE:HD12	1.94	0.50
21:W:19:SER:OG	21:W:77:ASP:OD1	2.21	0.50
28:e:43:LEU:HD23	31:h:163:ARG:HD2	1.93	0.50
9:I:153:ASP:OD1	9:I:155:THR:OG1	2.12	0.50
12:L:496:LEU:HD23	12:L:496:LEU:O	2.11	0.50
7:G:544:VAL:HG22	7:G:566:LEU:HD23	1.94	0.50
12:L:471:PHE:O	12:L:475:ILE:HG22	2.12	0.50
6:F:138:GLY:HA3	6:F:370:ILE:HD11	1.94	0.50
10:J:45:THR:HG22	10:J:46:LYS:N	2.26	0.50
12:L:327:ASP:OD1	12:L:329:ARG:N	2.42	0.50
15:O:266:SER:O	15:O:269:GLU:N	2.45	0.50
1:A:78:ILE:HG23	1:A:79:ILE:HD12	1.92	0.49
4:D:404:ALA:HB1	4:D:411:GLU:HG3	1.94	0.49
6:F:50:LEU:HD12	6:F:305:GLU:HA	1.93	0.49
10:J:41:THR:O	10:J:45:THR:OG1	2.16	0.49
13:M:103:THR:CG2	13:M:226:LEU:HD11	2.42	0.49
13:M:376:TRP:CZ3	36:m:87:LEU:HD21	2.44	0.49
14:N:61:PHE:O	14:N:65:VAL:HG12	2.12	0.49
16:P:95:ARG:NH1	49:P:501:NDP:O1X	2.44	0.49
19:T:111:HIS:CE1	19:T:134:LEU:HD11	2.43	0.49
23:Y:64:MET:N	23:Y:64:MET:HE2	2.27	0.49
30:g:107:GLN:O	32:i:124:LYS:NZ	2.45	0.49
4:D:335:TYR:O	4:D:339:VAL:HG23	2.12	0.49
24:Z:42:THR:O	24:Z:46:VAL:HG23	2.12	0.49
32:i:20:ARG:HG2	36:m:26:LEU:HD22	1.93	0.49
2:B:111:MET:HE3	2:B:116:VAL:HG12	1.95	0.49
3:C:202:ARG:NH1	4:D:130:GLU:OE2	2.39	0.49
4:D:261:ASP:OD1	4:D:343:ARG:NH2	2.41	0.49
9:I:142:ASP:OD1	9:I:144:SER:OG	2.26	0.49
12:L:65:PHE:HD1	12:L:302:LEU:HD13	1.78	0.49
16:P:41:ARG:NH1	16:P:276:ASP:OD1	2.43	0.49
23:Y:39:ASP:OD1	23:Y:42:THR:OG1	2.30	0.49
26:b:53:ARG:NH1	26:b:74:ASP:O	2.42	0.49
2:B:45:VAL:HG22	2:B:46:ALA:H	1.77	0.49
4:D:272:ILE:CD1	8:H:277:LEU:HD12	2.36	0.49
10:J:134:ASN:ND2	31:h:180:LEU:HD13	2.27	0.49
15:O:114:VAL:HG11	15:O:163:MET:CE	2.40	0.49
23:Y:87:ILE:O	23:Y:91:ILE:HD12	2.13	0.49
3:C:164:ALA:HB2	4:D:291:TYR:C	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:231:GLU:OE1	7:G:231:GLU:N	2.39	0.49
12:L:141:MET:HE1	44:L:601:3PE:C21	2.43	0.49
21:W:39:GLN:HB3	21:W:43:ILE:HD11	1.95	0.49
23:Y:139:PRO:HG2	23:Y:140:ILE:HD12	1.95	0.49
34:k:37:LEU:HD22	37:n:41:VAL:HG13	1.95	0.49
36:m:45:ASP:HB3	36:m:48:LEU:HD12	1.93	0.49
3:C:106:HIS:N	20:V:87:GLU:OE2	2.43	0.49
22:X:81:HIS:ND1	25:a:64:LEU:HD11	2.27	0.49
27:d:95:ASP:OD1	27:d:96:ASP:N	2.45	0.49
40:q:51:TYR:CE2	40:q:65:ILE:HD12	2.47	0.49
40:q:58:PHE:O	40:q:62:ASN:N	2.46	0.49
15:O:159:PHE:O	15:O:163:MET:N	2.35	0.49
16:P:405:CYS:SG	16:P:406:ILE:N	2.85	0.49
23:Y:73:THR:HG21	23:Y:95:ALA:HB2	1.95	0.49
31:h:80:ALA:CB	31:h:108:ILE:HD11	2.43	0.49
14:N:219:LYS:NZ	15:O:345:ASP:OD2	2.41	0.49
15:O:280:ILE:HG22	15:O:284:ALA:HB3	1.93	0.49
2:B:174:VAL:O	2:B:176:ARG:NH2	2.46	0.49
4:D:58:TYR:OH	12:L:539:TYR:OH	2.24	0.49
4:D:307:LEU:HD11	4:D:411:GLU:OE2	2.13	0.49
7:G:574:TYR:CZ	7:G:583:ALA:HB2	2.48	0.49
14:N:266:LEU:C	14:N:266:LEU:HD23	2.38	0.49
22:X:156:LEU:HD21	27:d:84:ALA:HB3	1.94	0.49
40:q:59:TYR:O	40:q:90:TYR:OH	2.25	0.49
4:D:56:VAL:HG13	14:N:167:ASN:OD1	2.13	0.48
4:D:148:SER:OG	4:D:187:ASN:ND2	2.45	0.48
15:O:357:VAL:O	15:O:361:VAL:HG23	2.13	0.48
19:U:135:LEU:N	19:U:139:ASP:OD2	2.43	0.48
20:V:90:LEU:O	20:V:94:MET:N	2.44	0.48
31:h:107:PRO:O	31:h:110:ARG:N	2.46	0.48
8:H:265:PHE:O	8:H:269:VAL:HG23	2.13	0.48
12:L:423:LEU:O	12:L:426:MET:N	2.46	0.48
13:M:62:ILE:HG23	13:M:101:ILE:CD1	2.43	0.48
14:N:136:ALA:O	14:N:140:LEU:HD23	2.14	0.48
15:O:231:LEU:HD12	15:O:285:GLU:O	2.14	0.48
16:P:98:ASP:OD1	16:P:99:SER:N	2.46	0.48
16:P:127:ARG:HG2	16:P:165:ILE:HG23	1.96	0.48
19:U:70:LEU:HD23	19:U:75:ILE:HD11	1.96	0.48
21:W:43:ILE:HD12	21:W:43:ILE:H	1.78	0.48
29:f:33:MET:HE1	31:h:122:GLN:O	2.13	0.48
7:G:447:ILE:HD12	7:G:449:LEU:HD21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:307:PHE:CE2	24:Z:51:LEU:HD22	2.48	0.48
16:P:328:LYS:O	16:P:331:SER:OG	2.30	0.48
34:k:22:VAL:O	34:k:24:GLN:N	2.46	0.48
4:D:68:VAL:HG23	4:D:68:VAL:O	2.12	0.48
11:K:3:MET:HE3	11:K:4:ILE:HD11	1.94	0.48
12:L:522:VAL:CG1	13:M:263:VAL:HG22	2.43	0.48
13:M:152:LEU:HB3	14:N:279:MET:HE2	1.96	0.48
14:N:321:MET:HE3	27:d:42:ILE:HA	1.94	0.48
15:O:172:ILE:HD13	15:O:346:LEU:HD13	1.95	0.48
18:R:102:ASN:OD1	18:R:103:LEU:N	2.45	0.48
19:T:79:VAL:HG11	19:T:141:ILE:HG13	1.95	0.48
20:V:100:TRP:NE1	20:V:101:GLU:OE2	2.46	0.48
21:W:17:ILE:HD12	21:W:74:ARG:HG3	1.95	0.48
22:X:6:ASN:OD1	22:X:7:THR:N	2.47	0.48
22:X:156:LEU:HD21	27:d:84:ALA:CB	2.43	0.48
30:g:45:LEU:HB2	37:n:119:GLU:CD	2.38	0.48
30:g:109:GLU:O	30:g:113:GLU:N	2.41	0.48
2:B:106:ALA:HB1	2:B:107:PRO:HD2	1.96	0.48
4:D:303:ILE:HD12	41:r:102:TRP:HZ3	1.79	0.48
7:G:44:VAL:HG11	7:G:106:VAL:HG11	1.93	0.48
8:H:133:ASN:O	8:H:137:LEU:HD23	2.12	0.48
13:M:239:GLN:HA	13:M:292:MET:HE1	1.95	0.48
14:N:20:ILE:HG13	28:e:11:LEU:HD21	1.95	0.48
16:P:137:ILE:HG22	16:P:139:LEU:CD2	2.43	0.48
35:l:172:THR:OG1	38:o:34:GLU:O	2.17	0.48
2:B:97:CYS:HB2	2:B:131:ALA:HB1	1.95	0.48
3:C:86:LEU:HD23	3:C:143:ILE:CD1	2.43	0.48
6:F:184:MET:HB2	6:F:212:MET:HE3	1.96	0.48
9:I:155:THR:HG21	9:I:185:HIS:HE2	1.77	0.48
13:M:170:PHE:HA	13:M:173:MET:HE2	1.94	0.48
15:O:115:ASP:CG	15:O:118:LEU:HD23	2.39	0.48
17:Q:115:GLU:OE1	17:Q:115:GLU:N	2.46	0.48
22:X:132:LYS:HB2	26:b:60:VAL:HG22	1.96	0.48
38:o:22:THR:HG22	38:o:22:THR:O	2.13	0.48
1:A:55:LEU:HD21	10:J:68:TYR:OH	2.13	0.48
7:G:280:ARG:HB3	7:G:285:LEU:HD11	1.96	0.48
14:N:236:LEU:HD11	27:d:44:TRP:CD1	2.49	0.48
24:Z:121:THR:HG21	28:e:33:LYS:HE3	1.95	0.48
32:i:25:ARG:O	32:i:29:ILE:HG23	2.13	0.48
2:B:72:LEU:HD13	2:B:219:TYR:HB2	1.96	0.48
6:F:192:TYR:HD1	6:F:197:ILE:HG23	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:42:LEU:HA	11:K:45:MET:HE2	1.96	0.48
12:L:285:MET:HE2	12:L:300:HIS:CE1	2.49	0.48
16:P:388:LEU:HD12	16:P:394:LEU:HD22	1.96	0.48
18:R:35:ASP:OD1	18:R:36:ILE:N	2.45	0.48
23:Y:74:THR:HG21	23:Y:89:TYR:CD1	2.48	0.48
24:Z:72:GLN:NE2	25:a:43:PHE:CG	2.81	0.48
32:i:31:MET:O	32:i:36:ARG:NH2	2.47	0.48
1:A:81:MET:HE2	8:H:308:LYS:CG	2.44	0.48
4:D:187:ASN:OD1	4:D:409:LYS:NZ	2.36	0.48
6:F:94:GLU:HA	6:F:97:THR:HG22	1.96	0.48
13:M:25:GLN:NE2	13:M:74:LEU:HD21	2.29	0.48
15:O:127:ASP:OD1	15:O:129:ARG:NH1	2.47	0.48
26:b:48:ASP:O	26:b:50:ASP:N	2.47	0.48
2:B:151:GLU:HB2	2:B:152:PRO:HA	1.96	0.47
4:D:459:LEU:HB3	4:D:461:VAL:HG23	1.95	0.47
7:G:432:ALA:HB3	7:G:438:LEU:HD22	1.94	0.47
11:K:13:LEU:HD13	11:K:41:MET:SD	2.54	0.47
15:O:195:PHE:HB2	15:O:198:MET:HE3	1.96	0.47
32:i:55:VAL:HG21	37:n:109:ALA:HB3	1.95	0.47
40:q:85:TYR:O	40:q:89:HIS:ND1	2.42	0.47
1:A:116:SER:OG	15:O:316:ILE:HD13	2.13	0.47
14:N:128:MET:HE3	14:N:132:TRP:HB3	1.96	0.47
21:W:17:ILE:HD13	21:W:78:MET:SD	2.53	0.47
22:X:56:ARG:HD2	24:Z:127:LEU:HD12	1.95	0.47
1:A:51:LEU:HD13	8:H:136:LEU:HD13	1.96	0.47
4:D:331:CYS:CB	4:D:458:THR:HG21	2.43	0.47
8:H:133:ASN:OD1	8:H:134:TYR:N	2.47	0.47
12:L:351:ALA:HB1	12:L:359:ALA:HB3	1.97	0.47
15:O:235:LEU:HD13	15:O:292:THR:OG1	2.14	0.47
19:T:134:LEU:C	19:T:134:LEU:HD12	2.39	0.47
4:D:391:THR:HG23	4:D:392:GLN:N	2.30	0.47
8:H:31:GLU:OE1	8:H:235:TYR:OH	2.25	0.47
9:I:214:HIS:CG	18:R:94:LEU:HD21	2.49	0.47
12:L:66:VAL:HG22	12:L:223:SER:HB3	1.96	0.47
26:b:44:TYR:OH	26:b:49:GLY:O	2.23	0.47
37:n:64:CYS:SG	37:n:65:GLY:N	2.87	0.47
1:A:48:SER:O	1:A:49:SER:OG	2.22	0.47
1:A:65:LEU:HD21	10:J:62:MET:HA	1.96	0.47
5:E:208:PRO:O	5:E:212:ARG:NH1	2.47	0.47
10:J:21:ILE:HD12	16:P:309:ARG:HH22	1.78	0.47
20:V:44:TYR:O	20:V:48:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:13:LYS:NZ	32:i:15:MET:SD	2.87	0.47
38:o:49:LEU:HD12	38:o:50:PRO:HD2	1.96	0.47
38:o:73:PRO:N	39:p:8:MET:HE1	2.28	0.47
3:C:139:TYR:CD1	41:r:99:VAL:HG22	2.50	0.47
21:W:92:GLU:OE1	21:W:94:TRP:CG	2.68	0.47
3:C:48:THR:O	4:D:167:ASP:N	2.47	0.47
3:C:185:ASP:OD1	21:W:88:LYS:NZ	2.48	0.47
6:F:265:VAL:HG12	6:F:269:ILE:HG12	1.96	0.47
7:G:264:SER:OG	7:G:265:ILE:N	2.47	0.47
7:G:398:LEU:HD21	7:G:522:LEU:HD23	1.97	0.47
12:L:562:LEU:HD11	12:L:566:PHE:CE2	2.50	0.47
13:M:13:PRO:O	13:M:17:ILE:HD12	2.15	0.47
13:M:144:LEU:HD21	13:M:148:LEU:HD12	1.97	0.47
15:O:282:THR:C	15:O:320:LYS:HZ3	2.22	0.47
16:P:127:ARG:HG3	16:P:165:ILE:HD12	1.97	0.47
21:W:39:GLN:CD	21:W:91:VAL:HG22	2.39	0.47
24:Z:102:MET:HB3	24:Z:105:VAL:HG21	1.97	0.47
37:n:19:TYR:CE2	37:n:23:LEU:HD11	2.49	0.47
37:n:31:ASP:OD1	37:n:32:ARG:N	2.48	0.47
4:D:133:THR:O	4:D:137:ALA:N	2.42	0.47
6:F:185:GLN:NE2	42:s:94:GLU:OE2	2.48	0.47
12:L:97:PHE:CE2	12:L:127:LEU:HD12	2.50	0.47
12:L:132:GLN:OE1	37:n:93:VAL:HG22	2.15	0.47
13:M:197:MET:HE3	13:M:197:MET:HA	1.97	0.47
14:N:303:GLU:OE1	15:O:371:ARG:NH1	2.48	0.47
25:a:65:ASP:OD1	25:a:65:ASP:N	2.48	0.47
29:f:4:GLY:C	29:f:5:LEU:HD22	2.40	0.47
6:F:212:MET:O	42:s:90:TYR:OH	2.33	0.47
7:G:164:THR:O	7:G:164:THR:HG22	2.15	0.47
13:M:241:MET:HE1	13:M:245:TYR:CD2	2.50	0.47
14:N:305:ASN:OD1	14:N:306:TRP:N	2.47	0.47
21:W:47:TYR:CE2	21:W:93:ILE:HG23	2.50	0.47
9:I:203:GLU:HB3	40:q:108:ILE:HD12	1.96	0.47
12:L:61:LEU:HD11	12:L:65:PHE:CE1	2.50	0.47
15:O:114:VAL:HG21	15:O:163:MET:HE3	1.97	0.47
18:R:85:VAL:HG22	18:R:103:LEU:HD11	1.97	0.47
19:T:132:GLU:N	19:T:132:GLU:OE1	2.47	0.47
19:T:140:ILE:O	19:T:144:VAL:N	2.48	0.47
33:j:42:LYS:HD2	33:j:46:ILE:HD12	1.96	0.47
12:L:303:THR:HG23	12:L:359:ALA:HB1	1.96	0.46
12:L:377:ASN:OD1	12:L:378:MET:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:40:THR:O	18:R:43:GLY:N	2.43	0.46
23:Y:84:ASP:OD1	23:Y:84:ASP:N	2.47	0.46
29:f:21:ILE:O	29:f:25:LEU:HD23	2.15	0.46
40:q:59:TYR:CE2	41:r:34:LEU:HD12	2.50	0.46
4:D:175:ILE:HD12	4:D:361:ILE:CD1	2.45	0.46
5:E:172:ALA:HB3	5:E:178:MET:HE3	1.96	0.46
10:J:82:MET:C	10:J:85:THR:HG1	2.23	0.46
11:K:53:LEU:HD13	11:K:56:GLU:CD	2.40	0.46
16:P:299:PHE:HA	16:P:302:LEU:HD12	1.98	0.46
4:D:179:PHE:HZ	4:D:222:VAL:HG11	1.80	0.46
4:D:409:LYS:HZ2	4:D:460:ASP:CG	2.23	0.46
6:F:51:ALA:O	6:F:54:ASP:N	2.48	0.46
12:L:155:LEU:HA	12:L:158:ILE:HD12	1.97	0.46
16:P:298:TRP:CE2	16:P:302:LEU:HD11	2.50	0.46
16:P:343:HIS:HD2	16:P:345:ALA:HB3	1.81	0.46
17:Q:88:ILE:HD12	17:Q:157:ALA:HB2	1.93	0.46
4:D:387:PHE:O	4:D:391:THR:HG22	2.15	0.46
5:E:125:ILE:H	5:E:125:ILE:HD12	1.80	0.46
11:K:49:TYR:CZ	14:N:79:MET:SD	3.09	0.46
13:M:155:LEU:HD11	13:M:159:PHE:CZ	2.50	0.46
15:O:74:THR:HG23	15:O:336:ARG:HD2	1.96	0.46
15:O:229:PRO:O	15:O:284:ALA:HB2	2.16	0.46
33:j:40:HIS:O	33:j:45:LYS:NZ	2.48	0.46
1:A:51:LEU:HD21	8:H:137:LEU:HD22	1.97	0.46
1:A:72:ALA:HB2	10:J:57:ILE:HD11	1.98	0.46
2:B:159:GLY:O	2:B:163:ASN:ND2	2.49	0.46
4:D:333:ASP:OD1	4:D:334:ARG:N	2.48	0.46
5:E:114:MET:HE1	6:F:217:GLY:N	2.31	0.46
12:L:65:PHE:HA	12:L:68:MET:HE2	1.96	0.46
12:L:96:MET:HE2	12:L:96:MET:HA	1.97	0.46
12:L:261:GLY:C	12:L:390:LEU:HD13	2.40	0.46
12:L:429:LEU:HD23	12:L:429:LEU:O	2.16	0.46
14:N:196:ILE:HG21	14:N:265:GLN:HG3	1.98	0.46
27:d:2:SER:OG	27:d:3:ALA:N	2.49	0.46
30:g:107:GLN:HA	39:p:78:GLU:OE2	2.15	0.46
39:p:106:MET:O	39:p:109:TYR:N	2.49	0.46
3:C:152:LEU:HD22	21:W:74:ARG:CD	2.45	0.46
4:D:165:ASN:O	4:D:166:ILE:HD13	2.16	0.46
4:D:461:VAL:HG13	4:D:466:ILE:CD1	2.45	0.46
7:G:395:ASN:OD1	7:G:672:GLY:N	2.49	0.46
9:I:43:TYR:OH	41:r:100:TYR:OH	2.32	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:28:LEU:O	10:J:32:ILE:HD12	2.16	0.46
12:L:251:LEU:HD21	35:l:146:TYR:CD2	2.51	0.46
33:j:30:VAL:HG23	33:j:30:VAL:O	2.14	0.46
1:A:96:PHE:O	1:A:100:LEU:HD23	2.16	0.46
44:B:302:3PE:O31	40:q:31:TYR:OH	2.34	0.46
12:L:45:ASN:ND2	36:m:112:PHE:O	2.48	0.46
12:L:403:MET:HE1	34:k:64:PHE:CZ	2.51	0.46
16:P:92:LEU:HD22	16:P:113:VAL:HG13	1.96	0.46
17:Q:87:HIS:HE2	17:Q:107:GLU:CD	2.20	0.46
22:X:14:GLU:O	22:X:63:LYS:NZ	2.44	0.46
30:g:45:LEU:HA	30:g:49:ASP:OD2	2.16	0.46
32:i:89:ARG:O	32:i:93:VAL:HG23	2.16	0.46
38:o:44:MET:HE3	38:o:54:ARG:HD3	1.98	0.46
2:B:176:ARG:O	2:B:180:ARG:NH2	2.49	0.46
13:M:200:VAL:HG12	13:M:200:VAL:O	2.15	0.46
13:M:367:ILE:HD12	13:M:367:ILE:H	1.81	0.46
14:N:19:LEU:CD2	28:e:11:LEU:HD23	2.45	0.46
38:o:47:ALA:HB2	38:o:62:ILE:HD13	1.98	0.46
5:E:193:ASP:OD1	5:E:194:MET:N	2.49	0.46
7:G:452:ASP:OD1	7:G:453:HIS:N	2.49	0.46
9:I:185:HIS:HB3	16:P:110:LEU:HD11	1.98	0.46
12:L:213:PRO:O	12:L:216:VAL:N	2.49	0.46
14:N:60:TYR:OH	14:N:133:GLN:NE2	2.44	0.46
39:p:100:VAL:HG12	39:p:101:LYS:HG2	1.98	0.46
6:F:61:TYR:OH	6:F:302:THR:O	2.13	0.46
12:L:430:LEU:HD11	12:L:434:ILE:HD11	1.97	0.46
34:k:32:LEU:O	34:k:35:GLN:N	2.49	0.46
37:n:23:LEU:O	37:n:36:TYR:OH	2.32	0.46
42:s:108:LEU:HD12	42:s:108:LEU:O	2.16	0.46
10:J:134:ASN:HD21	31:h:180:LEU:HD13	1.80	0.45
14:N:130:MET:HE1	14:N:179:SER:CB	2.46	0.45
17:Q:142:ILE:HG23	17:Q:152:TRP:CZ2	2.52	0.45
30:g:143:LEU:HD13	39:p:145:ARG:HH11	1.81	0.45
5:E:110:THR:HG21	7:G:212:THR:HB	1.99	0.45
6:F:259:ASN:OD1	6:F:260:VAL:N	2.48	0.45
6:F:384:ARG:NH1	6:F:387:SER:OG	2.49	0.45
7:G:104:MET:HE3	7:G:105:PRO:CD	2.46	0.45
12:L:10:SER:O	12:L:14:LEU:HD13	2.16	0.45
12:L:114:LEU:HD21	13:M:363:LEU:HD21	1.99	0.45
14:N:238:PHE:CE1	14:N:242:MET:HE1	2.51	0.45
16:P:265:ALA:O	16:P:269:ILE:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:71:ILE:HD12	21:W:78:MET:CB	2.46	0.45
38:o:71:THR:HG23	38:o:71:THR:O	2.15	0.45
1:A:56:ARG:O	1:A:60:ILE:HD12	2.16	0.45
6:F:426:MET:HE1	41:r:52:LEU:O	2.16	0.45
8:H:244:LEU:HA	8:H:247:VAL:HG22	1.99	0.45
11:K:18:LEU:HD23	11:K:38:ILE:HD13	1.97	0.45
12:L:114:LEU:CD2	13:M:363:LEU:HD21	2.46	0.45
19:T:71:SER:O	19:T:75:ILE:HD12	2.16	0.45
24:Z:28:VAL:HG13	24:Z:28:VAL:O	2.15	0.45
25:a:20:ILE:HD12	25:a:20:ILE:H	1.81	0.45
37:n:104:HIS:O	37:n:107:GLU:N	2.49	0.45
4:D:275:GLN:O	8:H:281:ARG:NH1	2.50	0.45
4:D:303:ILE:HG23	41:r:102:TRP:HE3	1.81	0.45
7:G:92:VAL:C	7:G:95:SER:HG	2.21	0.45
9:I:154:MET:HE1	9:I:190:TYR:CD2	2.52	0.45
12:L:203:SER:H	12:L:502:MET:HE1	1.81	0.45
13:M:293:THR:HB	36:m:113:ILE:HG21	1.99	0.45
14:N:98:MET:SD	14:N:146:ILE:HD13	2.57	0.45
14:N:108:ALA:HB3	14:N:109:PRO:CD	2.46	0.45
16:P:52:LYS:NZ	21:W:121:GLN:OE1	2.50	0.45
22:X:153:THR:O	31:h:158:GLN:NE2	2.49	0.45
25:a:23:MET:HE3	25:a:23:MET:HA	1.98	0.45
31:h:68:LEU:C	31:h:68:LEU:HD23	2.41	0.45
38:o:37:MET:HE2	38:o:37:MET:HA	1.99	0.45
4:D:190:MET:SD	4:D:212:ARG:NH2	2.87	0.45
47:M:501:CDL:O1	31:h:52:ARG:NH1	2.49	0.45
15:O:116:LEU:HD23	15:O:166:LEU:HD12	1.98	0.45
23:Y:66:MET:HE2	23:Y:100:PHE:HB2	1.98	0.45
29:f:34:THR:O	29:f:34:THR:HG23	2.17	0.45
1:A:77:MET:HE1	8:H:305:ILE:HD12	1.98	0.45
1:A:97:ILE:HD12	1:A:97:ILE:H	1.82	0.45
4:D:448:MET:HE3	4:D:448:MET:HA	1.99	0.45
6:F:150:PRO:O	6:F:154:VAL:HG23	2.17	0.45
6:F:392:GLU:O	6:F:442:LEU:HD21	2.17	0.45
12:L:96:MET:HB3	12:L:123:VAL:HG11	1.99	0.45
19:U:80:LEU:HD21	19:U:96:VAL:CG2	2.47	0.45
21:W:92:GLU:OE1	21:W:94:TRP:N	2.50	0.45
3:C:89:LEU:HD22	20:V:112:TRP:CE3	2.51	0.45
16:P:297:ASP:OD2	16:P:314:ARG:NH1	2.50	0.45
19:T:87:ASP:OD1	19:T:88:LYS:N	2.47	0.45
22:X:153:THR:HG21	31:h:162:TYR:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:r:49:SER:O	41:r:55:ASN:ND2	2.50	0.45
12:L:412:LEU:HD11	19:U:78:ARG:NH2	2.31	0.45
13:M:63:LEU:HD23	13:M:63:LEU:C	2.42	0.45
15:O:201:MET:SD	48:O:501:DGT:N2	2.89	0.45
16:P:180:LEU:HB3	16:P:221:ALA:HB2	1.99	0.45
20:V:56:ALA:O	20:V:59:VAL:HG12	2.16	0.45
29:f:37:ARG:NH1	29:f:56:TRP:O	2.50	0.45
41:r:11:LEU:O	41:r:15:ILE:HD12	2.16	0.45
10:J:94:PHE:HA	10:J:97:ILE:HG22	1.99	0.45
14:N:130:MET:HE1	14:N:179:SER:HB2	1.98	0.45
15:O:105:GLU:O	15:O:106:LEU:HD22	2.17	0.45
25:a:40:ASP:OD1	25:a:41:GLU:N	2.50	0.45
29:f:33:MET:HE2	29:f:56:TRP:CZ2	2.52	0.45
2:B:199:MET:HE1	9:I:91:TYR:HB3	1.99	0.45
3:C:126:ASN:OD1	20:V:111:GLN:NE2	2.47	0.45
4:D:280:ILE:HD11	8:H:281:ARG:CZ	2.46	0.45
8:H:277:LEU:HD21	9:I:75:PHE:CE1	2.52	0.45
12:L:28:PHE:O	12:L:32:ASP:N	2.48	0.45
12:L:552:MET:HE1	23:Y:43:LEU:HG	1.98	0.45
15:O:343:LYS:HA	15:O:346:LEU:HD12	1.99	0.45
24:Z:72:GLN:NE2	25:a:43:PHE:CE2	2.85	0.45
30:g:45:LEU:HB2	37:n:119:GLU:OE1	2.17	0.45
4:D:189:ILE:HD12	4:D:215:MET:HE1	1.99	0.44
10:J:66:PHE:O	10:J:70:THR:OG1	2.20	0.44
12:L:282:LEU:HA	12:L:285:MET:HE3	1.98	0.44
7:G:630:ARG:NH1	7:G:643:ASP:OD1	2.50	0.44
8:H:273:VAL:HG13	8:H:277:LEU:HD23	1.99	0.44
14:N:111:HIS:NE2	14:N:160:ILE:HD12	2.33	0.44
16:P:292:LEU:O	16:P:296:VAL:HG23	2.17	0.44
16:P:307:GLN:NE2	16:P:387:ALA:O	2.50	0.44
4:D:316:TYR:HA	4:D:319:VAL:HG22	2.00	0.44
5:E:187:GLU:N	5:E:187:GLU:OE1	2.50	0.44
6:F:426:MET:HE2	6:F:426:MET:HA	1.99	0.44
11:K:36:GLU:OE2	11:K:36:GLU:HA	2.17	0.44
11:K:61:MET:O	11:K:65:THR:HG23	2.18	0.44
31:h:45:GLN:NE2	32:i:46:GLN:O	2.49	0.44
7:G:104:MET:HE3	7:G:105:PRO:HD2	1.99	0.44
7:G:350:GLN:O	7:G:351:ILE:HD13	2.17	0.44
8:H:62:LEU:HD13	8:H:228:ALA:HB2	1.99	0.44
12:L:546:SER:O	14:N:167:ASN:ND2	2.50	0.44
13:M:85:TYR:OH	14:N:300:ASN:ND2	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:314:LEU:HD23	13:M:317:LEU:HD12	1.98	0.44
14:N:175:MET:HE2	14:N:212:THR:CG2	2.47	0.44
4:D:220:GLU:OE2	9:I:99:SER:N	2.49	0.44
5:E:136:ARG:HD3	5:E:176:ALA:HB3	2.00	0.44
6:F:129:VAL:HG11	6:F:227:LEU:CD2	2.47	0.44
6:F:407:MET:SD	6:F:450:VAL:HG21	2.58	0.44
10:J:105:THR:O	10:J:108:SER:N	2.43	0.44
12:L:103:LEU:HD23	12:L:115:LEU:CD2	2.47	0.44
21:W:39:GLN:NE2	21:W:91:VAL:HG22	2.32	0.44
4:D:222:VAL:HG23	4:D:223:SER:N	2.33	0.44
5:E:88:ILE:HD11	7:G:224:VAL:HG11	1.98	0.44
9:I:106:HIS:NE2	9:I:174:GLU:OE2	2.50	0.44
10:J:83:LYS:H	10:J:83:LYS:HD2	1.83	0.44
12:L:61:LEU:HD11	12:L:65:PHE:CZ	2.52	0.44
12:L:156:LEU:HB2	12:L:188:LEU:HD23	2.00	0.44
21:W:93:ILE:HG22	21:W:93:ILE:O	2.17	0.44
29:f:33:MET:HE3	31:h:126:LYS:CA	2.48	0.44
36:m:100:THR:HG23	39:p:153:MET:CE	2.43	0.44
39:p:95:ALA:O	39:p:98:HIS:NE2	2.50	0.44
4:D:61:GLU:HG2	4:D:62:VAL:HG13	1.98	0.44
4:D:143:ARG:NH2	4:D:228:HIS:ND1	2.66	0.44
6:F:309:ILE:HD11	6:F:313:GLU:OE1	2.18	0.44
7:G:350:GLN:C	7:G:351:ILE:HD13	2.42	0.44
8:H:156:ILE:HG22	8:H:160:PHE:HE2	1.81	0.44
13:M:301:TYR:CZ	13:M:305:ILE:HD11	2.53	0.44
17:Q:88:ILE:HD12	17:Q:157:ALA:HB1	1.99	0.44
26:b:65:ASP:O	26:b:68:ALA:N	2.50	0.44
30:g:129:TYR:CD2	30:g:130:VAL:HG13	2.52	0.44
1:A:86:ILE:HD13	26:b:44:TYR:CZ	2.53	0.44
6:F:337:SER:O	6:F:338:SER:OG	2.18	0.44
7:G:357:GLN:OE1	7:G:357:GLN:N	2.51	0.44
11:K:82:ILE:O	11:K:86:GLY:N	2.51	0.44
14:N:300:ASN:O	15:O:364:ALA:HB1	2.18	0.44
27:d:113:VAL:O	27:d:113:VAL:HG23	2.17	0.44
35:l:70:LEU:HD11	36:m:68:SER:HA	2.00	0.44
2:B:217:MET:HE1	16:P:97:ASP:N	2.32	0.44
5:E:173:CYS:N	45:E:301:FES:S1	2.91	0.44
6:F:441:ALA:HB3	46:F:501:FMN:HM81	1.99	0.44
11:K:81:MET:HE1	14:N:58:LEU:CD2	2.36	0.44
12:L:254:GLY:O	12:L:383:LEU:HD21	2.17	0.44
22:X:17:VAL:HG12	24:Z:85:ARG:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Z:68:MET:O	24:Z:72:GLN:N	2.49	0.44
27:d:11:LEU:CD1	31:h:143:LEU:HD13	2.48	0.44
33:j:60:ILE:HA	33:j:63:LEU:HD12	2.00	0.44
2:B:217:MET:HE1	16:P:96:GLY:CA	2.47	0.43
4:D:56:VAL:HG12	4:D:58:TYR:H	1.82	0.43
5:E:229:GLU:N	5:E:229:GLU:OE1	2.51	0.43
8:H:176:GLN:OE1	8:H:251:GLY:N	2.43	0.43
12:L:62:PHE:O	12:L:66:VAL:HG23	2.18	0.43
12:L:258:PHE:CE1	12:L:262:LEU:HD11	2.53	0.43
15:O:271:LEU:HD23	15:O:275:GLN:HG3	2.00	0.43
21:W:73:ILE:O	21:W:76:ILE:HG22	2.18	0.43
14:N:175:MET:HE2	14:N:212:THR:HG23	2.00	0.43
16:P:188:ASP:C	16:P:189:LEU:HD12	2.44	0.43
30:g:112:LEU:O	30:g:116:ARG:N	2.44	0.43
2:B:194:THR:HG23	2:B:197:ALA:H	1.82	0.43
2:B:205:LEU:O	2:B:209:VAL:HG23	2.18	0.43
10:J:31:LEU:HD12	10:J:59:LEU:HD11	2.00	0.43
13:M:121:ILE:CD1	14:N:250:LEU:HD23	2.36	0.43
14:N:220:LEU:HB3	14:N:226:LEU:HD22	2.00	0.43
14:N:331:LEU:O	14:N:334:ILE:N	2.49	0.43
19:T:102:ASN:OD1	19:T:102:ASN:N	2.50	0.43
19:T:116:MET:CE	21:W:34:LYS:HA	2.47	0.43
30:g:59:GLN:NE2	32:i:8:GLU:O	2.51	0.43
1:A:62:ILE:HG21	10:J:159:ILE:HG12	2.01	0.43
6:F:56:ILE:HG12	6:F:268:THR:HG21	2.00	0.43
8:H:156:ILE:HG21	8:H:192:TRP:HE3	1.83	0.43
8:H:271:ILE:O	8:H:274:ARG:N	2.52	0.43
9:I:185:HIS:CG	16:P:110:LEU:HD11	2.53	0.43
10:J:83:LYS:NZ	16:P:242:PHE:O	2.49	0.43
10:J:83:LYS:HD2	10:J:83:LYS:N	2.33	0.43
16:P:186:PRO:HB3	16:P:198:LEU:HD23	2.00	0.43
20:V:69:GLU:HG3	20:V:77:VAL:HG13	1.99	0.43
23:Y:16:ASP:OD2	23:Y:19:GLY:N	2.47	0.43
36:m:108:ARG:HB3	36:m:108:ARG:CZ	2.49	0.43
42:s:79:VAL:HG13	42:s:79:VAL:O	2.18	0.43
4:D:360:GLU:OE2	41:r:47:GLY:N	2.51	0.43
8:H:118:LEU:HD21	10:J:55:PHE:HE2	1.83	0.43
11:K:56:GLU:OE2	28:e:19:ILE:HB	2.18	0.43
13:M:26:ILE:HB	30:g:81:VAL:HG21	2.00	0.43
13:M:197:MET:O	13:M:201:HIS:N	2.51	0.43
14:N:183:LEU:HA	14:N:186:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:202:TYR:CE1	16:P:206:LEU:HD11	2.51	0.43
51:U:201:EHZ:S1	37:n:61:LEU:HD21	2.58	0.43
21:W:117:SER:HA	21:W:120:ILE:HG22	1.99	0.43
24:Z:134:GLU:OE1	28:e:66:GLN:NE2	2.48	0.43
30:g:140:ASP:OD1	30:g:141:GLU:N	2.52	0.43
38:o:73:PRO:CA	39:p:8:MET:HE1	2.49	0.43
2:B:167:TYR:HB2	9:I:158:ILE:CG2	2.48	0.43
6:F:65:ASP:OD2	6:F:66:TRP:N	2.52	0.43
11:K:53:LEU:HD22	11:K:56:GLU:OE1	2.19	0.43
13:M:325:LEU:HD21	13:M:414:PHE:CE1	2.53	0.43
24:Z:140:ASP:O	24:Z:143:SER:OG	2.36	0.43
38:o:49:LEU:HD11	38:o:53:PHE:HB2	1.99	0.43
4:D:179:PHE:CZ	4:D:222:VAL:HG11	2.54	0.43
10:J:142:ASN:OD1	10:J:143:PHE:N	2.52	0.43
12:L:109:ASN:OD1	12:L:110:LEU:N	2.52	0.43
12:L:269:ASP:O	12:L:272:LYS:N	2.52	0.43
12:L:284:LEU:CD2	12:L:367:ILE:HD13	2.49	0.43
13:M:144:LEU:CD2	13:M:148:LEU:HD12	2.49	0.43
13:M:194:LYS:NZ	13:M:226:LEU:HD23	2.33	0.43
14:N:129:LEU:O	14:N:129:LEU:HD23	2.18	0.43
2:B:103:HIS:O	2:B:106:ALA:HB3	2.18	0.43
3:C:87:GLU:OE2	3:C:144:ARG:NH1	2.47	0.43
4:D:218:PHE:CD1	4:D:249:ILE:HD13	2.54	0.43
12:L:237:ASN:CG	12:L:294:LEU:HD11	2.43	0.43
14:N:232:ASN:O	15:O:371:ARG:NH2	2.50	0.43
16:P:98:ASP:O	16:P:101:VAL:HG12	2.19	0.43
39:p:52:ASP:OD1	39:p:53:GLN:N	2.49	0.43
3:C:62:ASP:OD1	3:C:63:PHE:N	2.51	0.43
3:C:110:PHE:CD1	3:C:143:ILE:HG22	2.54	0.43
4:D:280:ILE:HD11	8:H:281:ARG:NH1	2.34	0.43
6:F:402:GLU:CD	6:F:403:GLY:N	2.76	0.43
7:G:465:ASP:OD1	7:G:466:VAL:HG23	2.19	0.43
7:G:656:ALA:HB1	7:G:658:HIS:NE2	2.33	0.43
8:H:203:THR:OG1	8:H:204:PRO:HA	2.19	0.43
10:J:1:MET:SD	10:J:2:ILE:N	2.92	0.43
10:J:103:ASP:OD1	28:e:74:ARG:NH2	2.52	0.43
13:M:30:PHE:CD1	30:g:85:LEU:HD21	2.54	0.43
13:M:156:ILE:H	13:M:156:ILE:HD12	1.82	0.43
14:N:127:LEU:HD11	14:N:209:PHE:HD2	1.84	0.43
20:V:44:TYR:CG	20:V:94:MET:HE2	2.53	0.43
30:g:107:GLN:HG2	32:i:124:LYS:HZ2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:i:68:ARG:O	32:i:68:ARG:NH2	2.52	0.43
39:p:29:SER:C	39:p:30:ILE:HD13	2.43	0.43
40:q:17:VAL:HG13	40:q:18:ARG:N	2.34	0.43
4:D:239:LEU:HD12	4:D:240:ASP:H	1.83	0.43
4:D:306:ASP:OD1	4:D:307:LEU:N	2.52	0.43
6:F:176:GLU:N	6:F:176:GLU:OE1	2.52	0.43
6:F:355:ASP:O	6:F:357:LEU:N	2.50	0.43
11:K:23:SER:OG	11:K:25:ARG:NH2	2.52	0.43
15:O:118:LEU:HD12	15:O:119:ILE:N	2.33	0.43
21:W:18:LEU:HD11	21:W:81:ILE:HD11	2.01	0.43
1:A:93:SER:O	1:A:97:ILE:HD12	2.19	0.42
4:D:106:LEU:HD11	4:D:111:VAL:HG22	2.00	0.42
6:F:345:ASN:OD1	6:F:345:ASN:N	2.51	0.42
13:M:436:ILE:HD12	13:M:436:ILE:H	1.84	0.42
18:R:36:ILE:HG23	18:R:36:ILE:O	2.19	0.42
30:g:122:VAL:HG12	30:g:123:ASP:N	2.34	0.42
36:m:12:LYS:O	36:m:15:HIS:N	2.51	0.42
4:D:303:ILE:HG23	41:r:102:TRP:CE3	2.55	0.42
7:G:159:ASP:OD1	41:r:60:ARG:NH1	2.49	0.42
7:G:323:MET:HA	7:G:323:MET:HE3	2.01	0.42
8:H:220:VAL:HG13	8:H:221:GLU:HG2	2.01	0.42
12:L:552:MET:O	12:L:555:ASN:ND2	2.49	0.42
15:O:312:PHE:HD2	15:O:321:MET:HG2	1.83	0.42
16:P:302:LEU:HD23	16:P:400:PRO:CG	2.48	0.42
24:Z:121:THR:HG22	28:e:56:ASP:OD2	2.19	0.42
27:d:115:VAL:HG23	27:d:116:ARG:N	2.35	0.42
32:i:121:TRP:O	32:i:124:LYS:HE2	2.19	0.42
4:D:303:ILE:HD12	41:r:102:TRP:CZ3	2.54	0.42
4:D:440:LEU:CD2	4:D:456:ILE:HD11	2.49	0.42
6:F:117:MET:HE1	6:F:254:PRO:O	2.18	0.42
8:H:197:LEU:HD23	8:H:204:PRO:HD2	2.01	0.42
9:I:149:ARG:HB2	40:q:128:THR:HG23	2.02	0.42
12:L:459:LEU:HD13	12:L:462:LEU:HD12	2.02	0.42
14:N:207:LEU:HD23	14:N:207:LEU:C	2.44	0.42
15:O:116:LEU:HD23	15:O:166:LEU:CD1	2.49	0.42
22:X:153:THR:HG23	22:X:153:THR:O	2.19	0.42
29:f:40:SER:OG	29:f:41:ALA:N	2.52	0.42
30:g:108:ARG:HB3	39:p:42:HIS:CE1	2.54	0.42
4:D:57:MET:HE1	14:N:167:ASN:C	2.44	0.42
4:D:377:LYS:NZ	18:R:95:GLY:O	2.36	0.42
6:F:133:ASP:OD1	6:F:135:GLY:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:311:LEU:N	7:G:311:LEU:HD12	2.34	0.42
12:L:473:TYR:CZ	12:L:477:LEU:HD11	2.53	0.42
13:M:231:MET:HA	13:M:234:VAL:HG12	2.02	0.42
16:P:181:ASN:HD22	16:P:352:VAL:HG11	1.84	0.42
16:P:362:THR:OG1	16:P:363:LEU:N	2.53	0.42
18:R:85:VAL:HG13	18:R:103:LEU:HD11	2.01	0.42
27:d:32:GLY:O	27:d:36:VAL:HG23	2.19	0.42
1:A:81:MET:HE2	8:H:308:LYS:HG2	2.02	0.42
1:A:87:MET:O	1:A:91:ILE:HD12	2.20	0.42
3:C:80:LEU:HD12	3:C:85:GLU:O	2.20	0.42
5:E:231:PRO:HB3	6:F:58:THR:HG21	2.01	0.42
7:G:230:THR:HG22	7:G:232:LEU:H	1.85	0.42
9:I:177:ASN:OD1	9:I:178:PHE:N	2.53	0.42
14:N:10:PHE:HB2	14:N:44:LEU:HD21	2.01	0.42
14:N:14:MET:HE2	14:N:128:MET:HE2	2.02	0.42
15:O:178:VAL:O	15:O:182:GLY:N	2.46	0.42
15:O:365:ASP:O	15:O:369:VAL:HG23	2.20	0.42
17:Q:131:MET:HE3	17:Q:132:ASN:H	1.84	0.42
10:J:26:LEU:HB3	11:K:33:LEU:HD23	2.00	0.42
12:L:181:GLU:OE1	12:L:181:GLU:N	2.41	0.42
12:L:273:ILE:HD12	12:L:273:ILE:H	1.85	0.42
12:L:530:SER:OG	13:M:202:LEU:HD21	2.19	0.42
27:d:112:TRP:HB3	39:p:134:MET:SD	2.59	0.42
32:i:141:GLU:OE1	32:i:141:GLU:N	2.50	0.42
1:A:60:ILE:HD12	1:A:60:ILE:H	1.84	0.42
4:D:240:ASP:O	9:I:216:TYR:OH	2.31	0.42
5:E:114:MET:HE1	6:F:217:GLY:CA	2.50	0.42
8:H:61:LYS:O	8:H:64:THR:OG1	2.32	0.42
10:J:31:LEU:CD1	10:J:59:LEU:HD11	2.49	0.42
11:K:79:VAL:HA	11:K:82:ILE:HD12	2.02	0.42
12:L:79:GLU:HB3	12:L:422:MET:HE3	2.02	0.42
15:O:135:LEU:HD12	15:O:366:ASP:OD2	2.20	0.42
15:O:142:TYR:HB2	15:O:155:LEU:CD2	2.50	0.42
16:P:139:LEU:HD13	16:P:177:LEU:HD12	2.01	0.42
22:X:22:LEU:O	25:a:50:ARG:NH2	2.53	0.42
28:e:61:VAL:HG13	28:e:62:GLY:N	2.35	0.42
30:g:84:THR:HG22	31:h:65:TYR:O	2.19	0.42
30:g:105:TRP:O	30:g:108:ARG:HB2	2.19	0.42
1:A:19:MET:HE1	8:H:79:TYR:CD1	2.54	0.42
1:A:89:TRP:CE3	8:H:309:ILE:HD11	2.55	0.42
4:D:121:LEU:O	4:D:123:2MR:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:205:TRP:O	12:L:208:ALA:N	2.53	0.42
13:M:66:LEU:HD23	13:M:97:LEU:HD11	2.01	0.42
14:N:96:ILE:HD12	14:N:96:ILE:H	1.83	0.42
15:O:230:HIS:CD2	15:O:321:MET:HE2	2.55	0.42
19:T:86:TYR:O	19:T:89:ILE:HG22	2.20	0.42
26:b:65:ASP:OD1	26:b:66:PRO:HD2	2.19	0.42
28:e:21:HIS:HE1	28:e:61:VAL:HG21	1.85	0.42
30:g:63:PHE:CE1	30:g:75:THR:HG23	2.55	0.42
32:i:129:VAL:HG12	32:i:130:ILE:N	2.35	0.42
37:n:43:LEU:HD11	37:n:47:PHE:HE2	1.85	0.42
40:q:51:TYR:HE2	40:q:65:ILE:HD12	1.85	0.42
4:D:144:LEU:O	4:D:152:ASN:ND2	2.53	0.42
7:G:60:LEU:C	7:G:60:LEU:HD23	2.45	0.42
10:J:32:ILE:HD12	10:J:32:ILE:H	1.84	0.42
12:L:44:LEU:HD21	13:M:368:TYR:CE2	2.55	0.42
24:Z:117:PRO:O	28:e:65:LYS:NZ	2.52	0.42
31:h:107:PRO:O	31:h:110:ARG:HB2	2.20	0.42
35:l:165:SER:O	35:l:168:VAL:HG12	2.19	0.42
36:m:14:LYS:O	36:m:18:THR:HG22	2.20	0.42
7:G:133:ASN:OD1	7:G:133:ASN:N	2.53	0.42
7:G:722:GLU:O	7:G:726:LYS:N	2.50	0.42
11:K:50:LEU:HB3	11:K:57:SER:HA	2.02	0.42
14:N:334:ILE:HG13	14:N:335:SER:N	2.34	0.42
1:A:51:LEU:CD2	8:H:136:LEU:HD22	2.50	0.41
2:B:48:VAL:O	2:B:52:LEU:HD13	2.19	0.41
7:G:292:ASN:O	7:G:296:ASN:N	2.52	0.41
10:J:16:ILE:HD11	10:J:88:SER:OG	2.20	0.41
14:N:130:MET:CE	14:N:179:SER:HB2	2.50	0.41
14:N:266:LEU:HD23	14:N:266:LEU:O	2.19	0.41
21:W:67:HIS:HB2	21:W:70:VAL:HG23	2.02	0.41
39:p:20:ASP:HA	39:p:23:ILE:HD11	2.02	0.41
1:A:11:ILE:HD11	8:H:94:MET:HE3	2.01	0.41
1:A:31:ILE:HG22	1:A:32:ASP:N	2.35	0.41
4:D:91:PRO:O	4:D:93:HIS:N	2.53	0.41
13:M:220:ALA:O	13:M:225:LYS:NZ	2.53	0.41
22:X:47:LEU:HD23	22:X:134:ILE:HD11	2.02	0.41
27:d:7:PRO:O	27:d:11:LEU:HD13	2.20	0.41
39:p:136:GLN:O	39:p:140:LEU:HD23	2.20	0.41
2:B:111:MET:CE	2:B:116:VAL:HG12	2.51	0.41
12:L:224:THR:O	12:L:227:THR:N	2.53	0.41
12:L:284:LEU:C	12:L:284:LEU:HD23	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:369:GLU:OE2	12:L:461:THR:HG21	2.21	0.41
13:M:7:PHE:CG	13:M:31:ILE:HD13	2.55	0.41
15:O:210:GLY:O	15:O:214:VAL:HG23	2.20	0.41
17:Q:139:GLU:OE1	17:Q:139:GLU:N	2.45	0.41
18:R:88:ASP:OD1	18:R:88:ASP:N	2.45	0.41
23:Y:87:ILE:CD1	23:Y:90:LEU:HD23	2.47	0.41
2:B:100:GLU:OE2	2:B:100:GLU:HA	2.20	0.41
6:F:290:LEU:HD12	6:F:290:LEU:N	2.36	0.41
7:G:624:GLU:OE1	7:G:626:TRP:NE1	2.52	0.41
9:I:153:ASP:OD1	9:I:155:THR:N	2.48	0.41
11:K:53:LEU:HD21	28:e:21:HIS:ND1	2.36	0.41
12:L:58:MET:HB3	12:L:298:MET:HE3	2.03	0.41
12:L:460:LEU:O	12:L:464:VAL:HG22	2.20	0.41
29:f:31:GLU:O	29:f:34:THR:HG22	2.20	0.41
40:q:94:LEU:HD23	40:q:99:ASP:HB3	2.02	0.41
6:F:397:CYS:C	6:F:401:ARG:HE	2.28	0.41
7:G:194:THR:HG1	7:G:198:ARG:HH11	1.69	0.41
12:L:4:LEU:HD23	12:L:9:ILE:HD13	2.02	0.41
13:M:117:GLU:HA	13:M:120:LEU:HD23	2.02	0.41
14:N:114:PHE:HB3	14:N:115:PRO:HD3	2.03	0.41
30:g:137:LEU:HD23	39:p:141:ILE:HD13	2.02	0.41
4:D:350:ASP:HB2	24:Z:23:ILE:HD13	2.01	0.41
15:O:237:LEU:HD11	15:O:291:TRP:HB2	2.03	0.41
18:R:85:VAL:HG13	18:R:103:LEU:CD1	2.51	0.41
19:U:75:ILE:HG23	19:U:122:PHE:HE1	1.85	0.41
28:e:34:MET:O	28:e:37:CYS:N	2.54	0.41
2:B:90:LEU:O	2:B:91:THR:OG1	2.36	0.41
3:C:165:ALA:O	3:C:168:TYR:N	2.54	0.41
6:F:330:LEU:HD23	6:F:378:VAL:CG1	2.51	0.41
12:L:201:PRO:HA	12:L:502:MET:HE3	2.02	0.41
15:O:108:MET:HE2	15:O:186:VAL:CG2	2.50	0.41
19:U:86:TYR:HD2	19:U:89:ILE:HD12	1.86	0.41
25:a:1:MET:SD	25:a:3:PHE:N	2.94	0.41
6:F:401:ARG:NH2	7:G:192:HIS:HB2	2.35	0.41
13:M:55:ASP:O	13:M:59:TYR:N	2.40	0.41
14:N:217:ILE:HD11	14:N:316:ASN:HB3	2.02	0.41
17:Q:86:ILE:HG12	17:Q:106:ILE:HG22	2.01	0.41
21:W:67:HIS:CD2	21:W:79:LEU:HD13	2.55	0.41
24:Z:69:ARG:O	24:Z:72:GLN:HB3	2.20	0.41
4:D:186:LEU:CD2	4:D:215:MET:HE3	2.47	0.41
5:E:113:THR:HG23	5:E:114:MET:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:120:THR:O	5:E:163:THR:OG1	2.35	0.41
7:G:490:ASP:OD2	7:G:688:ILE:HG22	2.20	0.41
9:I:95:LYS:NZ	40:q:89:HIS:CE1	2.89	0.41
10:J:158:VAL:HG11	11:K:73:LEU:HD21	2.03	0.41
12:L:129:ILE:HD11	13:M:404:HIS:CE1	2.56	0.41
12:L:214:THR:HG23	12:L:215:PRO:HD3	2.02	0.41
13:M:20:MET:O	13:M:24:VAL:HG23	2.21	0.41
13:M:235:ILE:HD13	13:M:289:LEU:HD21	2.01	0.41
13:M:317:LEU:HD22	13:M:347:TRP:CD1	2.56	0.41
15:O:64:TYR:CD2	15:O:337:ILE:HD12	2.56	0.41
15:O:380:MET:HG3	15:O:380:MET:O	2.21	0.41
21:W:24:GLU:OE2	21:W:28:ARG:NH2	2.50	0.41
23:Y:17:ALA:HB2	23:Y:75:LEU:HD21	2.03	0.41
26:b:31:LEU:O	26:b:35:VAL:HG23	2.21	0.41
32:i:97:THR:O	32:i:101:LEU:HD23	2.20	0.41
42:s:65:GLY:O	42:s:67:VAL:HG13	2.21	0.41
3:C:175:MET:HE3	3:C:190:LEU:CD1	2.46	0.41
6:F:330:LEU:HD23	6:F:378:VAL:HG13	2.03	0.41
7:G:229:LEU:HD11	7:G:719:GLN:OE1	2.21	0.41
8:H:156:ILE:HG21	8:H:192:TRP:CE3	2.56	0.41
9:I:159:TYR:CD1	9:I:159:TYR:N	2.89	0.41
15:O:214:VAL:HG22	15:O:354:ARG:NH2	2.36	0.41
16:P:394:LEU:O	16:P:396:GLU:N	2.49	0.41
19:U:75:ILE:CD1	19:U:150:VAL:HG21	2.51	0.41
22:X:18:GLN:NE2	22:X:19:GLU:O	2.54	0.41
22:X:43:ASN:HB3	22:X:134:ILE:HD13	2.01	0.41
40:q:94:LEU:HD12	40:q:94:LEU:N	2.36	0.41
2:B:199:MET:HE1	9:I:91:TYR:CD1	2.57	0.40
6:F:438:THR:HB	43:F:502:SF4:S4	2.61	0.40
7:G:398:LEU:HD11	7:G:522:LEU:HD23	2.01	0.40
8:H:1:MET:SD	8:H:4:MET:HG2	2.61	0.40
8:H:89:SER:O	8:H:92:VAL:HG12	2.21	0.40
16:P:106:VAL:O	16:P:106:VAL:HG12	2.20	0.40
18:R:40:THR:HG22	18:R:63:VAL:HG23	2.04	0.40
27:d:83:ASP:OD2	27:d:87:ARG:NE	2.50	0.40
4:D:121:LEU:O	4:D:122:HIS:C	2.64	0.40
6:F:250:VAL:HG22	6:F:255:THR:CG2	2.50	0.40
8:H:1:MET:HB2	25:a:56:ASP:O	2.21	0.40
13:M:269:ASP:O	13:M:273:LEU:HD23	2.21	0.40
13:M:284:ILE:CD1	13:M:387:LEU:HD21	2.51	0.40
13:M:325:LEU:HD22	13:M:411:VAL:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:P:135:VAL:HG22	16:P:173:ARG:HB2	2.03	0.40
16:P:406:ILE:O	16:P:406:ILE:HG23	2.22	0.40
24:Z:122:LEU:HB3	24:Z:126:THR:HG21	2.03	0.40
32:i:155:TYR:HB2	39:p:86:ARG:HG3	2.03	0.40
34:k:30:GLU:O	34:k:33:GLY:N	2.53	0.40
7:G:182:LEU:HD21	7:G:712:CYS:SG	2.62	0.40
7:G:601:ILE:HD11	7:G:649:ARG:CZ	2.51	0.40
8:H:132:SER:O	8:H:135:ALA:N	2.55	0.40
13:M:348:PHE:O	13:M:351:SER:OG	2.29	0.40
14:N:217:ILE:HG23	14:N:312:MET:HB2	2.02	0.40
16:P:265:ALA:HA	16:P:268:ILE:HD12	2.03	0.40
30:g:98:PRO:O	30:g:100:THR:HG23	2.22	0.40
33:j:78:ASN:OD1	33:j:79:SER:N	2.54	0.40
4:D:166:ILE:HG22	4:D:167:ASP:N	2.35	0.40
6:F:117:MET:HE1	6:F:254:PRO:C	2.46	0.40
6:F:159:ILE:HD12	6:F:267:PRO:HB3	2.03	0.40
9:I:39:VAL:HG12	9:I:45:TYR:CD1	2.56	0.40
9:I:89:ILE:HG21	9:I:95:LYS:HA	2.02	0.40
11:K:15:ILE:HG13	11:K:16:LEU:N	2.37	0.40
12:L:46:SER:HA	39:p:77:ASN:OD1	2.20	0.40
15:O:40:ILE:HD12	15:O:304:ILE:HG22	2.04	0.40
19:U:106:LEU:HD13	19:U:114:VAL:HG21	2.02	0.40
22:X:38:CYS:O	22:X:38:CYS:SG	2.80	0.40
1:A:61:THR:O	1:A:64:PHE:HB3	2.21	0.40
5:E:59:ILE:HD11	5:E:74:PRO:HB3	2.03	0.40
12:L:262:LEU:C	12:L:496:LEU:HD21	2.47	0.40
12:L:313:MET:HA	12:L:313:MET:HE3	2.04	0.40
13:M:218:ILE:HG22	13:M:223:MET:HE3	2.02	0.40
14:N:97:ILE:HG22	14:N:144:LEU:HD11	2.04	0.40
16:P:90:MET:HB3	16:P:92:LEU:HD13	2.03	0.40
16:P:101:VAL:O	16:P:101:VAL:HG22	2.21	0.40
21:W:76:ILE:HA	21:W:79:LEU:HD12	2.02	0.40
32:i:143:TYR:O	32:i:145:LYS:N	2.55	0.40
40:q:32:ARG:NH1	40:q:71:VAL:O	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	115/117 (98%)	110 (96%)	5 (4%)	0	100	100
2	B	180/182 (99%)	167 (93%)	12 (7%)	1 (1%)	21	52
3	C	207/209 (99%)	185 (89%)	22 (11%)	0	100	100
4	D	425/428 (99%)	397 (93%)	27 (6%)	1 (0%)	43	71
5	E	212/214 (99%)	195 (92%)	17 (8%)	0	100	100
6	F	437/439 (100%)	405 (93%)	32 (7%)	0	100	100
7	G	673/731 (92%)	622 (92%)	51 (8%)	0	100	100
8	H	313/315 (99%)	282 (90%)	31 (10%)	0	100	100
9	I	184/186 (99%)	174 (95%)	10 (5%)	0	100	100
10	J	165/167 (99%)	150 (91%)	15 (9%)	0	100	100
11	K	91/93 (98%)	84 (92%)	7 (8%)	0	100	100
12	L	575/577 (100%)	535 (93%)	40 (7%)	0	100	100
13	M	444/446 (100%)	412 (93%)	32 (7%)	0	100	100
14	N	339/341 (99%)	317 (94%)	22 (6%)	0	100	100
15	O	366/368 (100%)	328 (90%)	38 (10%)	0	100	100
16	P	375/377 (100%)	345 (92%)	30 (8%)	0	100	100
17	Q	128/130 (98%)	111 (87%)	17 (13%)	0	100	100
18	R	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
19	T	75/152 (49%)	70 (93%)	5 (7%)	0	100	100
19	U	83/152 (55%)	69 (83%)	14 (17%)	0	100	100
20	V	116/118 (98%)	110 (95%)	6 (5%)	0	100	100
21	W	112/114 (98%)	105 (94%)	7 (6%)	0	100	100
22	X	172/174 (99%)	157 (91%)	15 (9%)	0	100	100
23	Y	165/167 (99%)	157 (95%)	8 (5%)	0	100	100
24	Z	144/146 (99%)	138 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
25	a	71/73 (97%)	67 (94%)	4 (6%)	0	100	100
26	b	64/66 (97%)	58 (91%)	6 (9%)	0	100	100
27	d	113/115 (98%)	109 (96%)	4 (4%)	0	100	100
28	e	98/100 (98%)	92 (94%)	6 (6%)	0	100	100
29	f	54/56 (96%)	42 (78%)	12 (22%)	0	100	100
30	g	104/106 (98%)	95 (91%)	9 (9%)	0	100	100
31	h	143/145 (99%)	132 (92%)	11 (8%)	0	100	100
32	i	159/161 (99%)	147 (92%)	12 (8%)	0	100	100
33	j	57/59 (97%)	53 (93%)	4 (7%)	0	100	100
34	k	82/84 (98%)	64 (78%)	17 (21%)	1 (1%)	10	39
35	l	142/144 (99%)	125 (88%)	17 (12%)	0	100	100
36	m	106/108 (98%)	93 (88%)	13 (12%)	0	100	100
37	n	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
38	o	110/112 (98%)	99 (90%)	11 (10%)	0	100	100
39	p	149/151 (99%)	136 (91%)	13 (9%)	0	100	100
40	q	133/135 (98%)	123 (92%)	10 (8%)	0	100	100
41	r	85/103 (82%)	81 (95%)	4 (5%)	0	100	100
42	s	60/62 (97%)	51 (85%)	9 (15%)	0	100	100
All	All	8045/8346 (96%)	7397 (92%)	645 (8%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	CYS
34	k	38	LYS
4	D	122	HIS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	110/110 (100%)	110 (100%)	0	100	100
2	B	152/152 (100%)	152 (100%)	0	100	100
3	C	187/187 (100%)	187 (100%)	0	100	100
4	D	367/367 (100%)	367 (100%)	0	100	100
5	E	185/185 (100%)	185 (100%)	0	100	100
6	F	351/351 (100%)	351 (100%)	0	100	100
7	G	546/582 (94%)	546 (100%)	0	100	100
8	H	282/282 (100%)	282 (100%)	0	100	100
9	I	159/159 (100%)	159 (100%)	0	100	100
10	J	161/161 (100%)	161 (100%)	0	100	100
11	K	88/88 (100%)	88 (100%)	0	100	100
12	L	518/518 (100%)	518 (100%)	0	100	100
13	M	404/404 (100%)	404 (100%)	0	100	100
14	N	317/317 (100%)	317 (100%)	0	100	100
15	O	324/324 (100%)	324 (100%)	0	100	100
16	P	319/319 (100%)	319 (100%)	0	100	100
17	Q	114/114 (100%)	114 (100%)	0	100	100
18	R	77/77 (100%)	77 (100%)	0	100	100
19	T	71/136 (52%)	71 (100%)	0	100	100
19	U	79/136 (58%)	79 (100%)	0	100	100
20	V	97/97 (100%)	97 (100%)	0	100	100
21	W	107/107 (100%)	107 (100%)	0	100	100
22	X	150/150 (100%)	150 (100%)	0	100	100
23	Y	128/128 (100%)	128 (100%)	0	100	100
24	Z	128/128 (100%)	128 (100%)	0	100	100
25	a	65/65 (100%)	65 (100%)	0	100	100
26	b	52/52 (100%)	52 (100%)	0	100	100
27	d	93/93 (100%)	93 (100%)	0	100	100
28	e	88/88 (100%)	88 (100%)	0	100	100
29	f	43/43 (100%)	43 (100%)	0	100	100
30	g	95/95 (100%)	95 (100%)	0	100	100
31	h	130/130 (100%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	i	133/133 (100%)	133 (100%)	0	100	100
33	j	51/51 (100%)	51 (100%)	0	100	100
34	k	69/69 (100%)	69 (100%)	0	100	100
35	l	121/121 (100%)	121 (100%)	0	100	100
36	m	89/89 (100%)	89 (100%)	0	100	100
37	n	117/117 (100%)	117 (100%)	0	100	100
38	o	101/101 (100%)	101 (100%)	0	100	100
39	p	135/135 (100%)	135 (100%)	0	100	100
40	q	116/116 (100%)	116 (100%)	0	100	100
41	r	78/86 (91%)	78 (100%)	0	100	100
42	s	50/50 (100%)	50 (100%)	0	100	100
All	All	7047/7213 (98%)	7047 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	41	GLN
3	C	162	HIS
4	D	152	ASN
5	E	195	GLN
6	F	437	HIS
6	F	468	HIS
7	G	435	HIS
7	G	501	HIS
7	G	599	GLN
9	I	198	ASN
10	J	117	GLN
12	L	88	ASN
12	L	537	HIS
13	M	133	GLN
14	N	83	ASN
14	N	181	ASN
14	N	182	HIS
14	N	264	GLN
15	O	68	ASN
15	O	216	ASN

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Mol	Chain	Res	Type
15	O	230	HIS
15	O	245	GLN
16	P	134	ASN
16	P	138	ASN
16	P	148	ASN
16	P	343	HIS
18	R	64	ASN
19	T	95	ASN
19	T	111	HIS
19	U	76	ASN
20	V	22	HIS
20	V	83	GLN
21	W	13	GLN
21	W	39	GLN
22	X	172	HIS
27	d	93	HIS
28	e	58	GLN
30	g	104	ASN
31	h	63	HIS
31	h	118	ASN
32	i	46	GLN
34	k	44	ASN
35	l	98	HIS
39	p	38	GLN
40	q	33	ASN
40	q	70	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	2MR	D	123	4	10,12,13	2.42	2 (20%)	5,13,15	4.12	2 (40%)

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
4	2MR	D	123	4	-	1/10/13/15	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	123	2MR	CZ-NH2	5.44	1.44	1.33
4	D	123	2MR	CZ-NE	5.00	1.44	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	123	2MR	NE-CZ-NH2	-8.69	111.51	119.48
4	D	123	2MR	CG-CD-NE	-2.28	105.80	112.20

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	123	2MR	O-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	123	2MR	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 1 is monoatomic - leaving 21 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
43	SF4	I	302	9	0,12,12	-	-	-		
44	3PE	L	601	-	34,34,50	1.05	4 (11%)	37,39,55	1.24	2 (5%)
43	SF4	F	502	6	0,12,12	-	-	-		
47	CDL	M	501	-	54,54,99	1.16	6 (11%)	60,66,111	1.18	3 (5%)
44	3PE	B	302	-	41,41,50	0.97	4 (9%)	44,46,55	0.99	2 (4%)
43	SF4	G	802	7	0,12,12	-	-	-		
45	FES	G	803	7	0,4,4	-	-	-		
51	EHZ	T	201	19	31,36,37	1.55	5 (16%)	36,44,47	1.66	4 (11%)
45	FES	E	301	5	0,4,4	-	-	-		
44	3PE	Y	302	-	21,21,50	1.29	4 (19%)	24,26,55	1.31	2 (8%)
44	3PE	Y	301	-	19,19,50	1.30	3 (15%)	22,24,55	0.96	1 (4%)
48	DGT	O	501	-	32,33,33	3.45	15 (46%)	48,52,52	1.92	12 (25%)
43	SF4	I	301	9	0,12,12	-	-	-		
44	3PE	B	303	-	25,25,50	1.22	4 (16%)	28,30,55	1.36	2 (7%)
46	FMN	F	501	-	33,33,33	2.60	10 (30%)	48,50,50	1.71	12 (25%)
47	CDL	P	502	-	40,40,99	1.28	5 (12%)	46,52,111	1.13	4 (8%)
43	SF4	B	301	2	0,12,12	-	-	-		
49	NDP	P	501	-	51,52,52	3.91	26 (50%)	71,80,80	2.10	18 (25%)
51	EHZ	U	201	19	31,36,37	1.62	6 (19%)	36,44,47	1.64	7 (19%)
44	3PE	Y	303	-	24,24,50	1.24	4 (16%)	27,29,55	1.13	2 (7%)
43	SF4	G	801	7	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
43	SF4	I	302	9	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
44	3PE	L	601	-	-	16/38/38/54	-
47	CDL	M	501	-	-	34/64/64/110	-
43	SF4	F	502	6	-	-	0/6/5/5
44	3PE	B	302	-	-	18/45/45/54	-
43	SF4	G	802	7	-	-	0/6/5/5
45	FES	G	803	7	-	-	0/1/1/1
51	EHZ	T	201	19	-	9/42/44/45	-
45	FES	E	301	5	-	-	0/1/1/1
44	3PE	Y	302	-	-	11/25/25/54	-
44	3PE	Y	301	-	-	14/22/22/54	-
48	DGT	O	501	-	-	7/22/34/34	0/3/3/3
43	SF4	I	301	9	-	-	0/6/5/5
44	3PE	B	303	-	-	10/29/29/54	-
46	FMN	F	501	-	-	12/18/18/18	0/3/3/3
47	CDL	P	502	-	-	19/49/49/110	-
43	SF4	B	301	2	-	-	0/6/5/5
49	NDP	P	501	-	-	10/34/77/77	0/5/5/5
51	EHZ	U	201	19	-	9/42/44/45	-
44	3PE	Y	303	-	-	14/28/28/54	-
43	SF4	G	801	7	-	-	0/6/5/5

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	501	NDP	C2B-C1B	-9.29	1.30	1.53
49	P	501	NDP	PA-O3	9.00	1.69	1.59
48	O	501	DGT	C3'-C4'	-8.33	1.31	1.53
49	P	501	NDP	O4B-C1B	8.08	1.60	1.42
49	P	501	NDP	O4D-C1D	8.01	1.60	1.42
48	O	501	DGT	O4'-C4'	7.90	1.62	1.45
49	P	501	NDP	C7N-N7N	7.65	1.55	1.33
49	P	501	NDP	C2D-C1D	-7.35	1.30	1.53
49	P	501	NDP	C6N-C5N	7.02	1.54	1.33
49	P	501	NDP	O4D-C4D	-6.83	1.29	1.45
48	O	501	DGT	C4-N3	6.49	1.49	1.34
46	F	501	FMN	C10-N1	6.10	1.45	1.33
46	F	501	FMN	C4A-N5	5.92	1.43	1.30
48	O	501	DGT	C2-N3	5.58	1.46	1.33
49	P	501	NDP	P2B-O2B	5.53	1.69	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	P	501	NDP	C6A-N6A	5.37	1.47	1.34
49	P	501	NDP	O4B-C4B	-5.31	1.33	1.45
51	U	201	EHZ	C12-N1	5.26	1.45	1.33
48	O	501	DGT	PB-O3A	5.08	1.65	1.59
48	O	501	DGT	O4'-C1'	-5.06	1.31	1.42
48	O	501	DGT	PA-O3A	5.04	1.64	1.59
51	T	201	EHZ	C15-N2	5.03	1.45	1.33
51	U	201	EHZ	C15-N2	4.91	1.45	1.33
51	T	201	EHZ	C12-N1	4.91	1.45	1.33
46	F	501	FMN	C5A-N5	4.88	1.48	1.39
46	F	501	FMN	C9A-N10	4.77	1.49	1.41
46	F	501	FMN	C2-N1	4.67	1.47	1.36
48	O	501	DGT	C2-N2	4.66	1.45	1.34
48	O	501	DGT	PB-O3B	4.65	1.64	1.59
49	P	501	NDP	C5A-C4A	-4.60	1.30	1.39
46	F	501	FMN	C2-N3	4.30	1.48	1.39
49	P	501	NDP	C2N-C3N	4.29	1.47	1.35
49	P	501	NDP	C8A-N9A	-4.28	1.30	1.37
49	P	501	NDP	O7N-C7N	-4.17	1.14	1.24
49	P	501	NDP	PN-O3	3.75	1.63	1.59
49	P	501	NDP	O2D-C2D	3.61	1.51	1.43
46	F	501	FMN	C4-N3	3.55	1.45	1.38
46	F	501	FMN	C10-N10	3.35	1.44	1.37
46	F	501	FMN	O2-C2	-3.30	1.17	1.24
49	P	501	NDP	C4N-C3N	3.19	1.56	1.50
48	O	501	DGT	C5-N7	-3.08	1.32	1.39
44	Y	303	3PE	O21-C2	-2.96	1.39	1.46
44	B	302	3PE	O21-C2	-2.87	1.39	1.46
48	O	501	DGT	O3'-C3'	2.86	1.49	1.43
47	P	502	CDL	OA6-CA4	-2.82	1.40	1.46
47	M	501	CDL	OA6-CA4	-2.77	1.40	1.46
49	P	501	NDP	C5A-N7A	-2.76	1.34	1.39
49	P	501	NDP	C4N-C5N	2.74	1.56	1.49
47	M	501	CDL	OB6-CB4	-2.74	1.40	1.46
44	L	601	3PE	O21-C2	-2.71	1.40	1.46
48	O	501	DGT	O6-C6	-2.70	1.18	1.23
48	O	501	DGT	C2-N1	2.66	1.44	1.37
46	F	501	FMN	O4-C4	-2.64	1.18	1.23
44	Y	301	3PE	O21-C2	-2.64	1.40	1.46
44	B	303	3PE	O21-C2	-2.54	1.40	1.46
49	P	501	NDP	O3B-C3B	-2.46	1.36	1.43
44	Y	303	3PE	O31-C31	2.46	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	U	201	EHZ	C9-S1	2.46	1.82	1.76
47	M	501	CDL	OB6-CB5	2.45	1.41	1.34
51	U	201	EHZ	O4-C15	-2.45	1.18	1.23
44	B	303	3PE	O31-C3	-2.45	1.39	1.45
49	P	501	NDP	O3D-C3D	-2.43	1.36	1.43
44	Y	302	3PE	O31-C31	2.42	1.40	1.33
44	B	302	3PE	O31-C3	-2.42	1.39	1.45
47	P	502	CDL	OB6-CB5	2.38	1.41	1.34
49	P	501	NDP	C6N-N1N	2.38	1.43	1.37
47	M	501	CDL	OA8-CA7	2.37	1.40	1.33
48	O	501	DGT	C5-C6	2.35	1.53	1.44
51	T	201	EHZ	O4-C15	-2.34	1.18	1.23
51	U	201	EHZ	O3-C12	-2.33	1.18	1.23
51	T	201	EHZ	O3-C12	-2.30	1.18	1.23
44	B	302	3PE	O31-C31	2.29	1.40	1.33
44	Y	301	3PE	O31-C3	-2.28	1.40	1.45
44	Y	302	3PE	O21-C21	2.26	1.40	1.34
44	Y	302	3PE	O21-C2	-2.26	1.41	1.46
44	Y	302	3PE	O31-C3	-2.26	1.40	1.45
44	B	303	3PE	O21-C21	2.25	1.40	1.34
44	B	303	3PE	O31-C31	2.24	1.39	1.33
49	P	501	NDP	P2B-O1X	2.24	1.57	1.50
44	L	601	3PE	O31-C3	-2.22	1.40	1.45
44	Y	301	3PE	O21-C21	2.21	1.40	1.34
51	U	201	EHZ	O6-C20	-2.19	1.37	1.44
51	T	201	EHZ	C9-S1	2.18	1.81	1.76
44	L	601	3PE	O31-C31	2.18	1.39	1.33
47	M	501	CDL	OA8-CA6	-2.16	1.40	1.45
47	P	502	CDL	OA8-CA6	-2.16	1.40	1.45
44	L	601	3PE	O21-C21	2.15	1.40	1.34
47	P	502	CDL	OB6-CB4	-2.15	1.41	1.46
49	P	501	NDP	C7N-C3N	2.14	1.53	1.48
49	P	501	NDP	PA-O5B	2.12	1.67	1.59
47	P	502	CDL	OA6-CA5	2.09	1.40	1.34
44	B	302	3PE	O21-C21	2.09	1.40	1.34
47	M	501	CDL	OA6-CA5	2.06	1.40	1.34
44	Y	303	3PE	O31-C3	-2.04	1.40	1.45
44	Y	303	3PE	O21-C21	2.03	1.40	1.34
48	O	501	DGT	C6-N1	2.01	1.42	1.38

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	T	201	EHZ	C8-C9-S1	6.47	121.73	113.56
49	P	501	NDP	C4A-N9A-C1B	-5.80	113.06	126.63
49	P	501	NDP	N6A-C6A-N1A	-5.73	105.62	118.38
49	P	501	NDP	N3A-C2A-N1A	-5.57	120.16	128.58
48	O	501	DGT	C5-C4-N3	-5.43	119.75	128.39
49	P	501	NDP	C1B-N9A-C8A	5.11	138.43	127.09
49	P	501	NDP	C5A-C4A-N3A	-4.87	120.02	126.72
44	B	303	3PE	O21-C21-C22	4.70	121.66	111.48
49	P	501	NDP	C2B-C1B-N9A	-4.51	106.34	113.75
46	F	501	FMN	C9-C8-C7	4.44	126.20	119.69
44	L	601	3PE	O21-C21-C22	4.42	121.05	111.48
48	O	501	DGT	C2-N3-C4	4.41	119.89	112.30
48	O	501	DGT	C1'-N9-C4	-4.39	113.64	125.50
44	Y	302	3PE	O21-C21-C22	4.35	120.89	111.48
48	O	501	DGT	C1'-N9-C8	4.34	137.64	127.91
47	M	501	CDL	OA6-CA5-C11	4.30	120.78	111.48
49	P	501	NDP	N9A-C8A-N7A	-4.22	107.94	113.94
49	P	501	NDP	C5A-C6A-N6A	4.22	133.74	123.29
51	U	201	EHZ	C10-S1-C9	4.10	113.97	101.84
51	U	201	EHZ	C8-C9-S1	3.97	118.57	113.56
44	Y	303	3PE	O21-C21-C22	3.85	119.80	111.48
46	F	501	FMN	C7M-C7-C6	3.79	126.26	119.57
46	F	501	FMN	C4-N3-C2	-3.74	118.99	125.64
47	M	501	CDL	OB6-CB5-C51	3.73	119.55	111.48
48	O	501	DGT	N9-C4-N3	3.63	133.22	125.95
47	P	502	CDL	OB6-CB5-C51	3.57	119.20	111.48
44	B	302	3PE	O21-C21-C22	3.50	119.05	111.48
49	P	501	NDP	C2A-N3A-C4A	3.44	120.22	111.83
51	U	201	EHZ	C13-C14-N2	-3.31	104.96	112.00
51	T	201	EHZ	O2-C9-S1	-3.28	118.51	122.68
49	P	501	NDP	C3N-C2N-N1N	-3.26	118.42	123.20
48	O	501	DGT	C2-N1-C6	-3.21	119.28	125.11
46	F	501	FMN	C4A-C10-N10	3.17	121.02	116.48
44	L	601	3PE	O31-C31-C32	3.06	121.16	111.83
48	O	501	DGT	N9-C8-N7	-3.00	107.84	113.40
49	P	501	NDP	N3A-C4A-N9A	2.94	132.16	127.17
46	F	501	FMN	C8M-C8-C7	-2.93	114.77	120.76
44	Y	302	3PE	O31-C31-C32	2.92	120.01	111.15
44	B	303	3PE	O31-C31-C32	2.86	120.54	111.83
51	U	201	EHZ	C18-C17-C16	2.78	113.51	108.77
48	O	501	DGT	C2'-C3'-C4'	2.74	108.36	102.80
49	P	501	NDP	C4B-O4B-C1B	-2.71	103.47	109.47
48	O	501	DGT	C5-C6-N1	2.70	120.12	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	P	501	NDP	C5A-N7A-C8A	2.69	107.68	103.45
51	U	201	EHZ	C18-C17-C20	-2.67	103.82	108.22
51	U	201	EHZ	C14-C13-C12	-2.62	108.03	112.39
48	O	501	DGT	O6-C6-C5	-2.61	119.65	126.53
49	P	501	NDP	C4A-N9A-C8A	2.60	108.47	105.74
46	F	501	FMN	C6-C7-C8	-2.60	115.88	119.69
47	P	502	CDL	OA6-CA5-C11	2.57	120.38	110.93
44	B	302	3PE	O31-C31-C32	2.55	119.61	111.83
46	F	501	FMN	C6-C5A-C9A	2.55	122.55	119.05
51	T	201	EHZ	O2-C9-C8	-2.53	119.75	123.74
46	F	501	FMN	O4-C4-C4A	-2.51	119.91	126.53
49	P	501	NDP	P2B-O2B-C2B	-2.48	116.81	123.43
49	P	501	NDP	C3D-C2D-C1D	2.47	106.14	101.46
46	F	501	FMN	C4-C4A-C10	2.42	121.08	116.93
44	Y	301	3PE	O21-C21-C22	2.39	119.70	110.93
46	F	501	FMN	C5'-C4'-C3'	-2.38	107.73	112.22
47	M	501	CDL	OA8-CA7-C31	2.34	118.98	111.83
46	F	501	FMN	C4A-C4-N3	2.34	119.20	113.25
44	Y	303	3PE	O31-C31-C32	2.32	118.91	111.83
46	F	501	FMN	C10-C4A-N5	-2.22	120.28	124.81
47	P	502	CDL	OB6-CB4-CB3	2.19	116.20	108.34
49	P	501	NDP	C4A-C5A-N7A	-2.19	108.08	110.58
49	P	501	NDP	O4B-C1B-N9A	2.19	112.29	108.09
48	O	501	DGT	C2'-C1'-N9	-2.15	108.44	113.81
51	T	201	EHZ	C10-C11-N1	-2.12	107.98	112.41
51	U	201	EHZ	O2-C9-C8	-2.12	120.41	123.74
47	P	502	CDL	CB6-CB4-CB3	-2.08	106.93	111.78
48	O	501	DGT	C8-N7-C5	2.06	107.92	104.26

There are no chirality outliers.

All (183) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
44	B	303	3PE	O13-C11-C12-N
44	L	601	3PE	C1-O11-P-O12
44	L	601	3PE	C1-O11-P-O13
44	L	601	3PE	C1-O11-P-O14
44	Y	301	3PE	C1-O11-P-O12
44	Y	301	3PE	C1-O11-P-O13
44	Y	301	3PE	C1-O11-P-O14
44	Y	301	3PE	C11-O13-P-O11
44	Y	301	3PE	C11-O13-P-O14

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Mol	Chain	Res	Type	Atoms
44	Y	301	3PE	O13-C11-C12-N
44	Y	302	3PE	C22-C21-O21-C2
44	Y	303	3PE	C1-O11-P-O13
44	Y	303	3PE	C1-O11-P-O14
44	Y	303	3PE	C12-C11-O13-P
44	Y	303	3PE	O11-C1-C2-O21
44	Y	303	3PE	O22-C21-O21-C2
44	Y	303	3PE	C22-C21-O21-C2
46	F	501	FMN	C1'-C2'-C3'-C4'
46	F	501	FMN	O4'-C4'-C5'-O5'
46	F	501	FMN	C5'-O5'-P-O1P
46	F	501	FMN	C5'-O5'-P-O2P
46	F	501	FMN	C5'-O5'-P-O3P
47	M	501	CDL	O1-C1-CB2-OB2
47	M	501	CDL	CA2-OA2-PA1-OA3
47	M	501	CDL	CA2-OA2-PA1-OA5
47	M	501	CDL	OA7-CA5-OA6-CA4
47	M	501	CDL	CB3-OB5-PB2-OB2
47	M	501	CDL	CB3-OB5-PB2-OB3
47	M	501	CDL	CB3-OB5-PB2-OB4
47	P	502	CDL	C11-CA5-OA6-CA4
47	P	502	CDL	CB2-OB2-PB2-OB5
47	P	502	CDL	CB3-OB5-PB2-OB2
47	P	502	CDL	CB3-OB5-PB2-OB4
48	O	501	DGT	PB-O3B-PG-O2G
48	O	501	DGT	C5'-O5'-PA-O3A
48	O	501	DGT	C5'-O5'-PA-O1A
48	O	501	DGT	C5'-O5'-PA-O2A
49	P	501	NDP	C5B-O5B-PA-O1A
49	P	501	NDP	C5B-O5B-PA-O3
49	P	501	NDP	O4B-C4B-C5B-O5B
49	P	501	NDP	C2N-C3N-C7N-O7N
49	P	501	NDP	C2N-C3N-C7N-N7N
51	T	201	EHZ	C7-C8-C9-S1
51	U	201	EHZ	S1-C10-C11-N1
51	U	201	EHZ	C11-C10-S1-C9
44	Y	302	3PE	O22-C21-O21-C2
47	P	502	CDL	OA7-CA5-OA6-CA4
47	M	501	CDL	C11-CA5-OA6-CA4
44	Y	301	3PE	C32-C31-O31-C3
47	P	502	CDL	C51-CB5-OB6-CB4
44	Y	301	3PE	C2-C1-O11-P

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Mol	Chain	Res	Type	Atoms
47	P	502	CDL	CB4-CB3-OB5-PB2
44	L	601	3PE	C32-C31-O31-C3
44	Y	301	3PE	O32-C31-O31-C3
47	P	502	CDL	OB7-CB5-OB6-CB4
47	M	501	CDL	CA7-C31-C32-C33
47	M	501	CDL	CA2-C1-CB2-OB2
47	M	501	CDL	C51-CB5-OB6-CB4
49	P	501	NDP	O4D-C1D-N1N-C6N
47	M	501	CDL	OB7-CB5-OB6-CB4
44	L	601	3PE	O32-C31-O31-C3
47	P	502	CDL	CB3-CB4-OB6-CB5
51	U	201	EHZ	C5-C6-C7-O1
44	B	302	3PE	C22-C21-O21-C2
47	M	501	CDL	OB6-CB4-CB6-OB8
44	L	601	3PE	C22-C23-C24-C25
49	P	501	NDP	C3B-C4B-C5B-O5B
44	Y	303	3PE	C22-C23-C24-C25
47	P	502	CDL	C71-CB7-OB8-CB6
44	B	302	3PE	C28-C29-C2A-C2B
44	B	302	3PE	O22-C21-O21-C2
47	P	502	CDL	C51-C52-C53-C54
47	P	502	CDL	O1-C1-CB2-OB2
44	L	601	3PE	C22-C21-O21-C2
47	M	501	CDL	C51-C52-C53-C54
47	M	501	CDL	C11-C12-C13-C14
47	M	501	CDL	C13-C14-C15-C16
46	F	501	FMN	C3'-C4'-C5'-O5'
47	P	502	CDL	C1-CB2-OB2-PB2
44	L	601	3PE	C2-C3-O31-C31
51	T	201	EHZ	O4-C15-C16-O5
44	L	601	3PE	O22-C21-O21-C2
44	L	601	3PE	C1-C2-C3-O31
44	B	302	3PE	C24-C25-C26-C27
47	M	501	CDL	C53-C54-C55-C56
51	U	201	EHZ	C1-C21-C22-C23
46	F	501	FMN	O2'-C2'-C3'-C4'
47	M	501	CDL	C1-CB2-OB2-PB2
47	M	501	CDL	CB4-CB3-OB5-PB2
51	T	201	EHZ	S1-C10-C11-N1
51	T	201	EHZ	C21-C1-C2-C3
44	Y	303	3PE	O11-C1-C2-C3
44	B	302	3PE	C3B-C3C-C3D-C3E

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Mol	Chain	Res	Type	Atoms
51	T	201	EHZ	N2-C15-C16-C17
47	P	502	CDL	OB9-CB7-OB8-CB6
44	B	302	3PE	C1-C2-C3-O31
47	M	501	CDL	CB3-CB4-CB6-OB8
47	M	501	CDL	C54-C55-C56-C57
47	P	502	CDL	C31-CA7-OA8-CA6
51	U	201	EHZ	C1-C2-C3-C4
44	Y	302	3PE	O11-C1-C2-O21
51	U	201	EHZ	O1-C7-C8-C9
51	U	201	EHZ	O2-C9-S1-C10
44	B	302	3PE	O21-C2-C3-O31
44	B	302	3PE	C29-C2A-C2B-C2C
44	L	601	3PE	C28-C29-C2A-C2B
46	F	501	FMN	O2'-C2'-C3'-O3'
44	L	601	3PE	C32-C33-C34-C35
51	U	201	EHZ	C8-C9-S1-C10
44	Y	302	3PE	O11-C1-C2-C3
44	B	303	3PE	O11-C1-C2-O21
44	Y	301	3PE	C1-C2-C3-O31
44	B	303	3PE	C12-C11-O13-P
44	L	601	3PE	C12-C11-O13-P
44	Y	301	3PE	C12-C11-O13-P
44	B	302	3PE	C26-C27-C28-C29
44	Y	301	3PE	O21-C21-C22-C23
48	O	501	DGT	PA-O3A-PB-O2B
44	B	303	3PE	O11-C1-C2-C3
44	Y	301	3PE	O22-C21-C22-C23
44	L	601	3PE	O21-C2-C3-O31
44	Y	301	3PE	O21-C2-C3-O31
47	M	501	CDL	OA6-CA4-CA6-OA8
47	M	501	CDL	CA3-CA4-CA6-OA8
44	L	601	3PE	C34-C35-C36-C37
44	B	302	3PE	C1-O11-P-O12
44	B	302	3PE	C1-O11-P-O13
44	B	302	3PE	C1-O11-P-O14
44	B	303	3PE	C1-O11-P-O12
44	B	303	3PE	C1-O11-P-O13
44	B	303	3PE	C1-O11-P-O14
44	B	303	3PE	C11-O13-P-O12
44	Y	302	3PE	C1-O11-P-O12
44	Y	302	3PE	C1-O11-P-O13
44	Y	302	3PE	C1-O11-P-O14

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Mol	Chain	Res	Type	Atoms
44	Y	302	3PE	C11-O13-P-O11
44	Y	302	3PE	C11-O13-P-O12
44	Y	303	3PE	C1-O11-P-O12
44	Y	303	3PE	C11-O13-P-O11
44	Y	303	3PE	C11-O13-P-O12
47	P	502	CDL	CB2-OB2-PB2-OB3
49	P	501	NDP	C5B-O5B-PA-O2A
46	F	501	FMN	C2'-C3'-C4'-O4'
47	M	501	CDL	C15-C16-C17-C18
47	M	501	CDL	CA3-CA4-OA6-CA5
44	B	302	3PE	C34-C35-C36-C37
47	M	501	CDL	OA5-CA3-CA4-OA6
47	M	501	CDL	C52-C51-CB5-OB6
51	T	201	EHZ	C7-C8-C9-O2
51	T	201	EHZ	O4-C15-C16-C17
47	P	502	CDL	CA2-C1-CB2-OB2
44	B	302	3PE	C25-C26-C27-C28
51	U	201	EHZ	C2-C3-C4-C5
44	Y	303	3PE	C31-C32-C33-C34
44	Y	302	3PE	C3-C2-O21-C21
47	P	502	CDL	OA9-CA7-OA8-CA6
47	M	501	CDL	C71-CB7-OB8-CB6
44	B	302	3PE	C37-C38-C39-C3A
47	M	501	CDL	CA4-CA6-OA8-CA7
49	P	501	NDP	C3B-C2B-O2B-P2B
47	M	501	CDL	C17-C18-C19-C20
44	B	302	3PE	C23-C24-C25-C26
46	F	501	FMN	O3'-C3'-C4'-O4'
46	F	501	FMN	C1'-C2'-C3'-O3'
44	Y	302	3PE	C1-C2-O21-C21
47	M	501	CDL	OA5-CA3-CA4-CA6
47	M	501	CDL	C52-C53-C54-C55
48	O	501	DGT	PA-O3A-PB-O1B
44	Y	303	3PE	O31-C31-C32-C33
44	B	303	3PE	O31-C31-C32-C33
47	M	501	CDL	C12-C11-CA5-OA6
48	O	501	DGT	PB-O3B-PG-O3G
44	B	302	3PE	O31-C31-C32-C33
46	F	501	FMN	O3'-C3'-C4'-C5'
51	T	201	EHZ	C12-C13-C14-N2
44	Y	303	3PE	O32-C31-C32-C33
44	B	302	3PE	O32-C31-C32-C33

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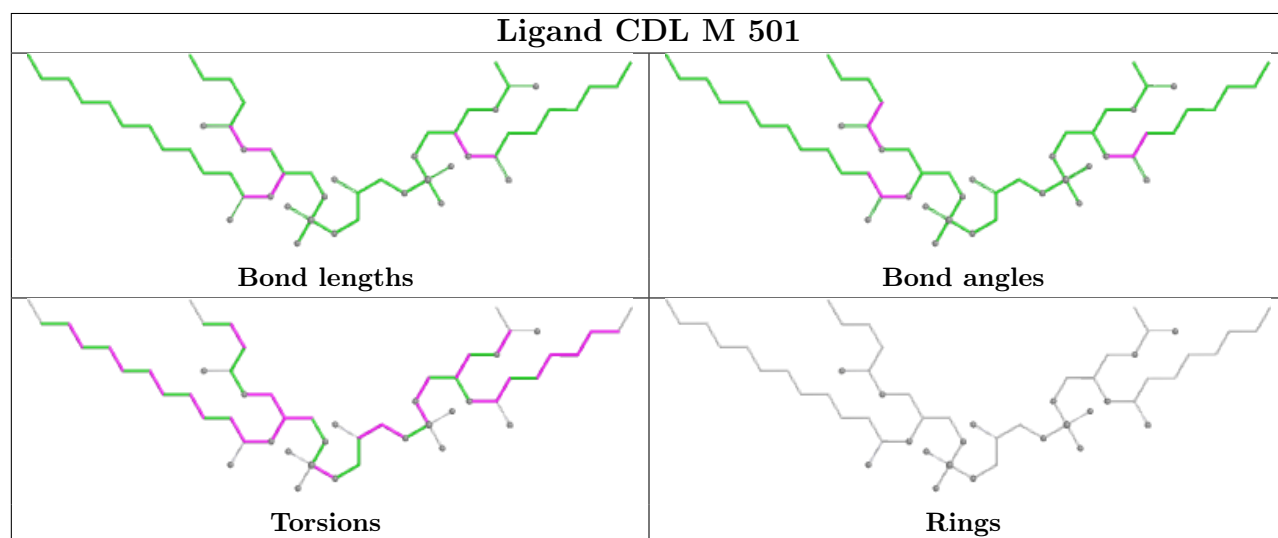
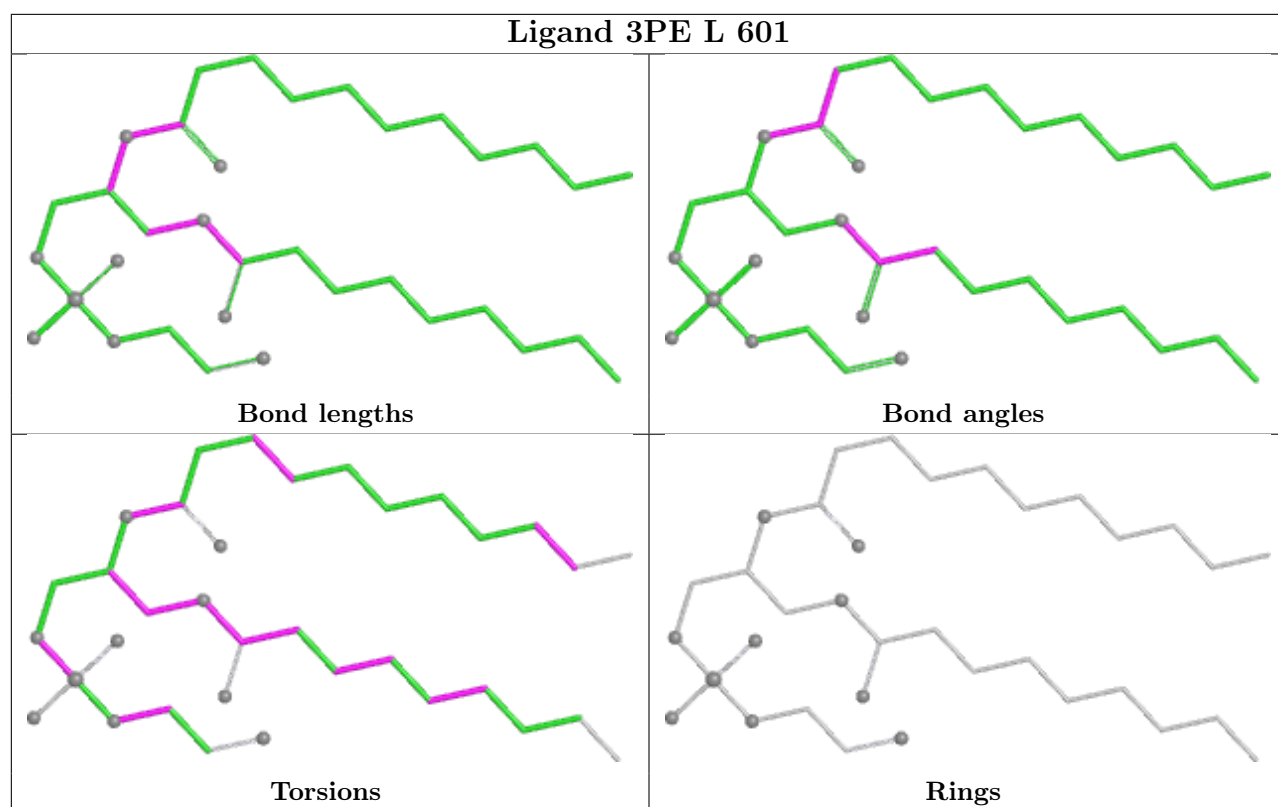
Mol	Chain	Res	Type	Atoms
47	P	502	CDL	CA3-CA4-CA6-OA8
51	T	201	EHZ	N2-C15-C16-O5
49	P	501	NDP	C1B-C2B-O2B-P2B
44	L	601	3PE	O31-C31-C32-C33
44	B	303	3PE	O32-C31-C32-C33
47	M	501	CDL	C12-C11-CA5-OA7

There are no ring outliers.

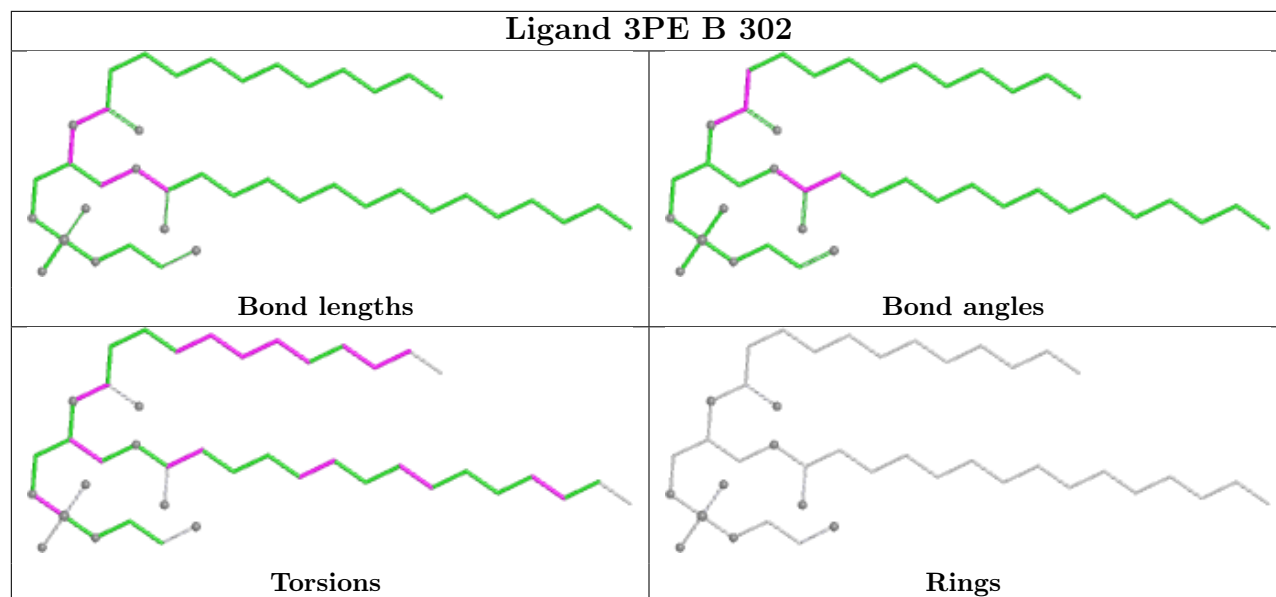
11 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
44	L	601	3PE	3	0
43	F	502	SF4	2	0
47	M	501	CDL	1	0
44	B	302	3PE	2	0
51	T	201	EHZ	1	0
45	E	301	FES	1	0
48	O	501	DGT	4	0
46	F	501	FMN	1	0
49	P	501	NDP	2	0
51	U	201	EHZ	1	0
43	G	801	SF4	2	0

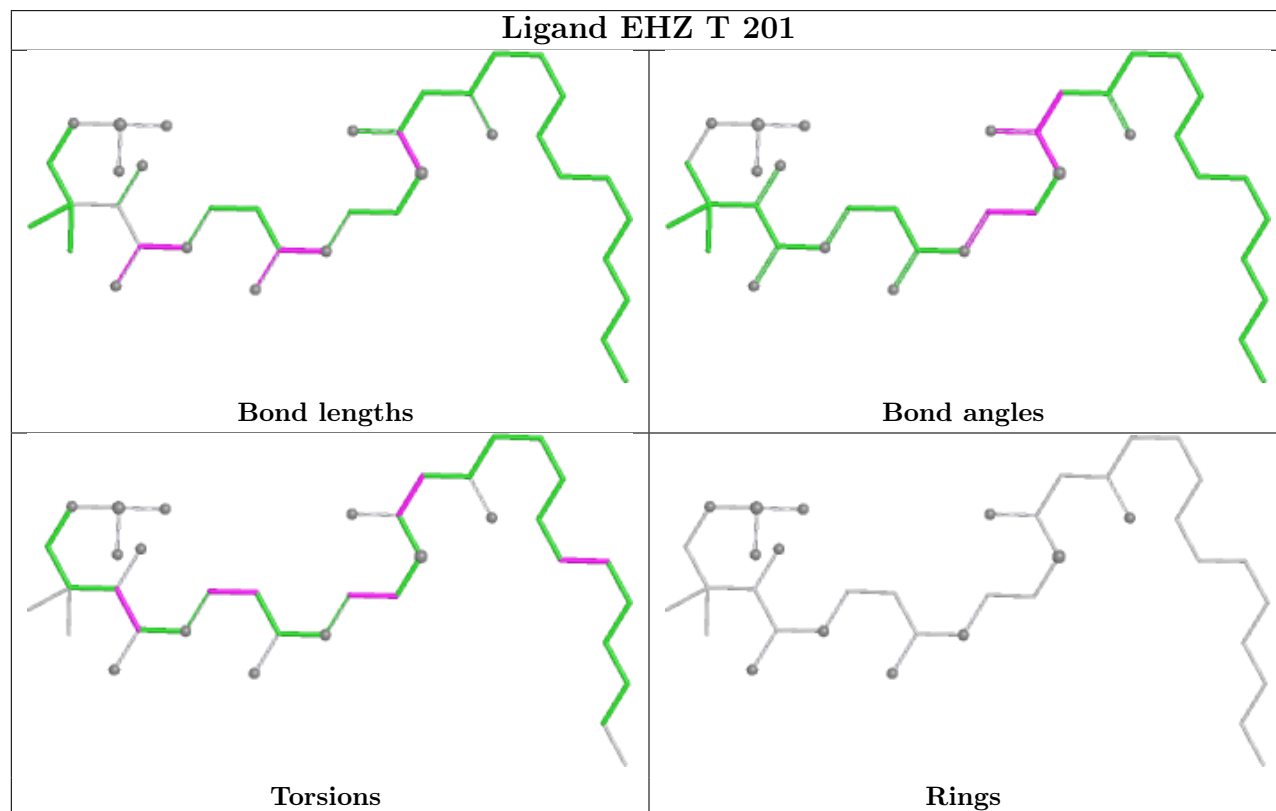
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



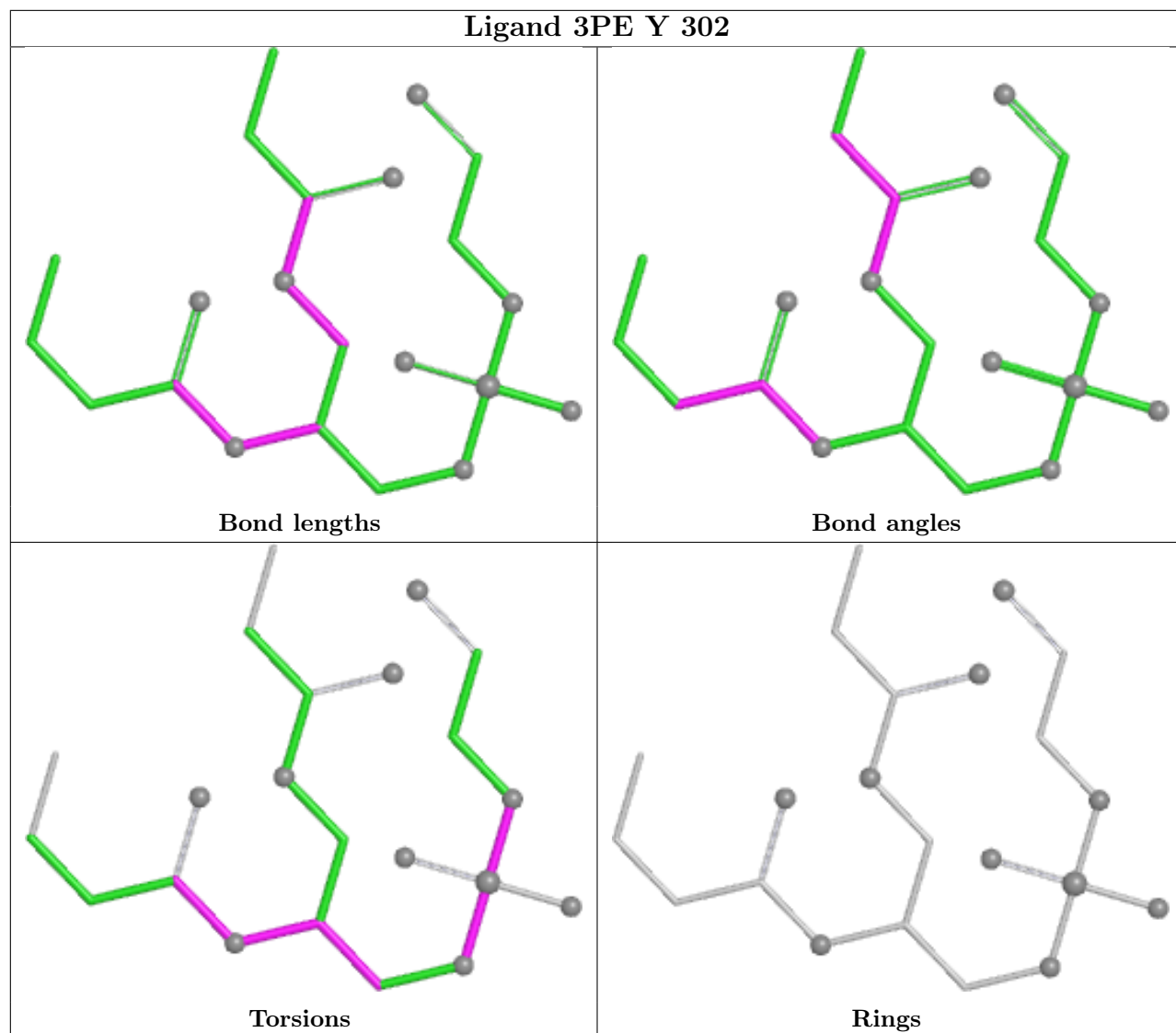
Ligand 3PE B 302

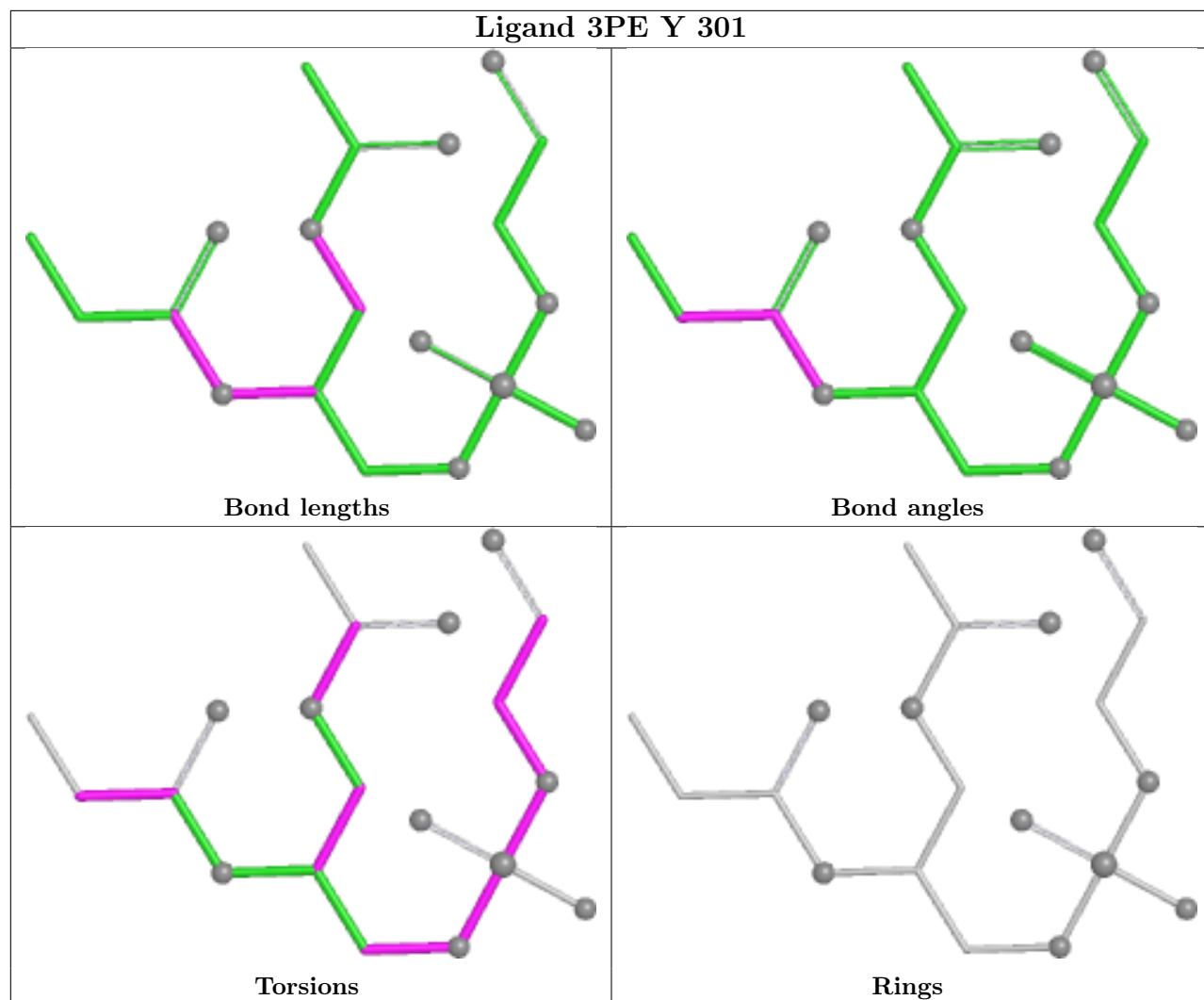


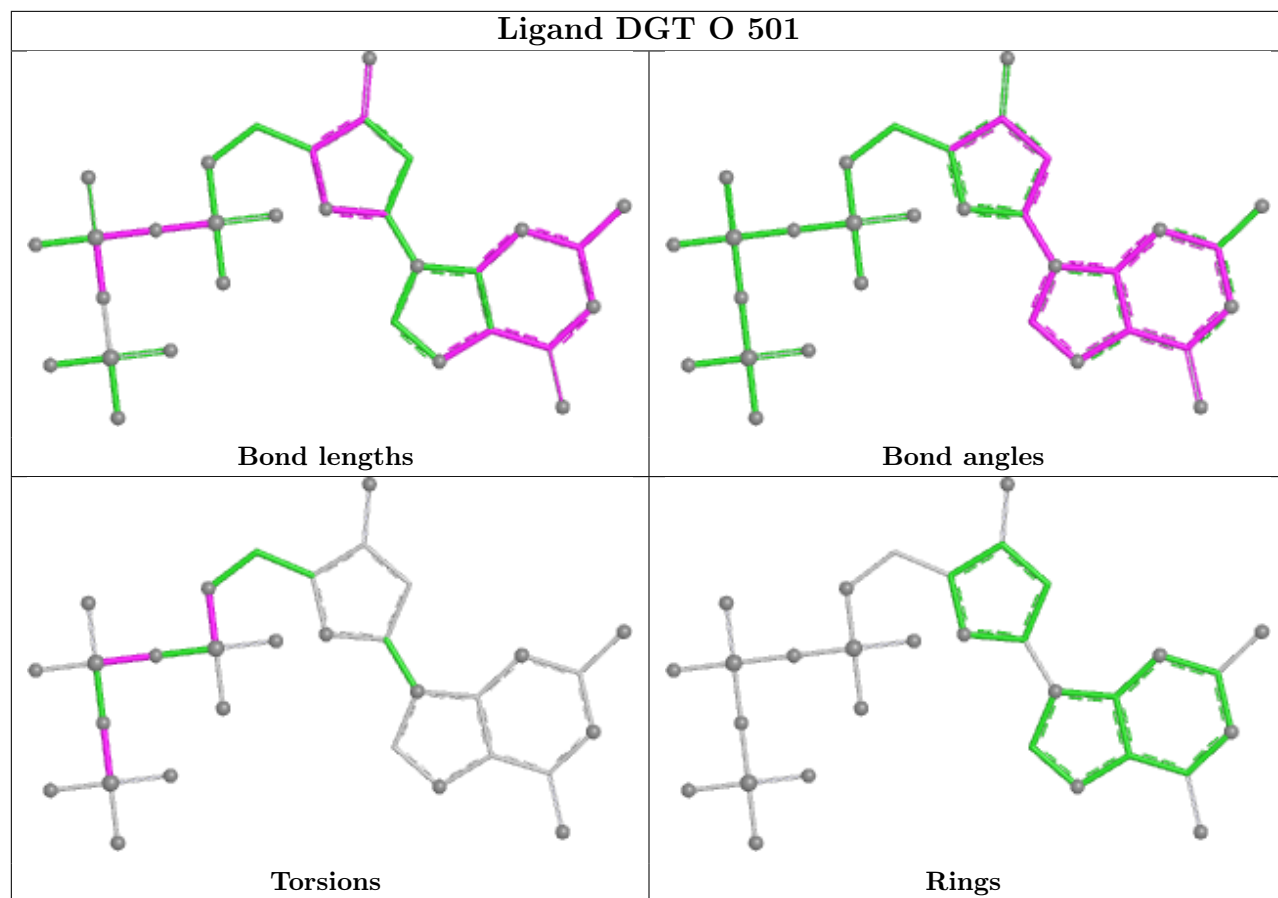
Ligand EHZ T 201

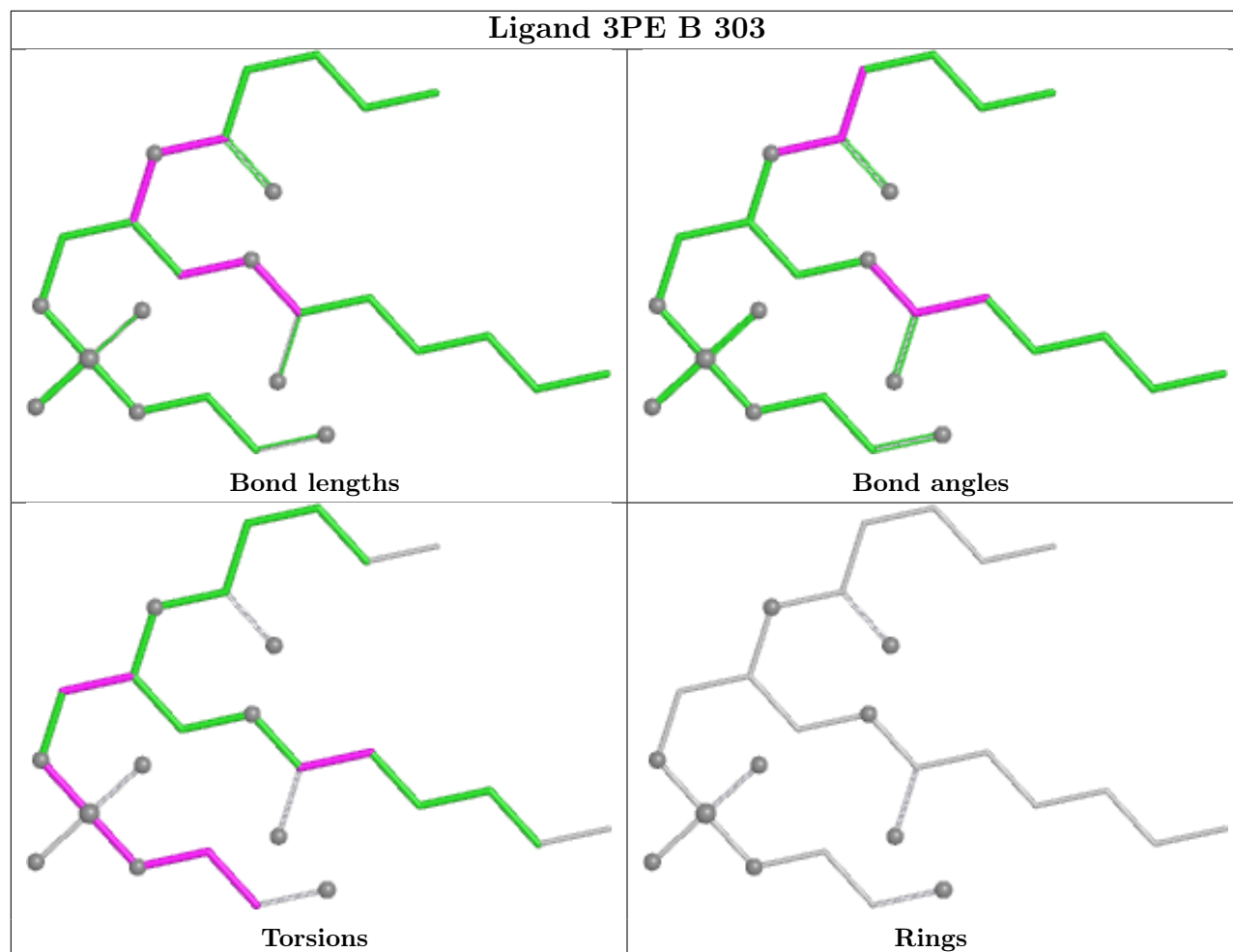


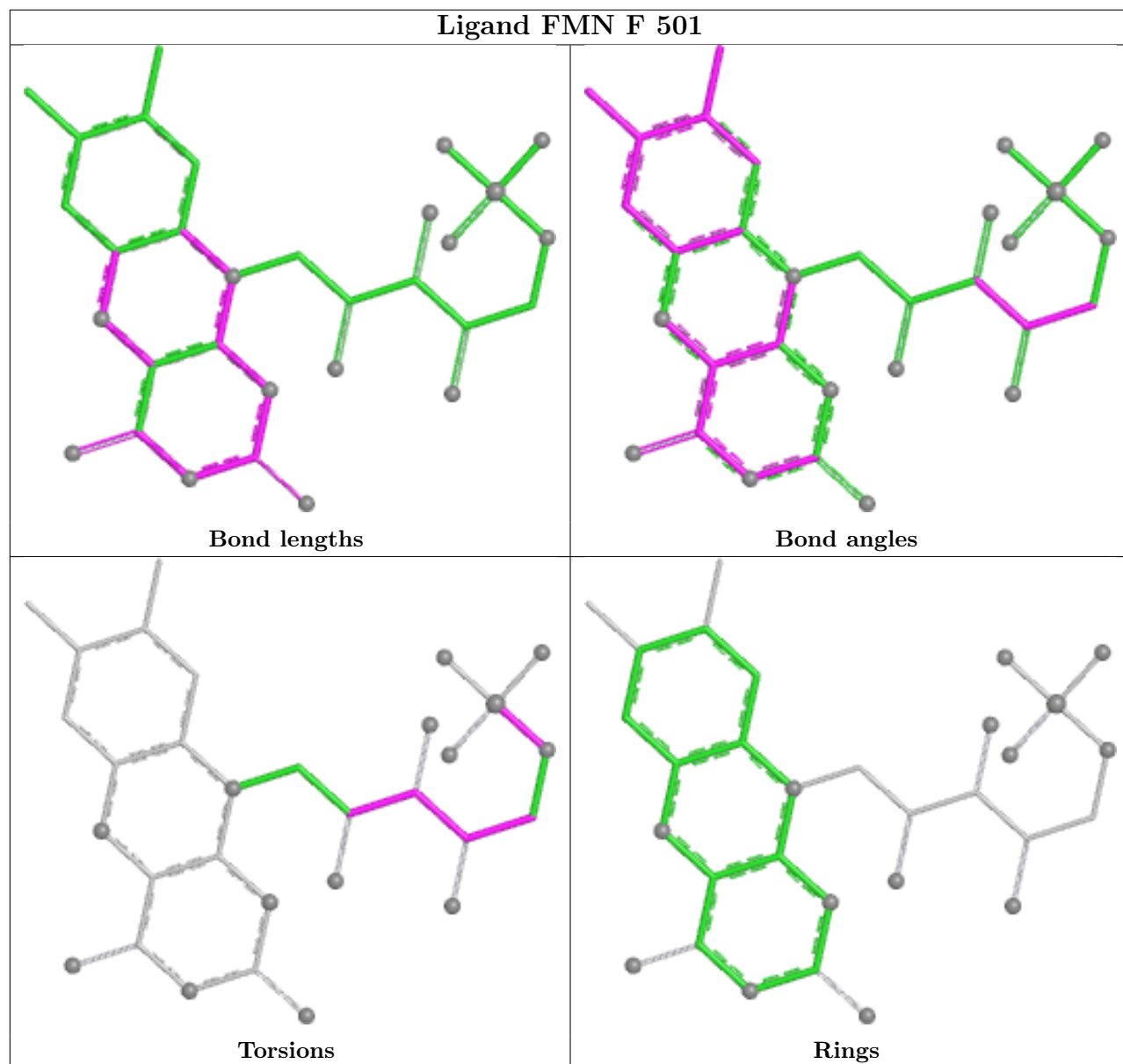
Ligand 3PE Y 302

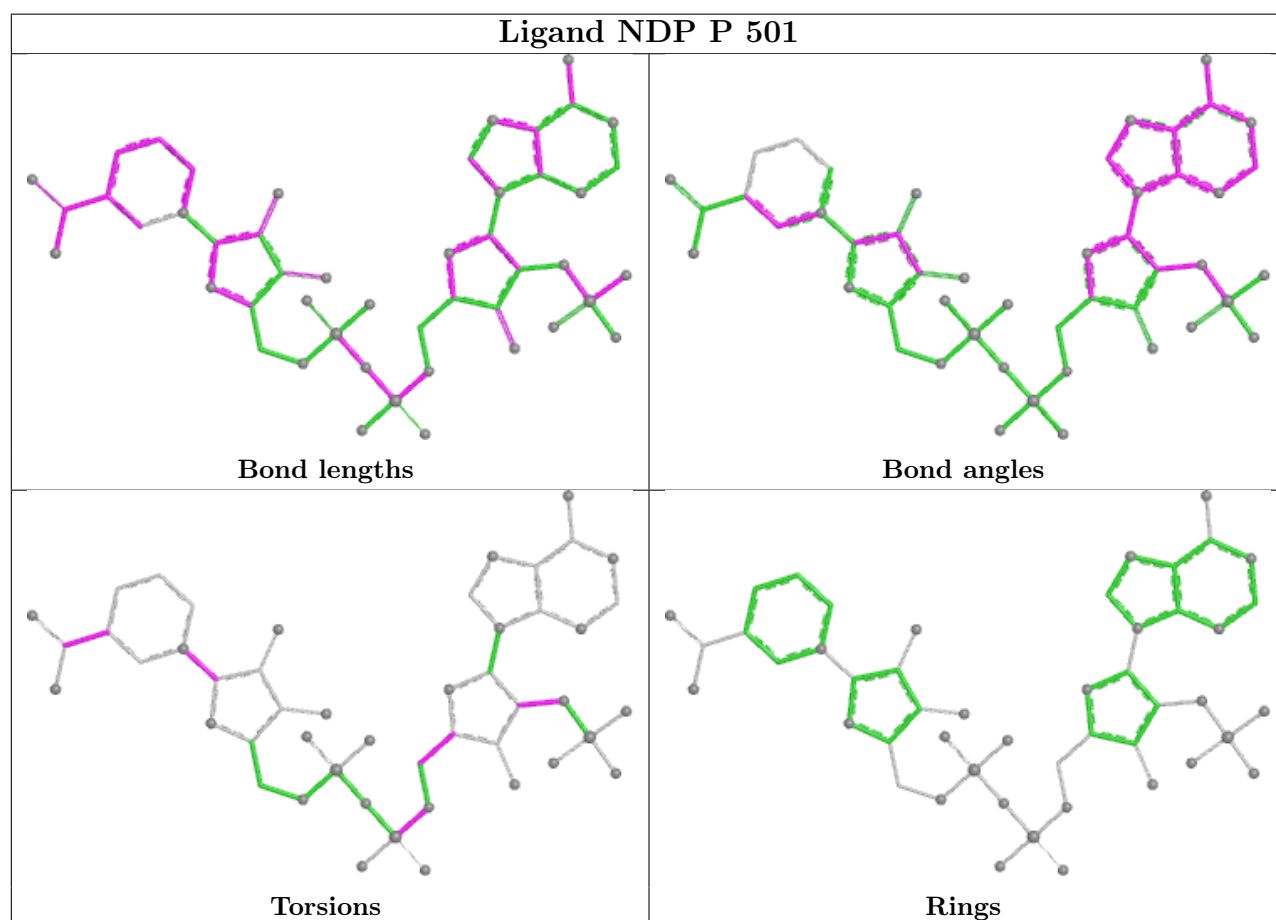
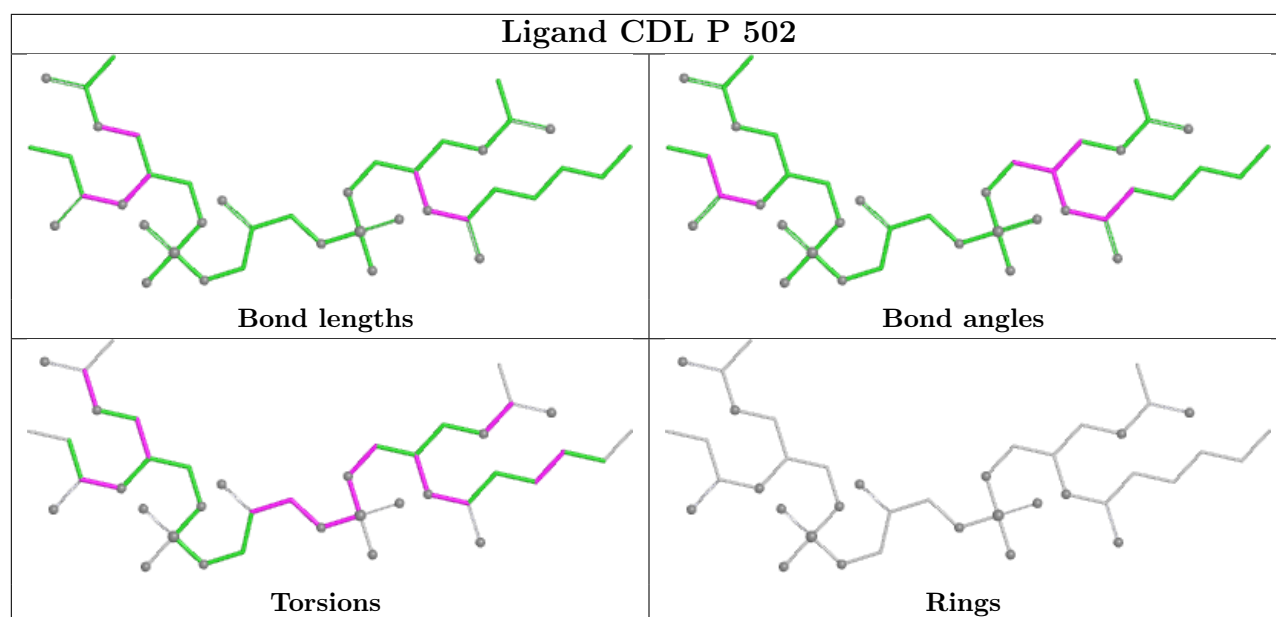


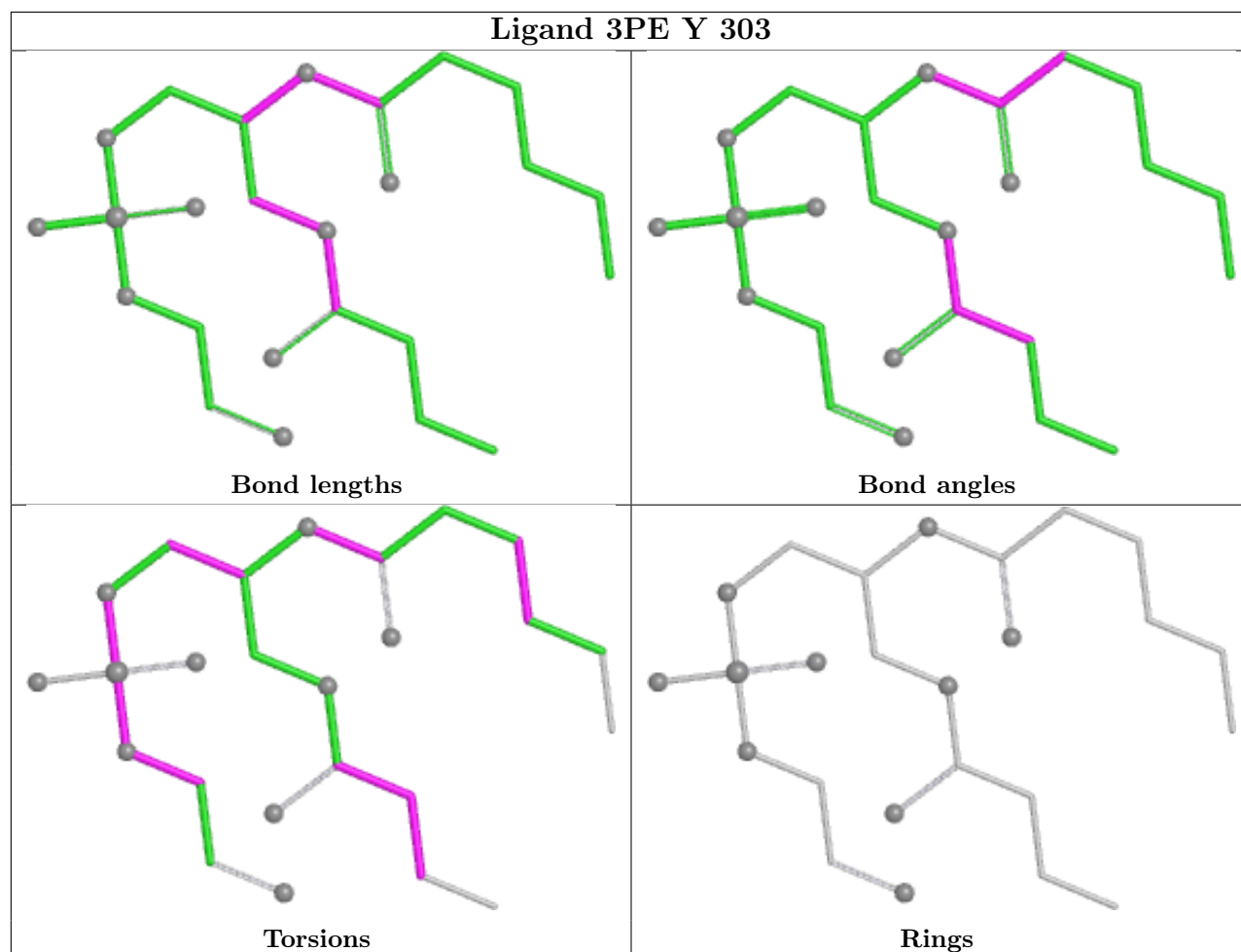
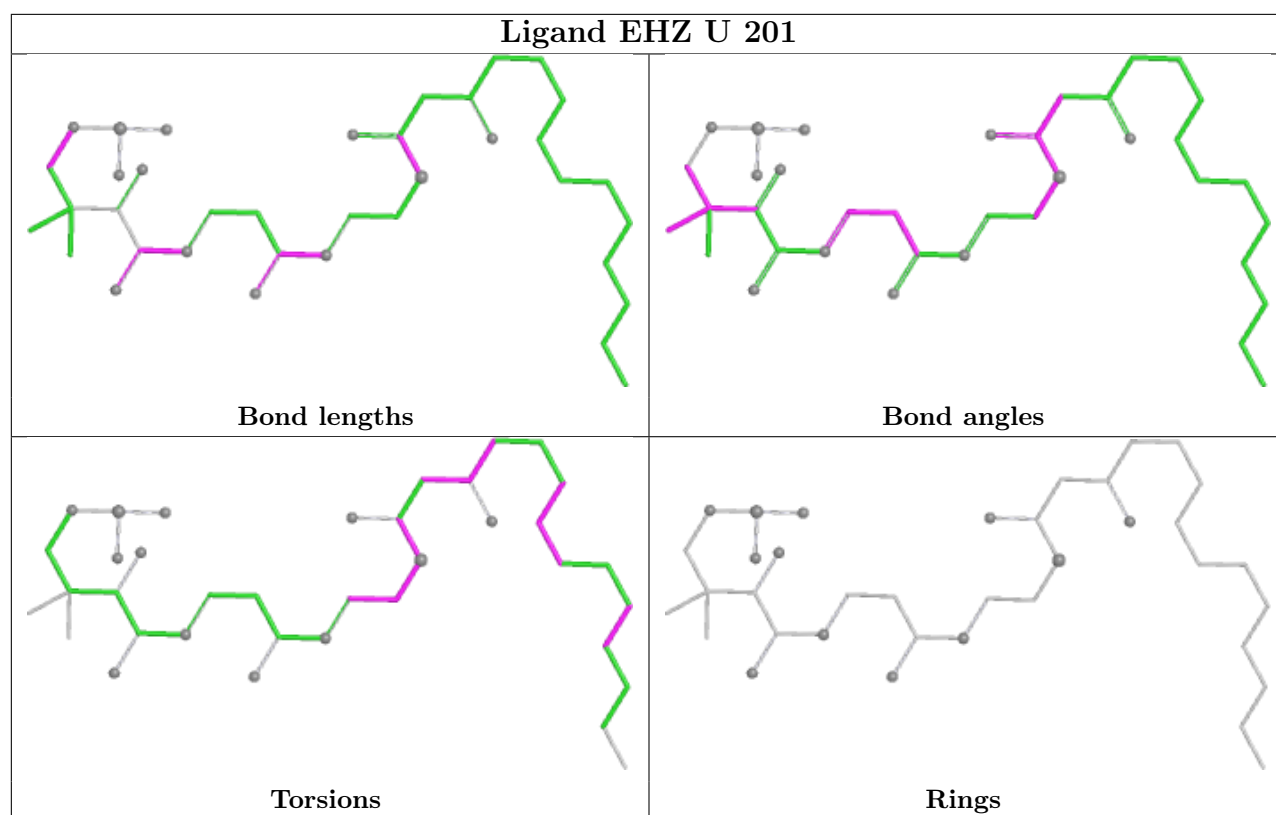












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

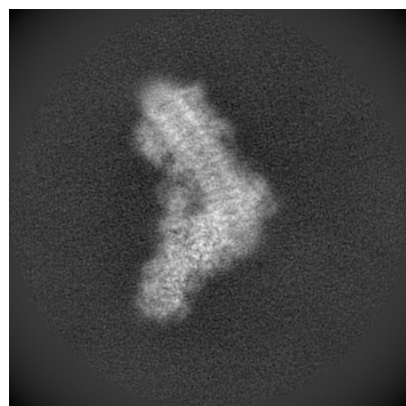
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-15937. These allow visual inspection of the internal detail of the map and identification of artifacts.

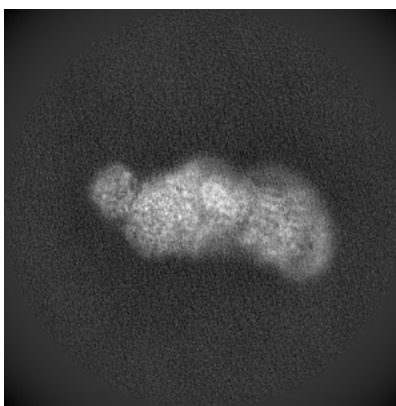
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

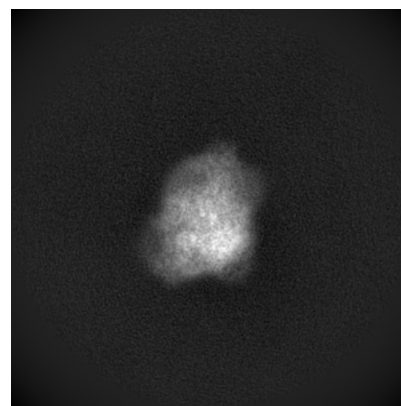
6.1.1 Primary map



X

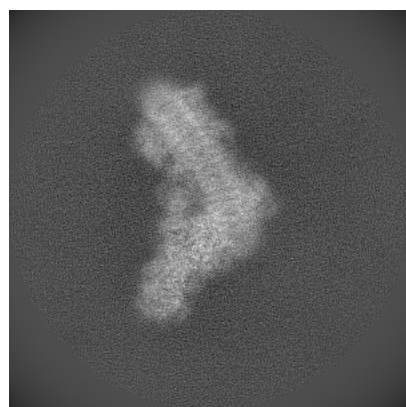


Y

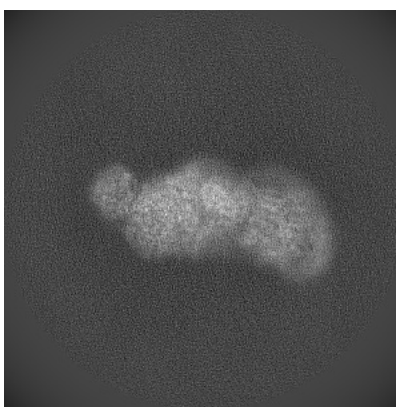


Z

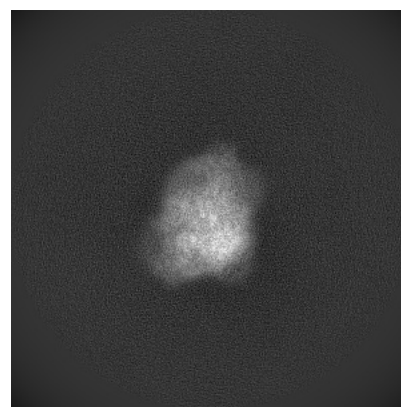
6.1.2 Raw map



X



Y

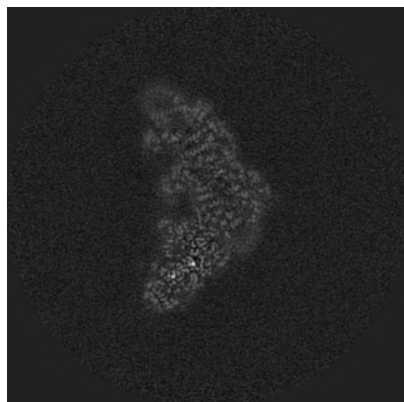


Z

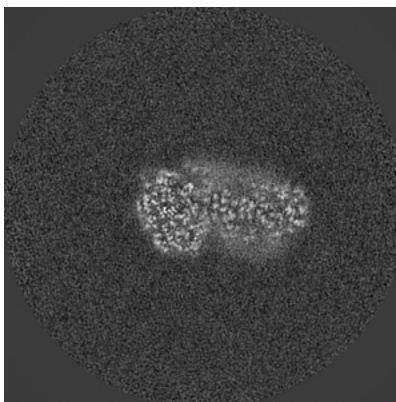
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

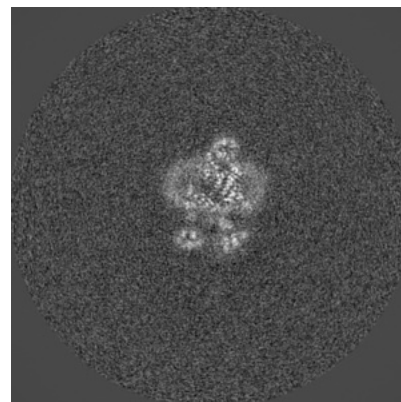
6.2.1 Primary map



X Index: 225

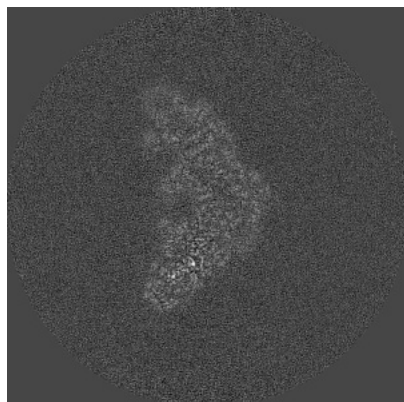


Y Index: 225

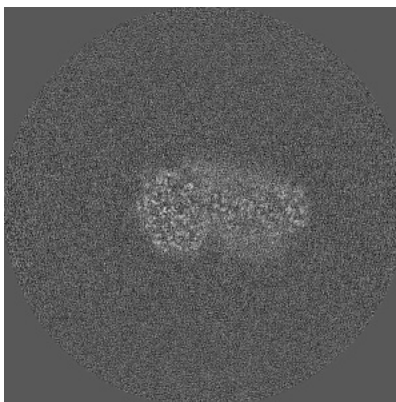


Z Index: 225

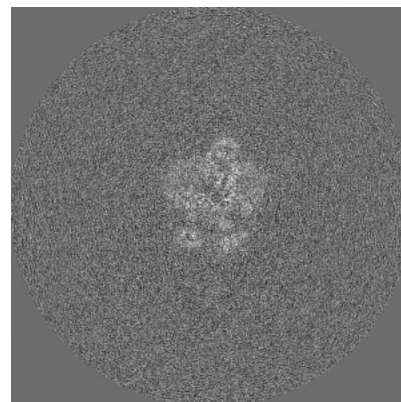
6.2.2 Raw map



X Index: 225



Y Index: 225

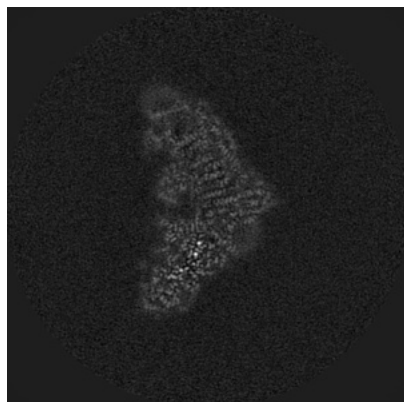


Z Index: 225

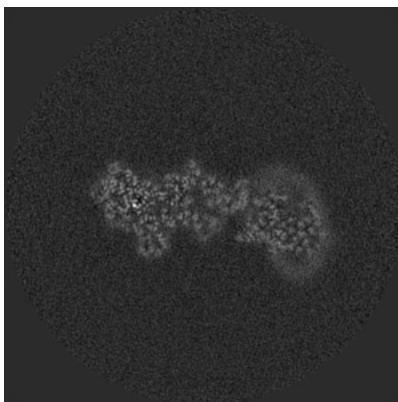
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

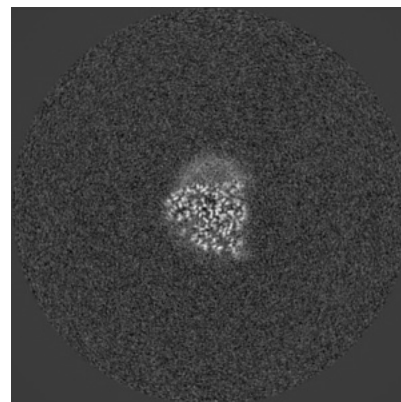
6.3.1 Primary map



X Index: 228

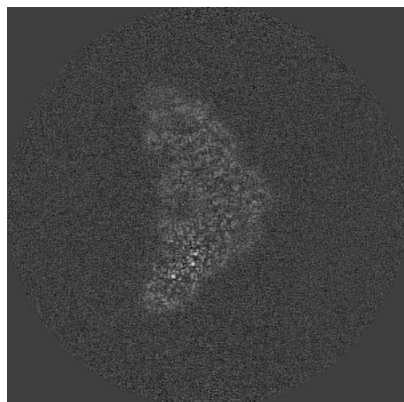


Y Index: 188

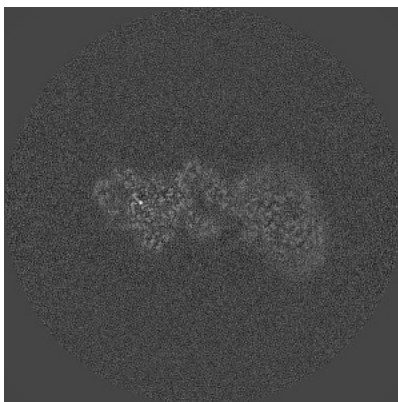


Z Index: 188

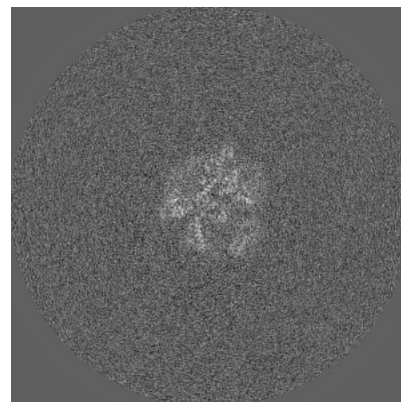
6.3.2 Raw map



X Index: 226



Y Index: 195

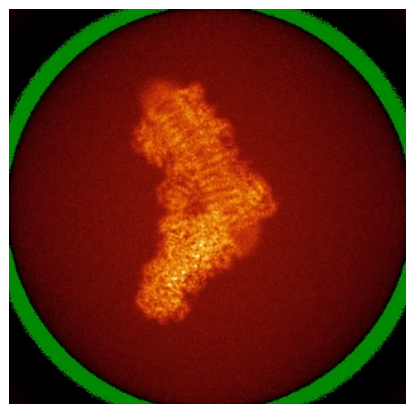


Z Index: 215

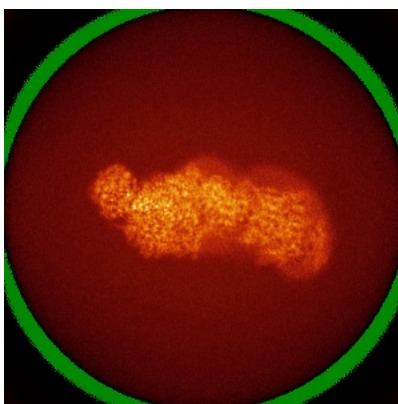
The images above show the largest variance slices of the map in three orthogonal directions.

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

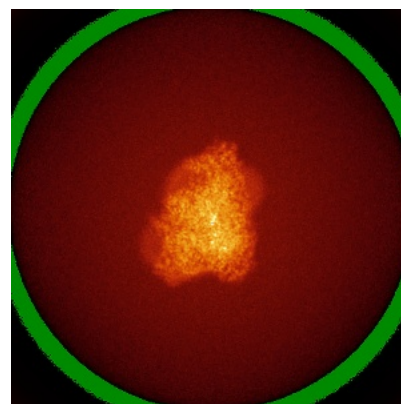
6.4.1 Primary map



X

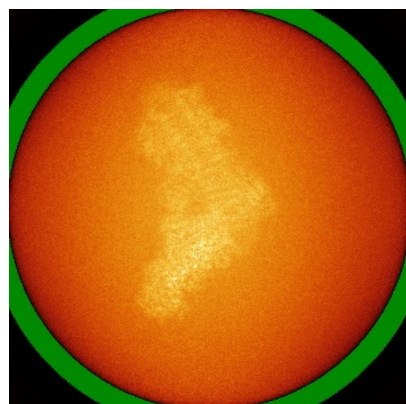


Y

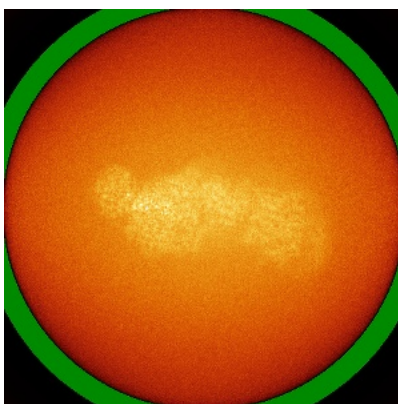


Z

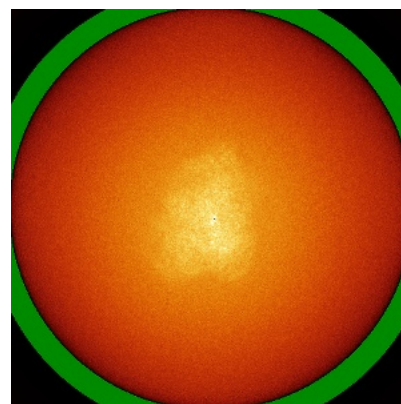
6.4.2 Raw map



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](#)

This section was not generated.

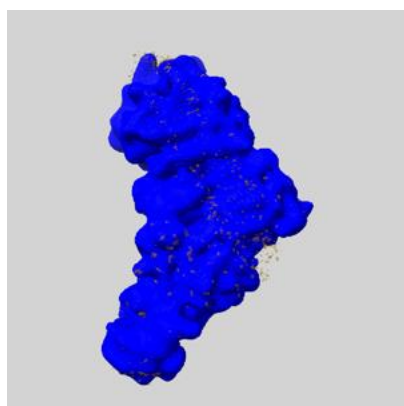
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

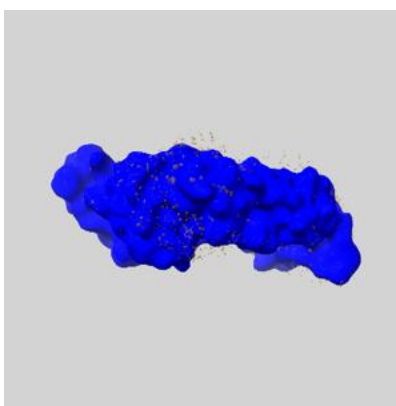
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

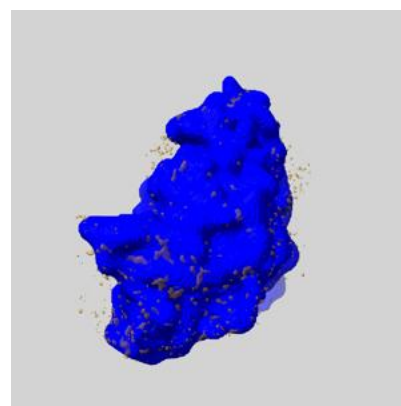
6.6.1 emd_15937_msk_1.map [i](#)



X



Y

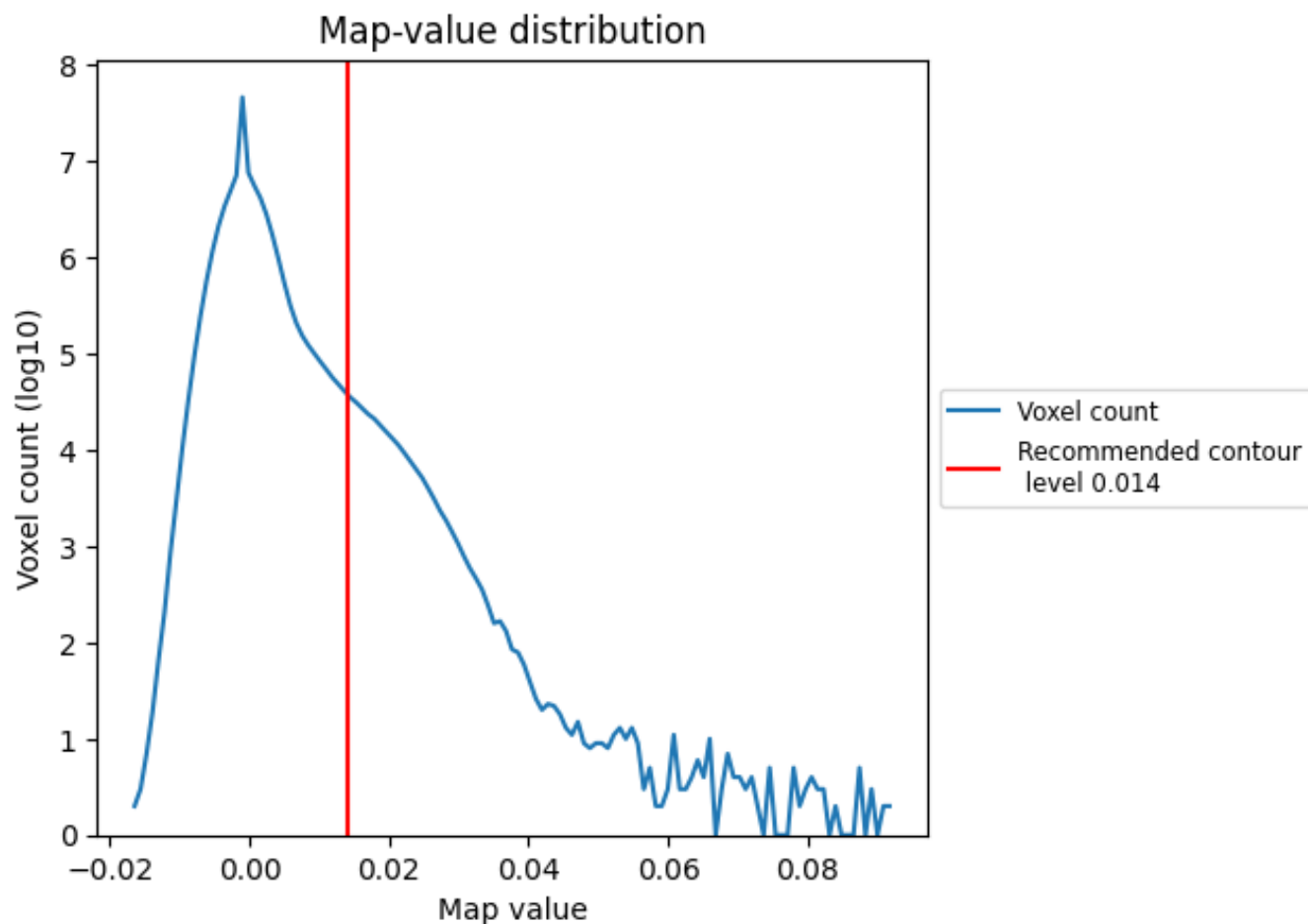


Z

7 Map analysis [i](#)

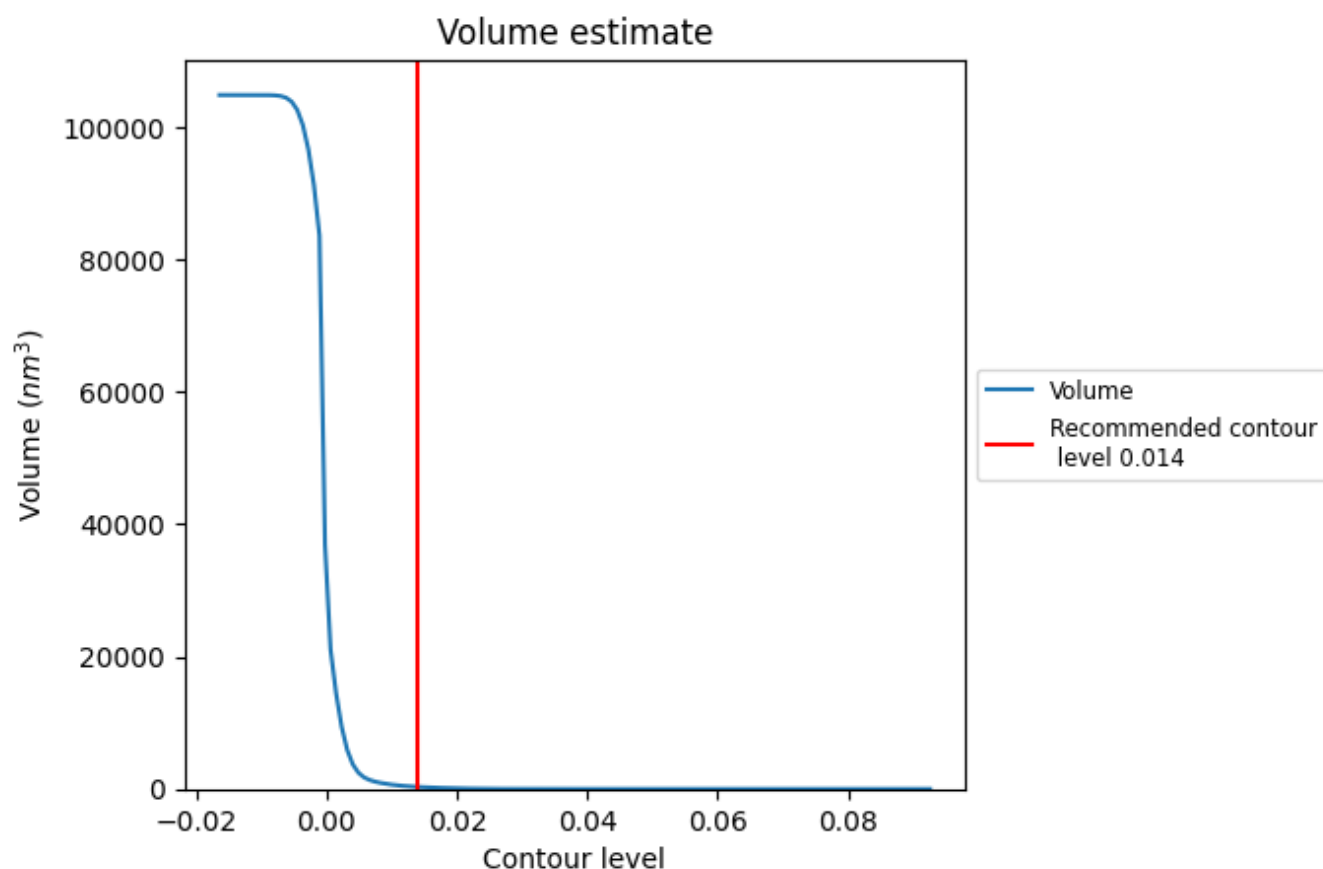
This section contains the results of statistical analysis of the map.

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.

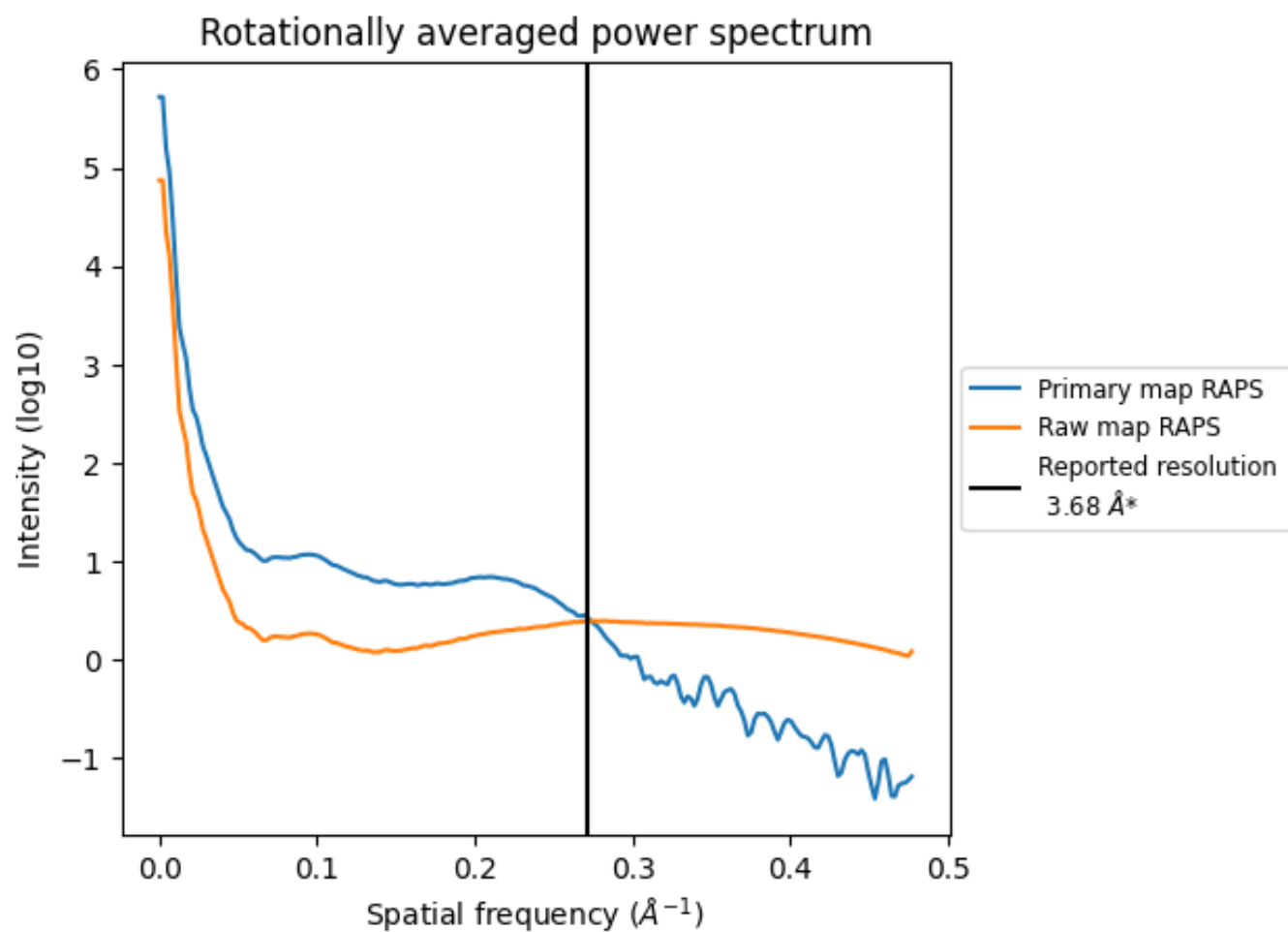
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 306 nm^3 ; this corresponds to an approximate mass of 277 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 ⓘ

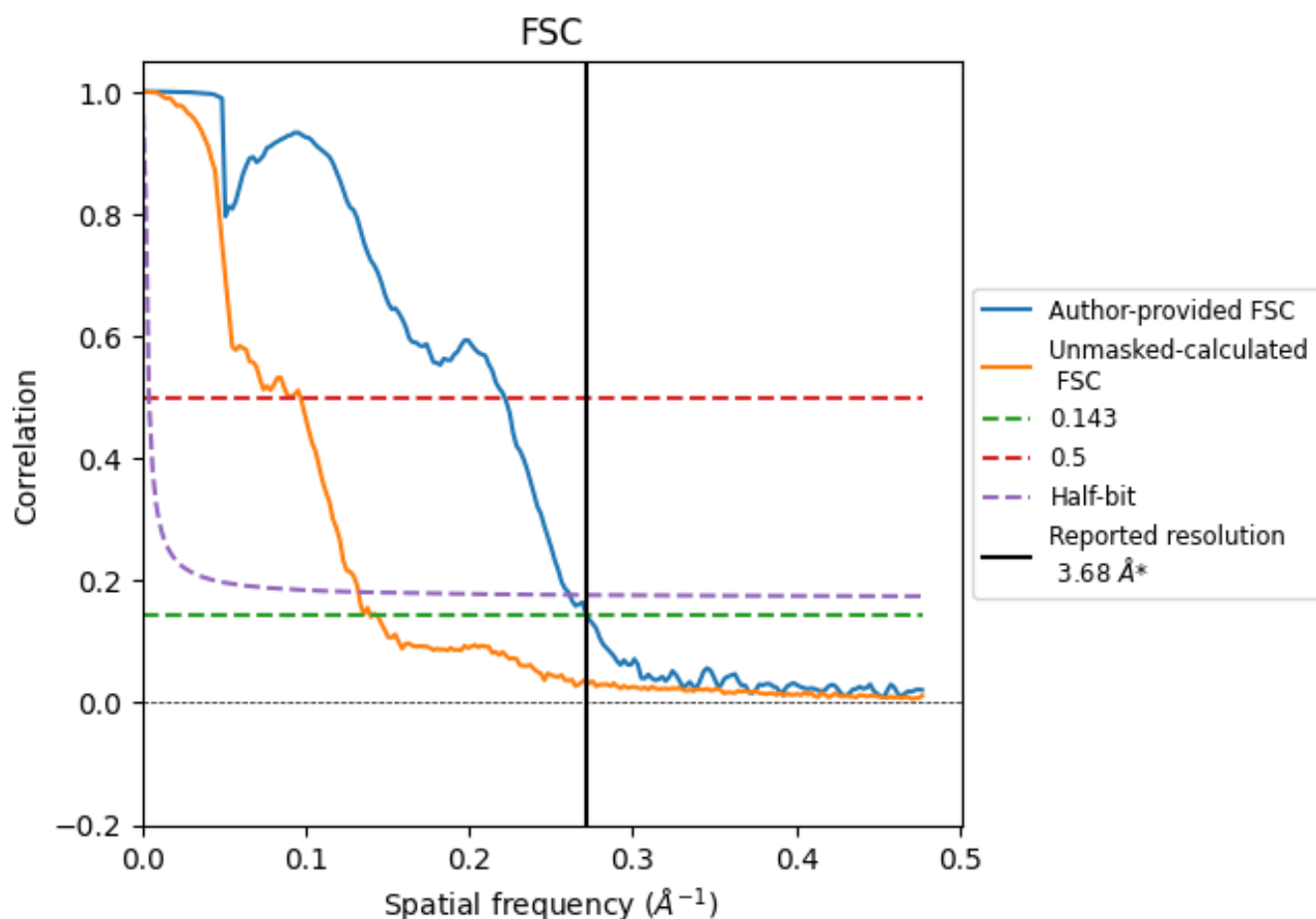


*Reported resolution corresponds to spatial frequency of 0.272 $\text{\AA}^{-1}$

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 0.272 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.68	-	-
Author-provided FSC curve	3.68	4.51	3.82
Unmasked-calculated*	7.16	10.34	7.56

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.16 differs from the reported value 3.68 by more than 10 %

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-15937 and PDB model 8BA0. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)

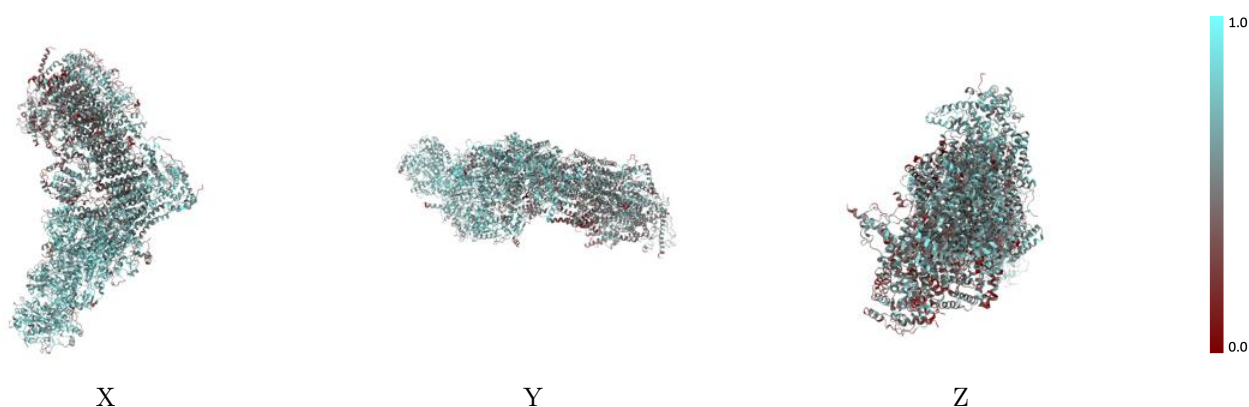
This section was not generated.

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



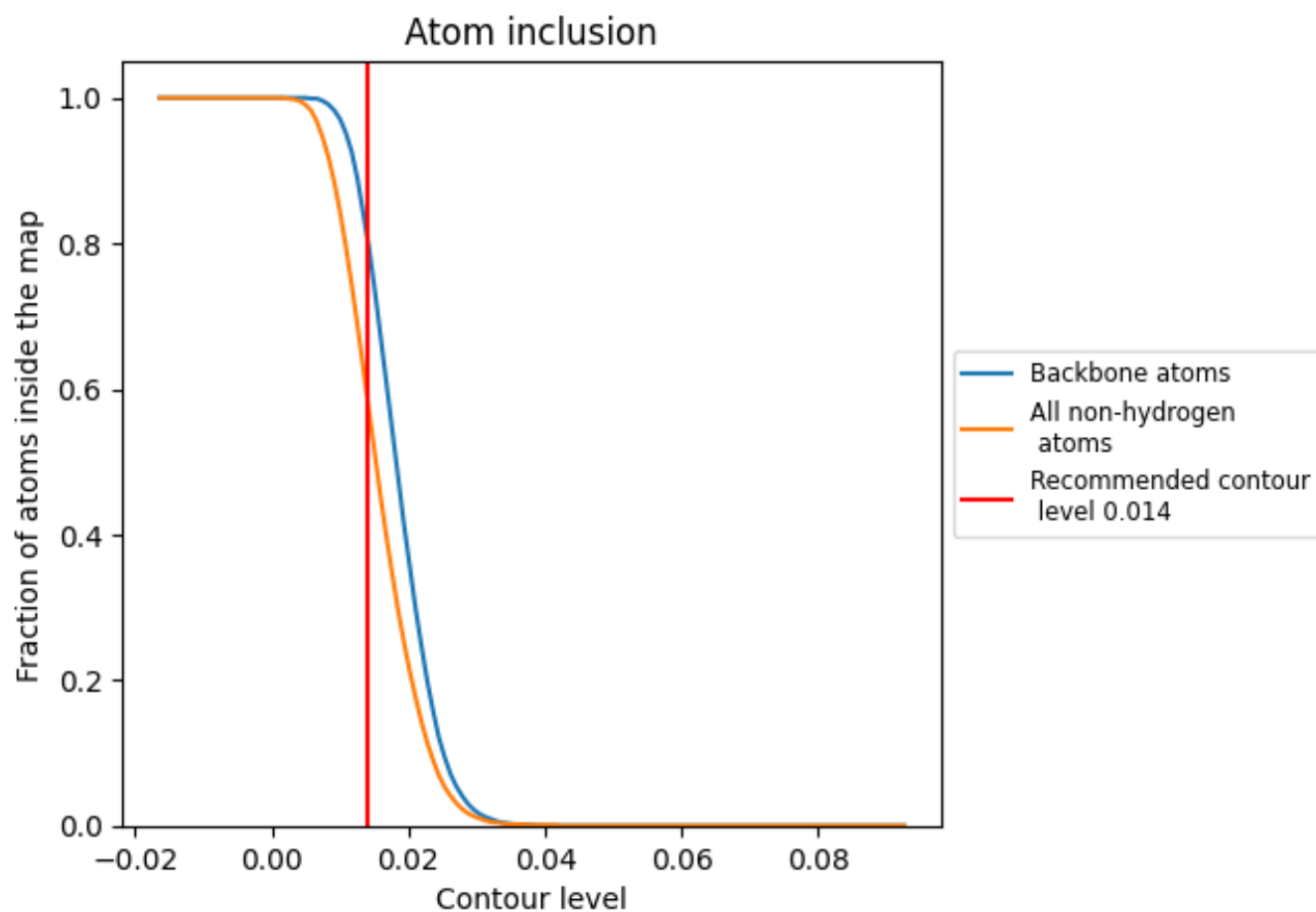
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.014).

9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 59% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.014) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5860	 0.4350
A	 0.5360	 0.4170
B	 0.6870	 0.4910
C	 0.6970	 0.4850
D	 0.6480	 0.4690
E	 0.6550	 0.4450
F	 0.6990	 0.4630
G	 0.6740	 0.4700
H	 0.6250	 0.4540
I	 0.7260	 0.4840
J	 0.5520	 0.4190
K	 0.5080	 0.3880
L	 0.5020	 0.4150
M	 0.5280	 0.4370
N	 0.5530	 0.4160
O	 0.5270	 0.3950
P	 0.6500	 0.4570
Q	 0.6790	 0.4770
R	 0.7190	 0.4840
T	 0.3900	 0.3360
U	 0.3560	 0.3490
V	 0.6260	 0.4280
W	 0.6280	 0.4340
X	 0.5960	 0.4400
Y	 0.3630	 0.3980
Z	 0.6770	 0.4570
a	 0.6050	 0.4390
b	 0.6110	 0.4360
d	 0.5470	 0.4220
e	 0.6250	 0.4280
f	 0.4200	 0.4020
g	 0.4780	 0.4170
h	 0.5780	 0.4270
i	 0.4700	 0.3860
j	 0.4530	 0.3710



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Chain	Atom inclusion	Q-score
k	 0.4210	 0.3490
l	 0.4920	 0.4160
m	 0.5080	 0.4120
n	 0.4850	 0.3810
o	 0.5100	 0.3770
p	 0.6110	 0.4220
q	 0.6420	 0.4640
r	 0.5670	 0.4520
s	 0.5100	 0.4130