



Full wwPDB EM Validation Report ⓘ

Jul 28, 2025 – 06:32 PM EDT

PDB ID : 9CWT / pdb_00009cwt
EMDB ID : EMD-45974
Title : Human kidney respiratory complex I
Authors : Zhang, Z.; Lyu, M.
Deposited on : 2024-07-30
Resolution : 3.44 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev126
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

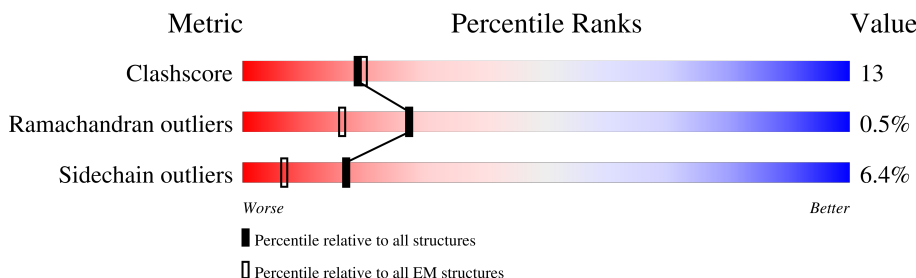
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.44 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.


















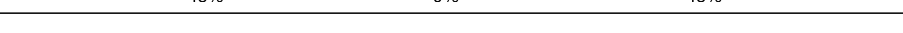





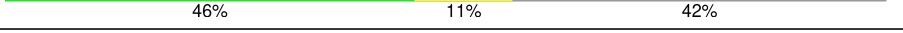



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	464	
2	B	210	
3	C	213	
4	E	128	
5	F	99	
6	G	156	
6	X	156	
7	H	116	













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Mol	Chain	Length	Quality of chain
8	I	113	
9	J	377	
10	K	108	
11	L	175	
12	M	727	
13	N	145	
14	O	249	
15	P	264	
16	Q	463	
17	S	70	
18	T	124	
19	U	84	
20	V	141	
21	W	144	
22	Y	105	
23	Z	98	
24	a	189	
25	b	128	
26	c	186	
27	d	172	
28	e	153	
29	f	76	
30	g	119	
31	h	106	
32	j	115	

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Mol	Chain	Length	Quality of chain
33	k	98	
34	l	603	
35	m	174	
36	n	58	
37	o	129	
38	p	179	
39	r	459	
40	s	318	
41	u	172	
42	v	137	
43	D	22	
44	i	347	

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
45	SF4	A	501	-	-	X	-
45	SF4	B	302	-	-	X	-
45	SF4	C	301	-	-	X	-

2 Entry composition

There are 49 unique types of molecules in this entry. The entry contains 60914 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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	431	Total	C	N	O	S	0	0
			3316	2093	591	612	20		

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	176	Total	C	N	O	S	0	0
			1420	893	243	271	13		

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	156	Total	C	N	O	S	0	0
			1249	794	227	214	14		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	113	Total	C	N	O	S	0	0
			968	623	178	162	5		

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	83	Total	C	N	O	S	0	0
			670	422	124	122	2		

- Molecule 6 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	G	83	Total	C	N	O	S	0	0
			647	416	96	130	5		
6	X	85	Total	C	N	O	S	0	0
			686	442	101	138	5		

- Molecule 7 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	H	112	Total	C	N	O	S	0	0
			922	593	157	169	3		

- Molecule 8 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	95	Total	C	N	O	S	0	0
			769	483	146	138	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	313	Total	C	N	O	S	0	0
			2486	1598	447	433	8		

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	30	Total	C	N	O	S	0	0
			247	157	42	47	1		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	117	Total	C	N	O	S	0	0
			955	602	171	178	4		

- Molecule 12 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	686	Total	C	N	O	S	0	0
			5261	3302	915	1006	38		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	143	Total	C	N	O	S	0	0
			1188	764	210	211	3		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	212	Total	C	N	O	S	0	0
			1637	1044	273	310	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	207	Total	C	N	O	S	0	0
			1721	1112	296	310	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	384	Total	C	N	O	S	0	0
			3073	1961	534	556	22		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	70	Total	C	N	O	S	0	0
			568	367	101	96	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	95	Total	C	N	O	S	0	0
			742	459	138	142	3		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	U	83	Total	C	N	O	S	0	0
			647	427	105	113	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	140	Total	C	N	O	S	0	0
			1038	668	178	187	5		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	138	Total	C	N	O	S	0	0
			1116	715	195	200	6		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	Y	58	Total	C	N	O	S	0	0
			510	338	83	88	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	72	Total	C	N	O	S	0	0
			582	382	102	96	2		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	138	Total	C	N	O	S	0	0
			1174	771	199	202	2		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	120	Total	C	N	O	S	0	0
			1022	674	175	169	4		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	138	Total	C	N	O	S	0	0
			1094	708	178	197	11		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	166	Total	C	N	O	S	0	0
			1393	870	257	254	12		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	e	88	Total	C	N	O	S	0	0
			731	472	121	134	4		

- Molecule 29 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	f	47	Total	C	N	O	0	0
			405	269	69	67		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	119	Total	C	N	O	S	0	0
			1004	658	173	169	4		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	104	Total	C	N	O	S	0	0
			840	531	154	149	6		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	92	Total	C	N	O	S	0	0
			732	507	103	116	6		

- Molecule 33 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	k	84	Total	C	N	O	S	0	0
			627	413	95	107	12		

- Molecule 34 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	l	565	Total	C	N	O	S	0	0
			4383	2882	697	774	30		

- Molecule 35 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	m	166	Total	C	N	O	S	0	0
			1239	830	184	215	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
36	n	56	Total	C	N	O	S	0	0
			473	305	85	80	3		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	102	Total	C	N	O	S	0	0
			841	538	156	145	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
38	p	171	Total	C	N	O	S	0	0
			1480	950	264	259	7		

- Molecule 39 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	r	459	Total	C	N	O	S	0	0
			3623	2404	569	620	30		

- Molecule 40 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	s	318	Total	C	N	O	S	0	0
			2494	1667	375	436	16		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	u	169	Total	C	N	O	S	0	0
			1394	886	247	252	9		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	v	112	Total	C	N	O	S	0	0
			887	546	178	154	9		

- Molecule 43 is a protein called Unknow peptide.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	D	22	Total	C	N	O	0	0
			110	66	22	22		

- Molecule 44 is a protein called NADH-ubiquinone oxidoreductase chain 2.

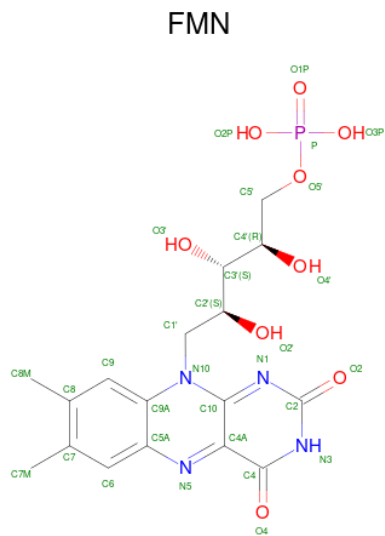
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	306	Total	C	N	O	S	0	0
			2385	1595	359	409	22		

- Molecule 45 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



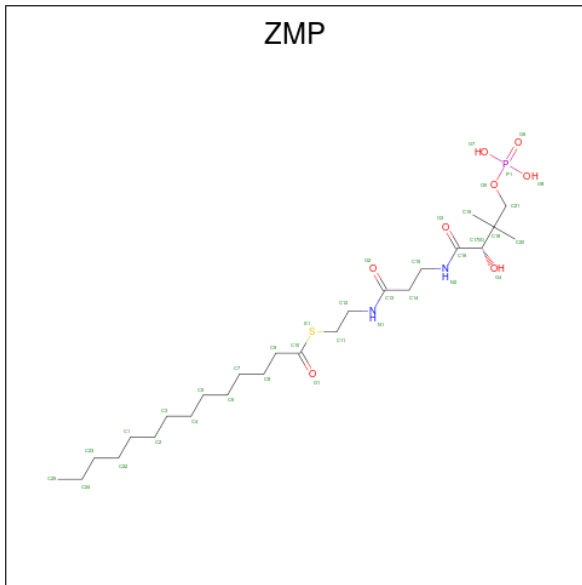
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	B	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	
45	M	1	Total	Fe	S	0
			8	4	4	

- Molecule 46 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$).



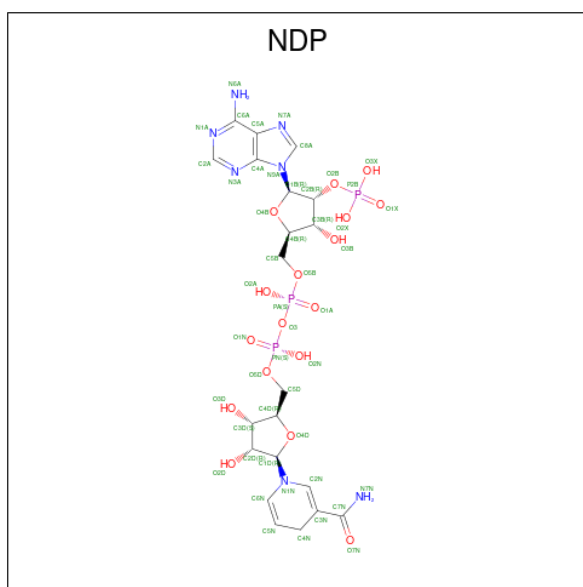
Mol	Chain	Residues	Atoms					AltConf
46	A	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 47 is S-[2-($\{N-[(2S)-2\text{-hydroxy-}3,3\text{-dimethyl-}4\text{-(phosphonooxy)butanoyl}]\text{-beta-alaninyl}\}$ amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: $C_{25}H_{49}N_2O_8PS$).



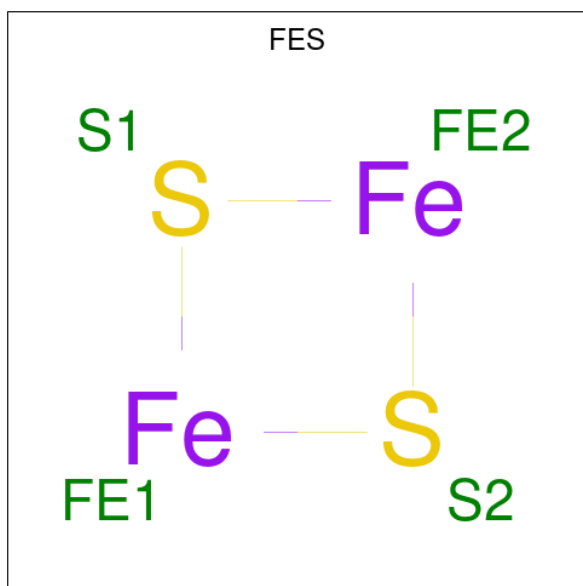
Mol	Chain	Residues	Atoms					AltConf	
47	E	1	Total 30	C 18	N 2	O 8	P 1	S 1	0

- Molecule 48 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



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

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

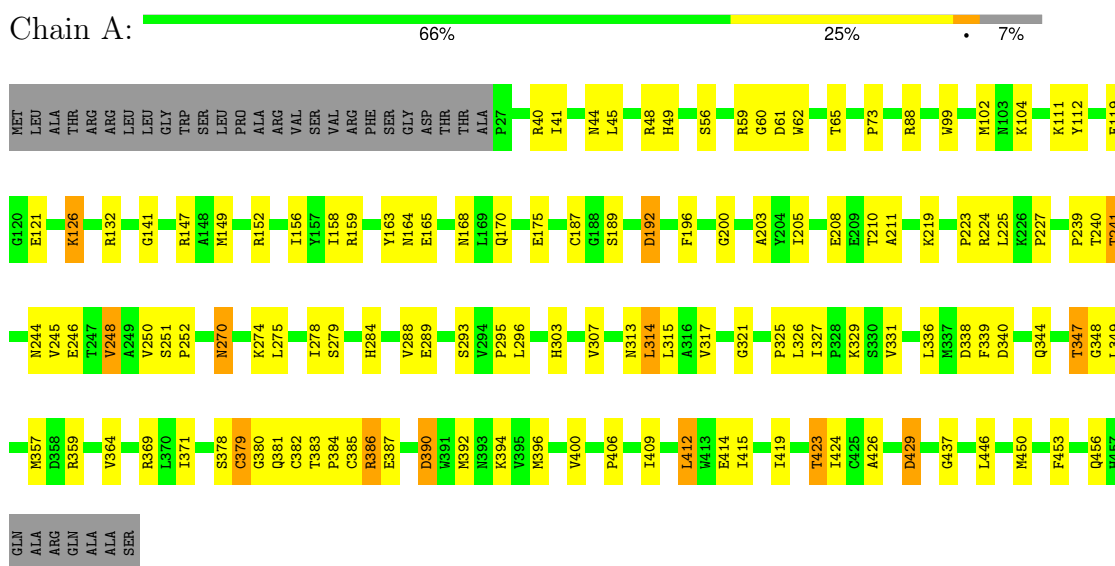


Mol	Chain	Residues	Atoms			AltConf
49	M	1	Total 4	Fe 2	S 2	0
49	O	1	Total 4	Fe 2	S 2	0

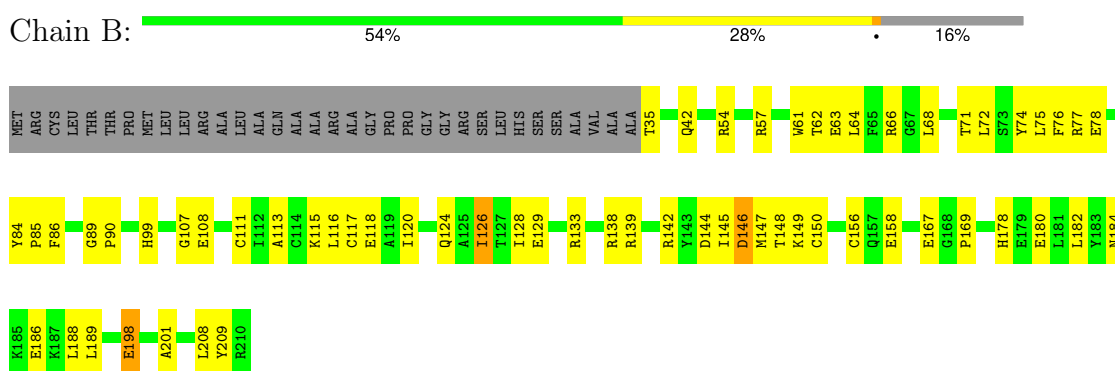
3 Residue-property plots [i](#)

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 dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

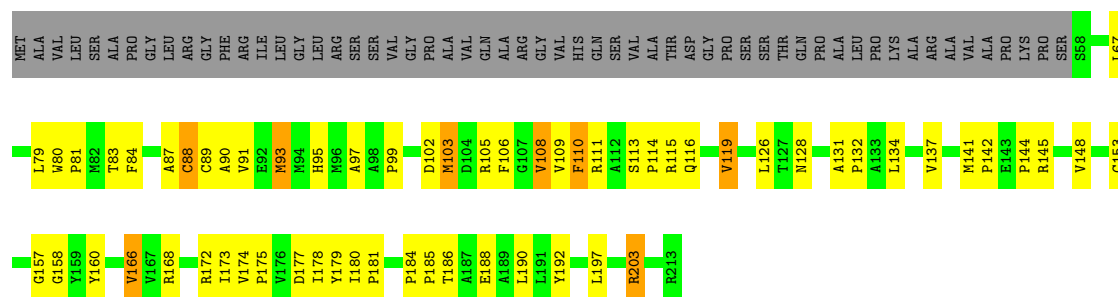


- Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



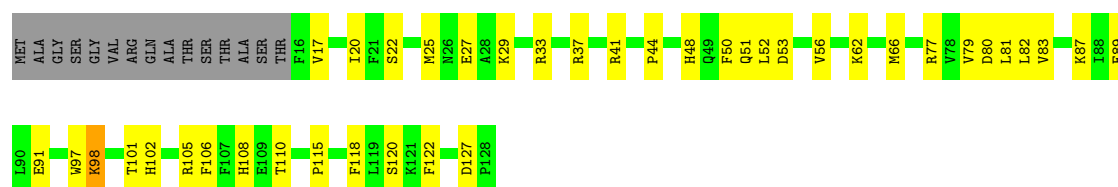
- Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial





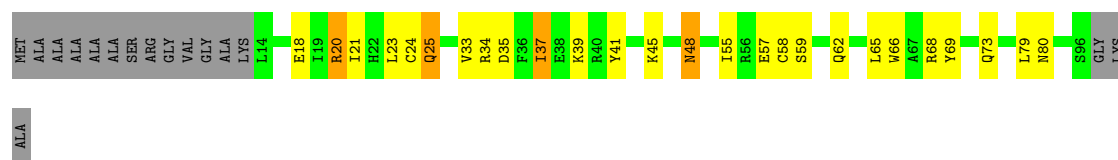
- Molecule 4: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain E: 57% 30% 12%



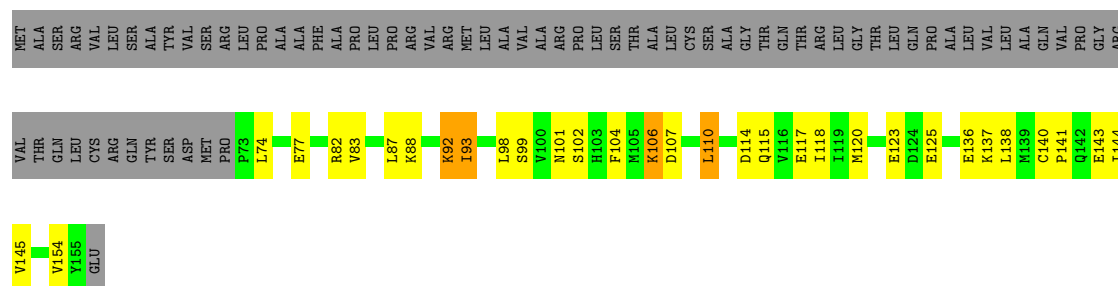
- Molecule 5: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

Chain F: 58% 22% 16%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain G: 33% 18% 47%



- Molecule 6: Acyl carrier protein, mitochondrial

Chain X: 39% 15% 46%

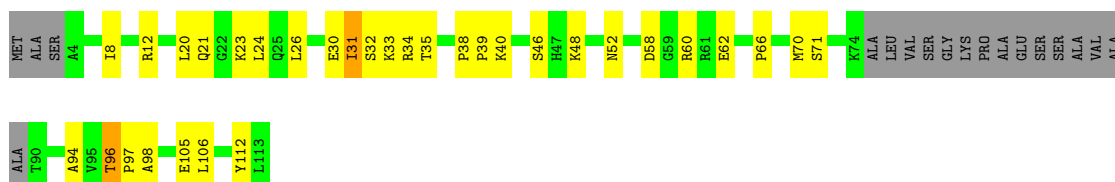




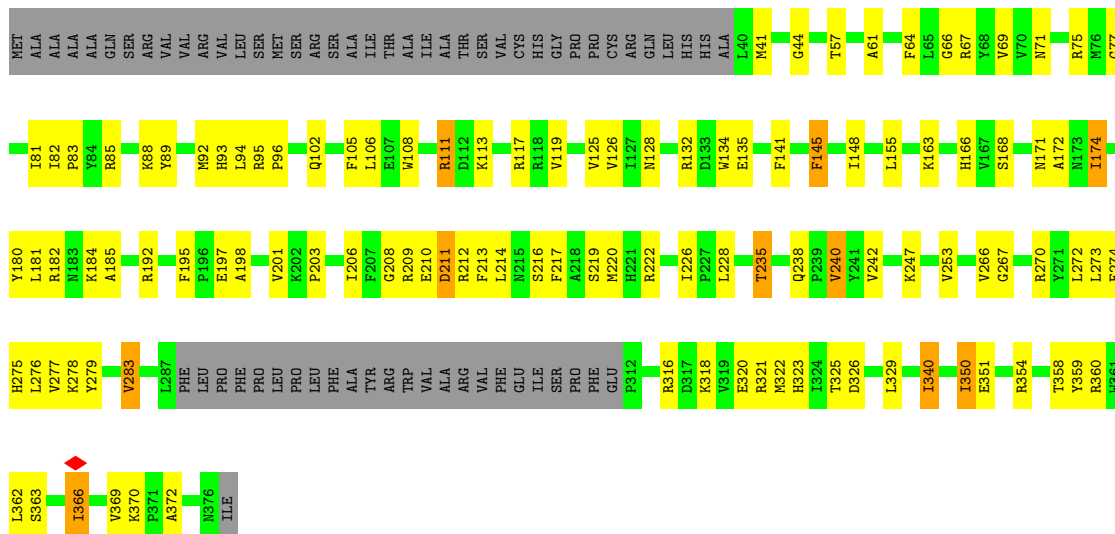
- Molecule 7: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



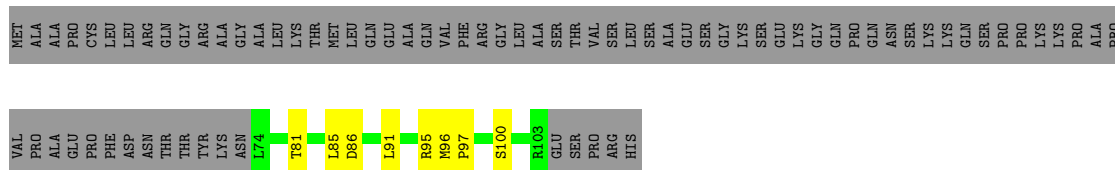
- Molecule 8: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



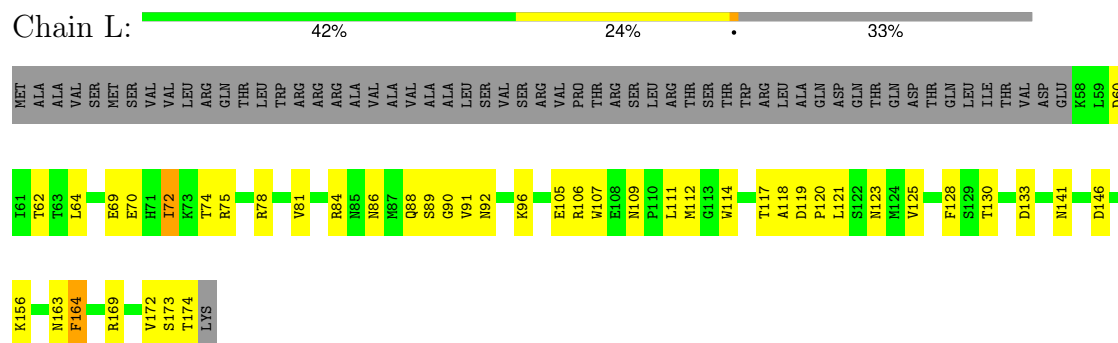
- Molecule 9: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial



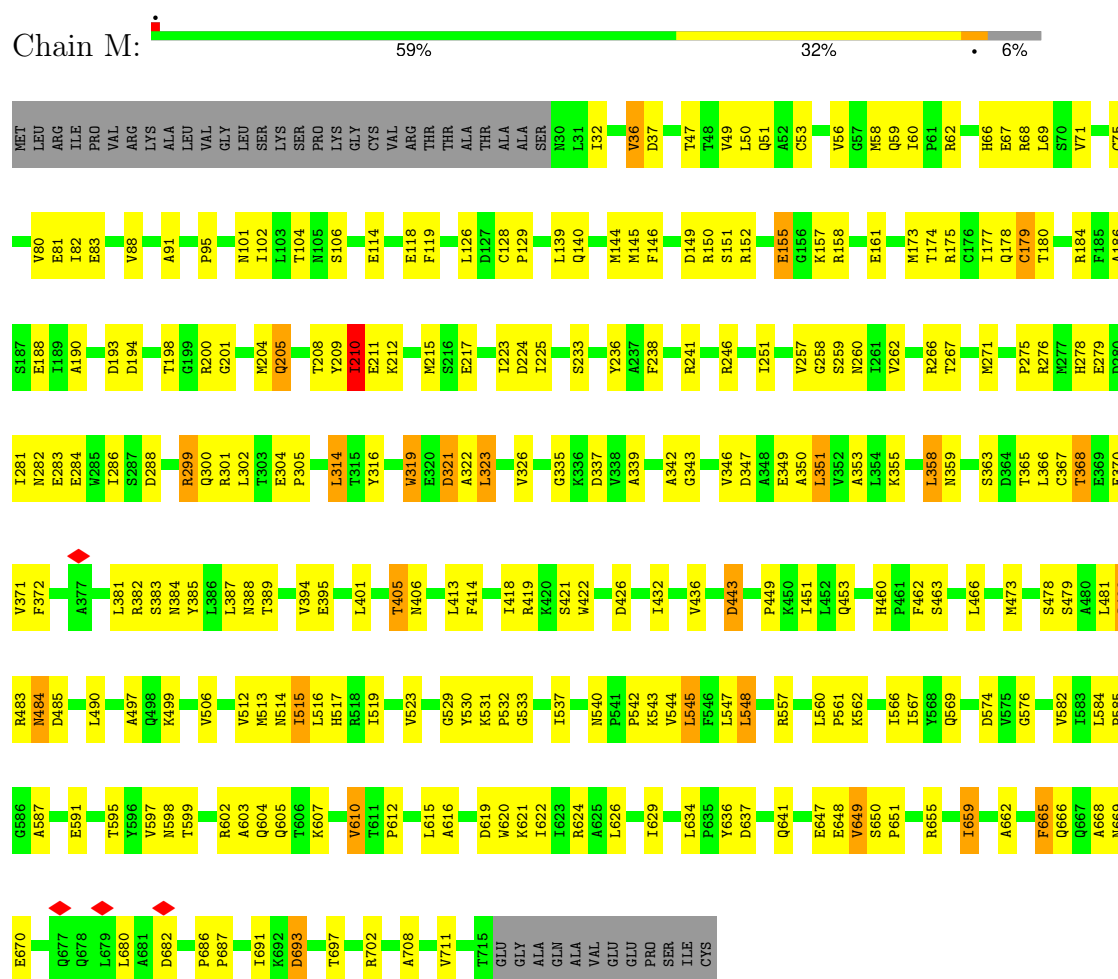
- Molecule 10: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



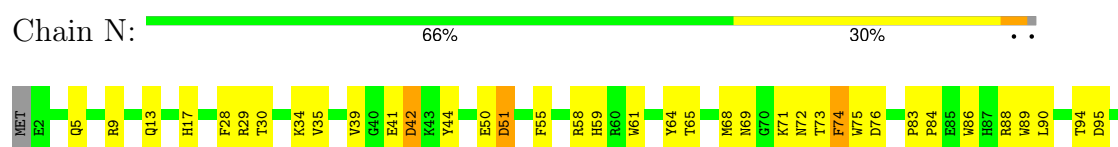
- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



- Molecule 12: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



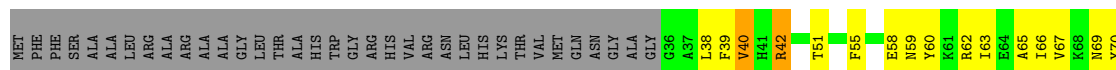
- Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12





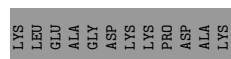
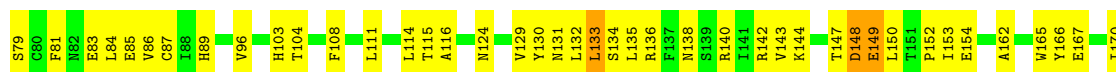
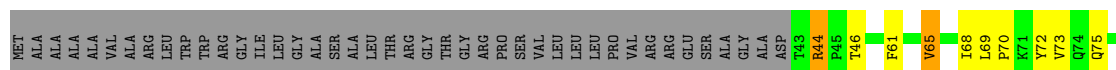
- Molecule 14: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain O: 52% 30% 15%



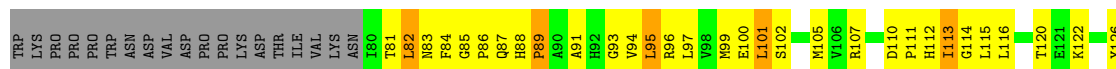
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain P: 44% 32% 22%



- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

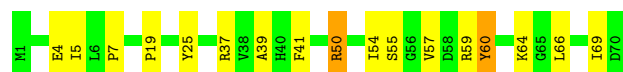
Chain Q: 50% 30% 17%





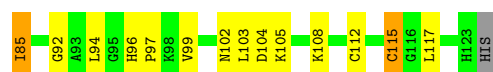
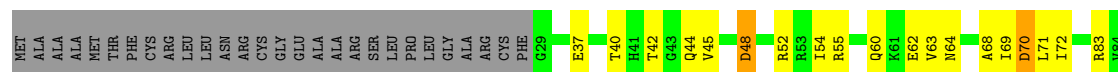
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1

Chain S: 76% 21%



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

Chain T: 50% 23% 23%



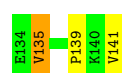
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain U: 79% 18%



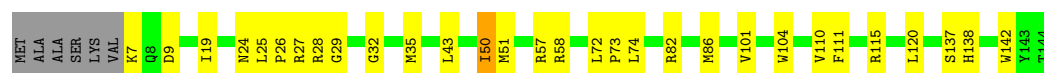
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain V: 73% 23%



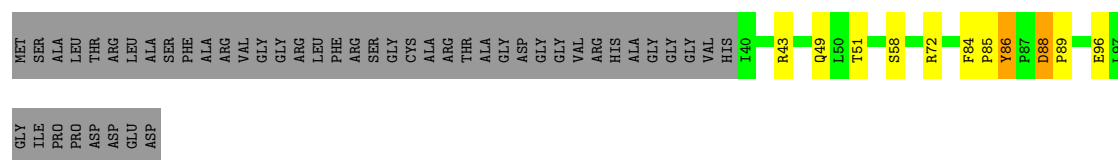
- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain W: 75% 20%



- Molecule 22: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

Chain Y: 



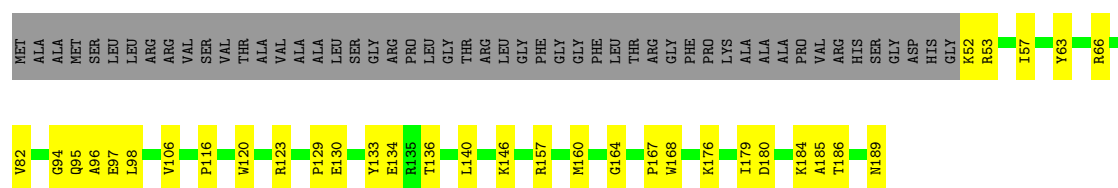
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

Chain Z: 



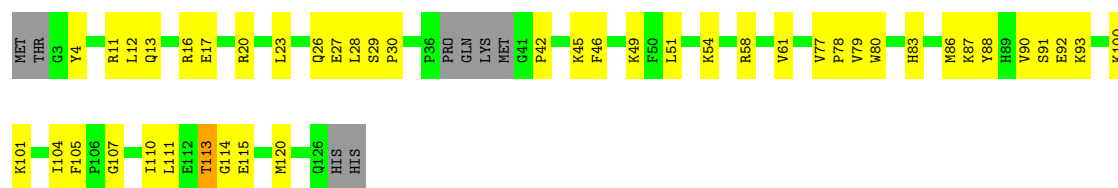
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain a: 



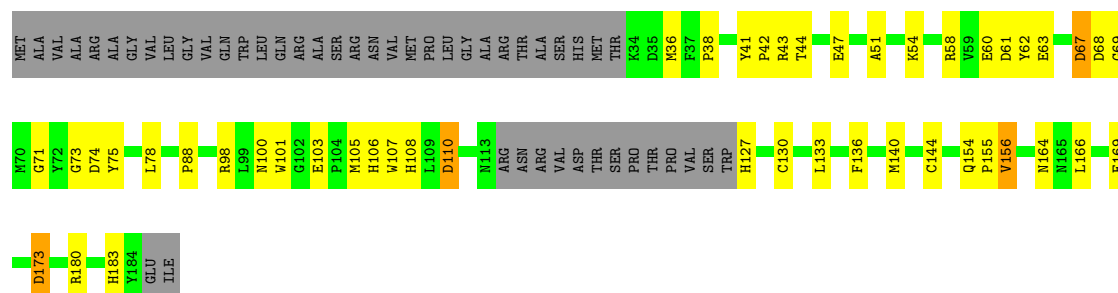
- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain b: 



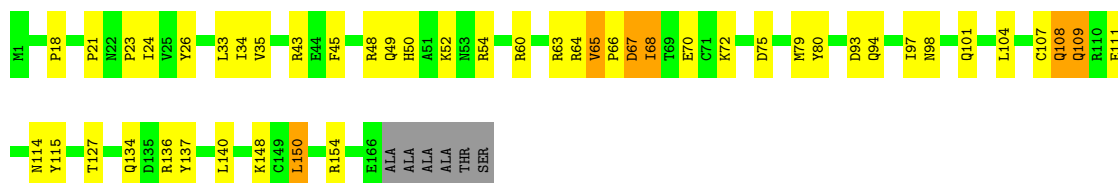
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial

Chain c: 



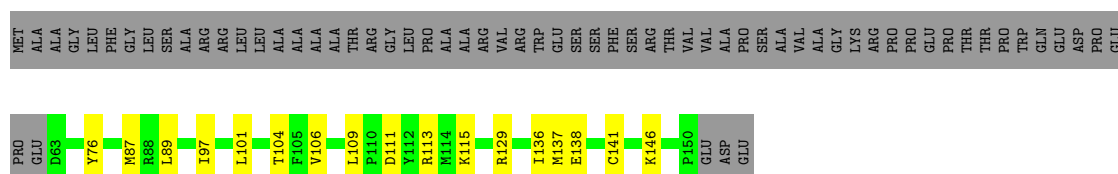
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10

Chain d: 



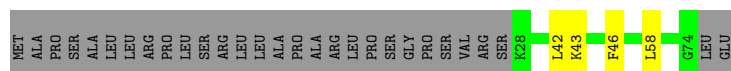
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

Chain e: 




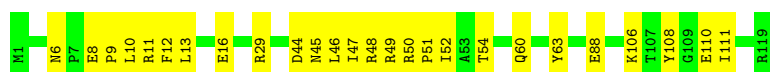
- Molecule 29: NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial

Chain f: 



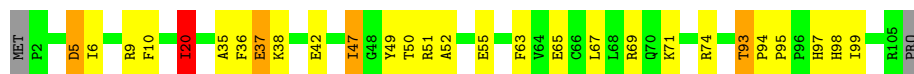
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 subunit C2

Chain g: 



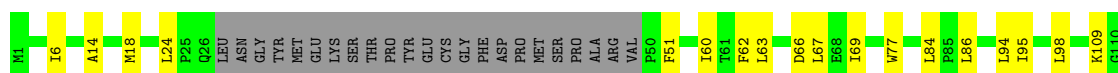
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain h: 



- Molecule 32: NADH-ubiquinone oxidoreductase chain 3

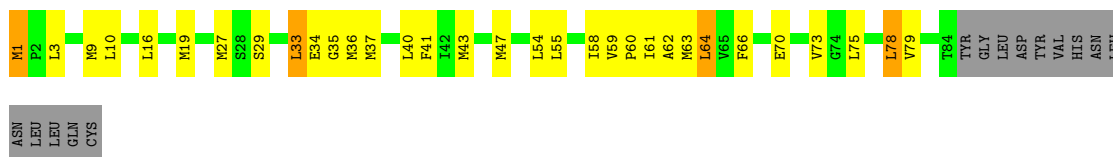
Chain j: 





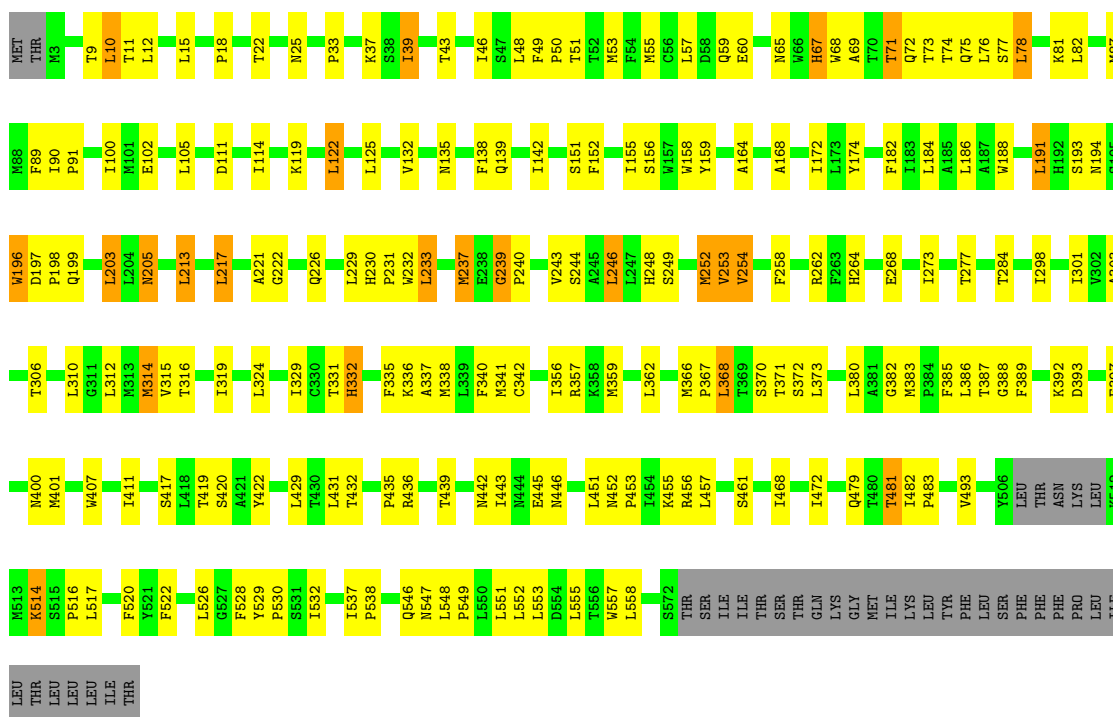
- Molecule 33: NADH-ubiquinone oxidoreductase chain 4L

Chain k: 53% 29% 14%



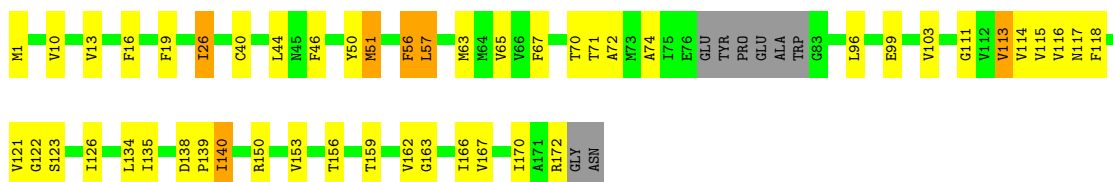
- Molecule 34: NADH-ubiquinone oxidoreductase chain 5

Chain l: 60% 29% 6%



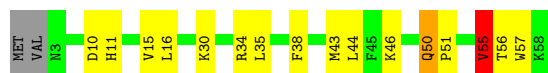
- Molecule 35: NADH-ubiquinone oxidoreductase chain 6

Chain m: 67% 25% 5%



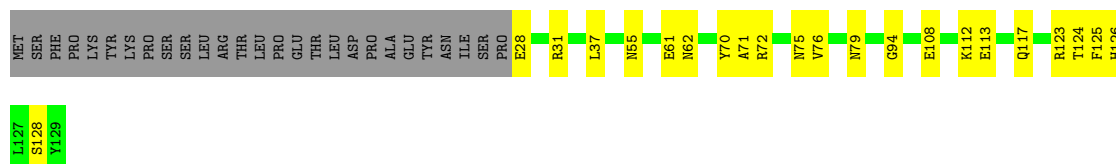
- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain n: 



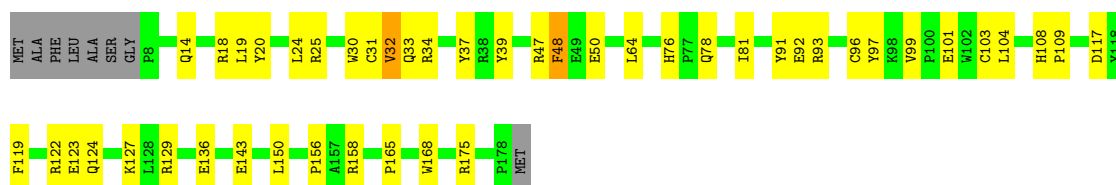
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain o: 



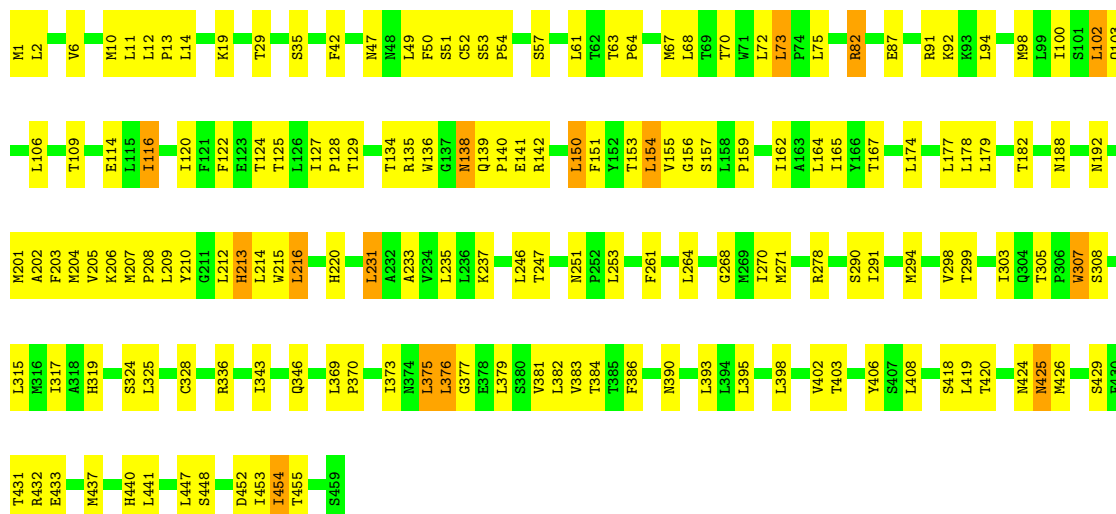
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain p: 



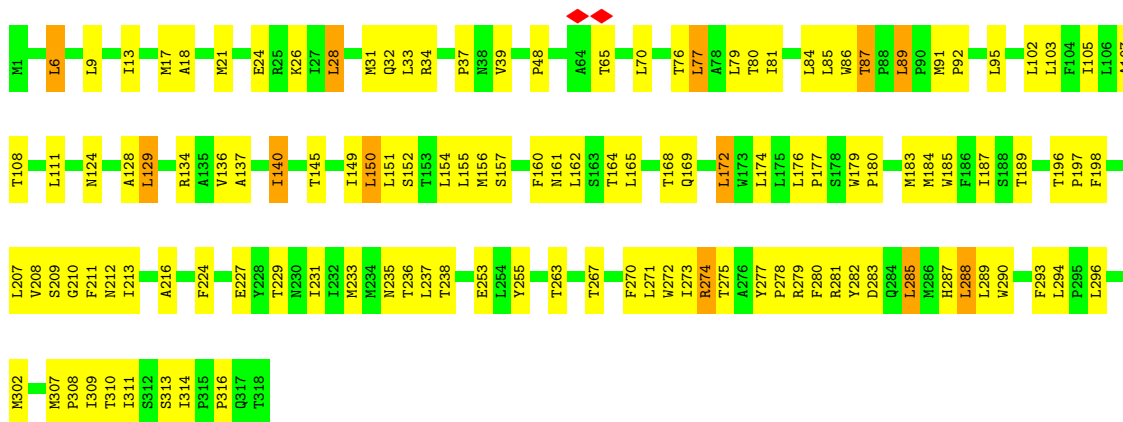
- Molecule 39: NADH-ubiquinone oxidoreductase chain 4

Chain r: 



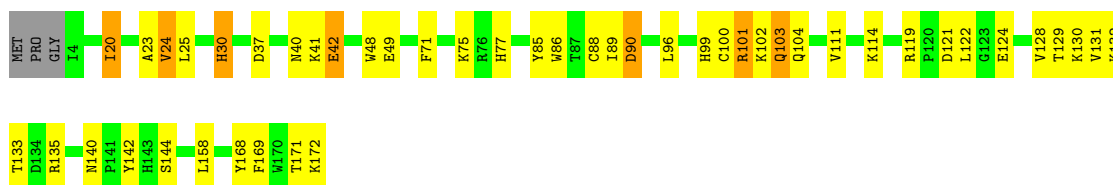
- Molecule 40: NADH-ubiquinone oxidoreductase chain 1

Chain s: 



- Molecule 41: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain u: 71% 23%



- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain v: 61% 20% 18%



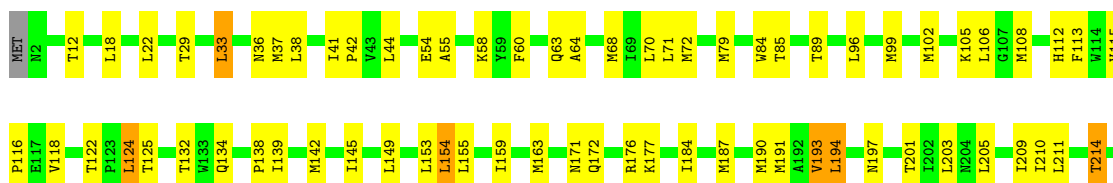
- Molecule 43: Unknow peptide

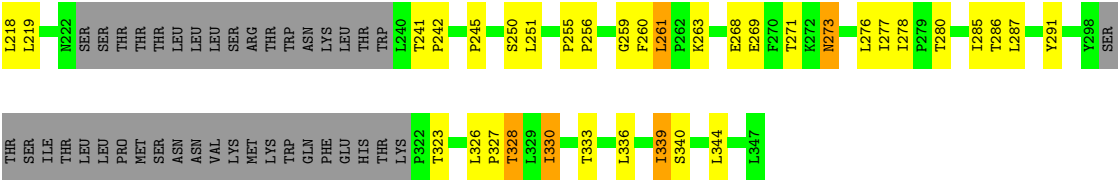
Chain D: 100%

There are no outlier residues recorded for this chain.

- Molecule 44: NADH-ubiquinone oxidoreductase chain 2

Chain i: 58% 27% 12%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	16097	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 ($e^-/\text{\AA}^2$)	38	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.246	Depositor
Minimum map value	-0.386	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.042	Depositor
Recommended contour level	0.135	Depositor
Map size (Å)	547.84, 547.84, 547.84	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.07, 1.07, 1.07	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, SF4, FES, NDP, ZMP

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	0.25	0/3392	0.44	0/4583
2	B	0.37	0/1452	0.58	0/1964
3	C	0.57	0/1280	0.76	0/1732
4	E	0.18	0/993	0.36	0/1335
5	F	0.20	0/682	0.33	0/922
6	G	0.08	0/657	0.27	0/890
6	X	0.23	0/698	0.39	0/942
7	H	0.12	0/941	0.34	0/1275
8	I	0.20	0/788	0.44	0/1066
9	J	0.21	0/2544	0.35	1/3437 (0.0%)
10	K	0.11	0/253	0.24	0/341
11	L	0.28	0/978	0.43	0/1320
12	M	0.35	0/5349	0.50	0/7250
13	N	0.12	0/1228	0.35	0/1670
14	O	0.17	0/1676	0.34	0/2282
15	P	0.17	0/1771	0.39	0/2412
16	Q	0.51	0/3146	0.70	0/4255
17	S	0.27	0/583	0.47	0/785
18	T	0.37	0/755	0.47	0/1017
19	U	0.42	0/670	0.58	0/920
20	V	0.19	0/1065	0.32	0/1450
21	W	0.44	0/1147	0.61	0/1557
22	Y	0.13	0/533	0.39	0/727
23	Z	0.09	0/601	0.25	0/806
24	a	0.21	0/1209	0.36	0/1639
25	b	0.12	0/1056	0.33	0/1427
26	c	0.17	0/1139	0.32	0/1558
27	d	0.15	0/1420	0.31	0/1910
28	e	0.12	0/751	0.31	0/1017
29	f	0.16	0/418	0.26	0/566
30	g	0.11	0/1035	0.27	0/1398
31	h	0.22	0/860	0.43	0/1153

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	j	0.45	0/749	0.72	0/1022
33	k	0.49	0/635	0.71	0/861
34	l	0.42	0/4495	0.58	1/6146 (0.0%)
35	m	0.49	0/1266	0.69	0/1721
36	n	0.22	0/484	0.36	0/652
37	o	0.10	0/859	0.29	0/1160
38	p	0.25	0/1533	0.38	0/2077
39	r	0.35	0/3717	0.50	0/5082
40	s	0.60	0/2563	0.81	0/3518
41	u	0.18	0/1433	0.34	0/1937
42	v	0.10	0/898	0.48	2/1198 (0.2%)
44	i	0.25	0/2447	0.42	1/3350 (0.0%)
All	All	0.33	0/62149	0.49	5/84330 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	B	0	2
12	M	0	1
14	O	0	1
16	Q	0	1
40	s	0	3
All	All	0	10

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	v	27	PRO	N-CA-CB	11.54	110.55	102.35
42	v	26	PRO	N-CA-CB	7.25	110.11	103.08
9	J	44	GLY	CA-C-O	-6.10	118.02	122.23
44	i	84	TRP	N-CA-C	-5.66	106.18	114.39
34	l	237	MET	N-CA-C	-5.12	107.41	113.97

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	48	ARG	Sidechain
1	A	59	ARG	Sidechain
2	B	54	ARG	Sidechain
2	B	66	ARG	Sidechain
12	M	158	ARG	Sidechain
14	O	42	ARG	Sidechain
16	Q	333	ARG	Sidechain
40	s	134	ARG	Sidechain
40	s	274	ARG	Sidechain
40	s	279	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3316	0	3274	85	0
2	B	1420	0	1365	61	0
3	C	1249	0	1253	51	0
4	E	968	0	982	37	0
5	F	670	0	679	22	0
6	G	647	0	623	23	0
6	X	686	0	676	18	0
7	H	922	0	950	22	0
8	I	769	0	788	27	0
9	J	2486	0	2531	74	0
10	K	247	0	234	8	0
11	L	955	0	949	33	0
12	M	5261	0	5292	194	0
13	N	1188	0	1148	29	0
14	O	1637	0	1633	60	0
15	P	1721	0	1679	72	0
16	Q	3073	0	3056	127	0
17	S	568	0	567	13	0
18	T	742	0	721	22	0
19	U	647	0	653	16	0
20	V	1038	0	1027	24	0
21	W	1116	0	1087	27	0
22	Y	510	0	456	11	0
23	Z	582	0	569	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	a	1174	0	1177	29	0
25	b	1022	0	1037	34	0
26	c	1094	0	946	39	0
27	d	1393	0	1353	36	0
28	e	731	0	710	12	0
29	f	405	0	407	2	0
30	g	1004	0	1008	16	0
31	h	840	0	821	29	0
32	j	732	0	794	17	0
33	k	627	0	684	31	0
34	l	4383	0	4510	159	0
35	m	1239	0	1272	39	0
36	n	473	0	480	9	0
37	o	841	0	851	20	0
38	p	1480	0	1424	32	0
39	r	3623	0	3817	111	0
40	s	2494	0	2596	102	0
41	u	1394	0	1367	39	0
42	v	887	0	817	21	0
43	D	110	0	24	0	0
44	i	2385	0	2517	72	0
45	A	8	0	0	2	0
45	B	16	0	0	4	0
45	C	8	0	0	4	0
45	M	16	0	0	1	0
46	A	31	0	19	2	0
47	E	30	0	30	1	0
48	J	48	0	26	1	0
49	M	4	0	0	0	0
49	O	4	0	0	0	0
All	All	60914	0	60879	1536	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1536) 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)
34:l:246:LEU:HD11	34:l:337:ALA:HA	1.20	1.10
2:B:99:HIS:CD2	45:B:302:SF4:S4	2.61	0.93
40:s:28:LEU:O	40:s:32:GLN:HB2	1.69	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:CYS:HG	45:B:301:SF4:FE1	0.73	0.91
14:O:183:ALA:HB3	14:O:195:ASP:HA	1.57	0.84
40:s:102:LEU:HD12	40:s:154:LEU:HD21	1.59	0.84
12:M:405:THR:HG1	12:M:479:SER:HG	1.26	0.83
41:u:24:VAL:HG22	41:u:86:TRP:HE1	1.42	0.83
39:r:336:ARG:HH22	39:r:429:SER:HA	1.44	0.82
34:l:246:LEU:HD13	34:l:340:PHE:HB2	1.60	0.81
1:A:385:CYS:HB3	45:A:501:SF4:S2	2.21	0.81
40:s:28:LEU:HD22	40:s:275:THR:HG22	1.63	0.80
3:C:105:ARG:HA	40:s:37:PRO:HA	1.64	0.80
26:c:133:LEU:HD12	34:l:532:ILE:HD12	1.64	0.79
26:c:73:GLY:HA3	37:o:79:ASN:HD22	1.48	0.79
3:C:88:CYS:SG	45:C:301:SF4:FE3	1.73	0.79
35:m:162:VAL:HG21	44:i:12:THR:HG21	1.64	0.79
31:h:47:ILE:HB	31:h:52:ALA:HB2	1.65	0.78
12:M:305:PRO:HD3	12:M:615:LEU:HD22	1.66	0.78
2:B:113:ALA:HB3	2:B:138:ARG:HB3	1.65	0.77
39:r:308:SER:HB3	39:r:384:THR:HG21	1.65	0.77
16:Q:314:VAL:HG11	16:Q:343:ILE:HG23	1.67	0.77
34:l:248:HIS:HA	34:l:252:MET:HB3	1.65	0.77
9:J:111:ARG:HH12	9:J:148:ILE:HD11	1.50	0.77
27:d:34:ILE:HG13	27:d:35:VAL:HG13	1.67	0.76
3:C:89:CYS:SG	45:C:301:SF4:FE2	1.76	0.76
4:E:51:GLN:HE22	9:J:362:LEU:HG	1.51	0.76
15:P:75:GLN:H	15:P:87:CYS:HB3	1.51	0.76
12:M:337:ASP:HB3	12:M:542:PRO:HD2	1.67	0.75
12:M:406:ASN:HB3	12:M:436:VAL:HG21	1.68	0.75
39:r:162:ILE:HD13	44:i:280:THR:HG22	1.67	0.75
24:a:53:ARG:HH22	25:b:30:PRO:HA	1.50	0.75
32:j:60:ILE:HG21	35:m:167:VAL:HG11	1.69	0.74
14:O:40:VAL:HG22	14:O:42:ARG:H	1.52	0.74
12:M:53:CYS:HB2	12:M:60:ILE:HD11	1.69	0.74
12:M:275:PRO:HB3	12:M:286:ILE:HB	1.70	0.74
32:j:109:LYS:HA	32:j:112:ASP:HB2	1.69	0.74
1:A:371:ILE:HD12	1:A:396:MET:HG3	1.70	0.73
2:B:156:CYS:N	45:B:302:SF4:S2	2.62	0.73
12:M:173:MET:C	12:M:175:ARG:H	1.96	0.73
3:C:114:PRO:HB3	3:C:137:VAL:HG13	1.70	0.73
39:r:102:LEU:HG	39:r:128:PRO:HB2	1.70	0.72
1:A:357:MET:HG2	14:O:142:LEU:HD21	1.72	0.72
2:B:117:CYS:HA	2:B:120:ILE:HG22	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:113:LYS:HG3	9:J:155:LEU:HD11	1.71	0.71
26:c:133:LEU:HD11	34:l:529:TYR:HA	1.72	0.71
34:l:174:TYR:HD2	34:l:232:TRP:HB3	1.55	0.71
28:e:76:TYR:H	39:r:432:ARG:HD2	1.55	0.71
9:J:206:ILE:HB	9:J:242:VAL:HG22	1.73	0.70
12:M:299:ARG:HD3	12:M:300:GLN:HG2	1.72	0.70
27:d:154:ARG:NH2	30:g:108:TYR:O	2.24	0.70
34:l:222:GLY:HA2	34:l:229:LEU:HD12	1.72	0.70
34:l:67:HIS:HA	34:l:77:SER:HA	1.72	0.70
21:W:120:LEU:HD11	31:h:69:ARG:HG3	1.73	0.70
6:X:76:LEU:H	6:X:156:GLU:HG3	1.57	0.70
12:M:624:ARG:HE	12:M:637:ASP:HA	1.55	0.70
7:H:7:LYS:HG2	7:H:8:THR:HG23	1.74	0.69
12:M:50:LEU:HD11	12:M:62:ARG:HE	1.57	0.69
26:c:183:HIS:HA	42:v:36:GLU:HA	1.72	0.69
10:K:86:ASP:OD1	14:O:62:ARG:NH1	2.26	0.69
9:J:283:VAL:HG13	9:J:369:VAL:HG11	1.74	0.69
12:M:326:VAL:HG23	12:M:626:LEU:HD13	1.72	0.69
34:l:155:ILE:HA	34:l:240:PRO:HB3	1.74	0.69
1:A:152:ARG:NH2	10:K:97:PRO:O	2.25	0.69
40:s:157:SER:HA	40:s:168:THR:HG21	1.74	0.69
9:J:201:VAL:HG12	9:J:203:PRO:HD3	1.75	0.68
16:Q:116:LEU:HD12	16:Q:458:PHE:HB2	1.75	0.68
31:h:93:THR:O	31:h:95:PRO:HD3	1.93	0.68
5:F:25:GLN:HB3	12:M:662:ALA:HB2	1.75	0.68
3:C:81:PRO:HG2	3:C:110:PHE:HD1	1.57	0.68
16:Q:174:PHE:HZ	16:Q:217:VAL:HG11	1.59	0.68
12:M:323:LEU:HB3	12:M:629:ILE:HD12	1.75	0.67
14:O:72:GLU:HA	14:O:75:LYS:HE2	1.75	0.67
18:T:105:LYS:HD3	18:T:108:LYS:HE2	1.76	0.67
19:U:14:ASP:N	19:U:14:ASP:OD1	2.27	0.67
4:E:101:THR:HG22	15:P:218:ARG:HB2	1.76	0.67
2:B:142:ARG:NH2	11:L:112:MET:O	2.27	0.67
18:T:96:HIS:HE1	18:T:99:VAL:HG12	1.58	0.67
39:r:72:LEU:HD13	39:r:233:ALA:HB1	1.77	0.67
16:Q:232:VAL:HB	16:Q:356:ILE:HG22	1.77	0.67
33:k:41:PHE:HA	33:k:63:MET:HE1	1.75	0.66
16:Q:140:ASP:HB2	16:Q:147:ASN:HD21	1.60	0.66
1:A:274:LYS:HE3	1:A:349:LEU:HD21	1.78	0.66
26:c:38:PRO:HG2	37:o:71:ALA:HB2	1.76	0.66
39:r:102:LEU:HD11	39:r:129:THR:HG22	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HE21	10:K:91:LEU:HD12	1.61	0.66
12:M:49:VAL:HG13	12:M:102:ILE:HD13	1.77	0.66
16:Q:432:LEU:HG	16:Q:456:ILE:HG21	1.76	0.66
34:l:237:MET:HG3	34:l:303:ALA:HB2	1.78	0.66
12:M:205:GLN:HE21	14:O:39:PHE:HB2	1.59	0.66
12:M:481:LEU:HD11	12:M:515:ILE:HD11	1.78	0.66
16:Q:180:LEU:HD22	16:Q:251:PHE:HE2	1.59	0.66
7:H:87:GLU:OE1	15:P:103:HIS:ND1	2.29	0.65
12:M:666:GLN:HA	12:M:669:ASN:HB3	1.77	0.65
16:Q:82:LEU:N	16:Q:99:MET:O	2.30	0.65
9:J:318:LYS:HE3	9:J:321:ARG:HH21	1.60	0.65
41:u:96:LEU:HD11	41:u:99:HIS:CD2	2.31	0.65
34:l:82:LEU:HB3	34:l:87:MET:HE1	1.77	0.65
3:C:173:ILE:HG22	3:C:174:VAL:HG13	1.77	0.65
24:a:63:TYR:HD1	24:a:66:ARG:HH21	1.45	0.65
17:S:69:ILE:HD13	41:u:71:PHE:HB3	1.79	0.65
20:V:135:VAL:HG22	44:i:277:ILE:HD12	1.78	0.65
34:l:514:LYS:HG3	34:l:516:PRO:HD2	1.79	0.65
31:h:49:TYR:HA	31:h:52:ALA:HB3	1.77	0.64
1:A:41:ILE:HG21	1:A:250:VAL:HG23	1.78	0.64
8:I:60:ARG:HG3	16:Q:392:PRO:HG3	1.79	0.64
34:l:142:ILE:HA	39:r:370:PRO:HG2	1.77	0.64
2:B:99:HIS:H	2:B:147:MET:HE1	1.63	0.64
33:k:43:MET:HG3	33:k:47:MET:HE3	1.79	0.64
28:e:113:ARG:HH21	28:e:115:LYS:HE2	1.63	0.64
6:X:85:TYR:OH	23:Z:22:TRP:NE1	2.27	0.64
6:X:91:ASP:HB3	23:Z:47:ARG:HH21	1.63	0.64
12:M:83:GLU:HB2	12:M:101:ASN:HB3	1.80	0.63
1:A:164:ASN:O	1:A:168:ASN:ND2	2.31	0.63
36:n:55:VAL:HG12	36:n:56:THR:H	1.64	0.63
12:M:180:THR:OG1	12:M:184:ARG:NH1	2.31	0.63
17:S:50:ARG:HH21	41:u:25:LEU:HD11	1.63	0.63
20:V:12:ILE:HG21	20:V:17:ASP:HB2	1.80	0.63
31:h:5:ASP:N	31:h:5:ASP:OD1	2.30	0.63
35:m:56:PHE:HB3	40:s:107:ALA:HB1	1.81	0.63
5:F:58:CYS:SG	12:M:651:PRO:HB2	2.38	0.63
12:M:194:ASP:OD1	12:M:212:LYS:NZ	2.26	0.63
15:P:44:ARG:O	16:Q:162:ARG:NH2	2.32	0.63
33:k:34:GLU:HG2	35:m:63:MET:HE2	1.79	0.63
14:O:183:ALA:HB1	14:O:184:PRO:HD2	1.81	0.63
16:Q:251:PHE:HA	16:Q:254:ARG:HE	1.63	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:48:ASP:OD1	18:T:48:ASP:N	2.31	0.63
26:c:107:TRP:O	37:o:72:ARG:NH1	2.32	0.63
9:J:238:GLN:NE2	9:J:267:GLY:O	2.32	0.63
2:B:126:ILE:HG12	2:B:145:ILE:HB	1.81	0.62
24:a:136:THR:HG22	39:r:51:SER:H	1.63	0.62
28:e:129:ARG:NH1	28:e:136:ILE:O	2.32	0.62
15:P:233:PHE:O	16:Q:418:ARG:NH2	2.32	0.62
42:v:113:LYS:HG2	42:v:117:LYS:HE3	1.80	0.62
3:C:184:PRO:HG3	16:Q:222:MET:HE2	1.80	0.62
34:l:71:THR:OG1	34:l:72:GLN:N	2.33	0.62
34:l:231:PRO:HD3	34:l:529:TYR:CE2	2.34	0.62
39:r:127:ILE:HB	39:r:128:PRO:HD3	1.80	0.62
12:M:276:ARG:O	12:M:282:ASN:ND2	2.31	0.62
14:O:130:TYR:HA	14:O:189:ASN:HD21	1.65	0.62
7:H:44:TYR:H	7:H:100:TRP:HE1	1.48	0.62
5:F:37:ILE:HG12	5:F:55:ILE:HD13	1.81	0.62
21:W:27:ARG:C	21:W:29:GLY:H	2.07	0.62
34:l:49:PHE:HB2	34:l:50:PRO:HD3	1.82	0.62
34:l:240:PRO:HB2	34:l:244:SER:HB2	1.82	0.62
3:C:172:ARG:NH1	15:P:209:GLU:OE2	2.33	0.62
32:j:94:LEU:HD12	35:m:153:VAL:HG13	1.81	0.61
12:M:262:VAL:HG23	12:M:276:ARG:HB2	1.83	0.61
14:O:158:ILE:HG23	14:O:162:GLU:HB3	1.82	0.61
26:c:67:ASP:OD1	26:c:67:ASP:N	2.31	0.61
34:l:419:THR:HA	34:l:422:TYR:CE2	2.35	0.61
1:A:40:ARG:NH1	1:A:289:GLU:O	2.33	0.61
4:E:81:LEU:HD23	11:L:64:LEU:HD22	1.82	0.61
16:Q:113:ILE:HG12	16:Q:114:GLY:H	1.64	0.61
25:b:93:LYS:NZ	34:l:65:ASN:O	2.33	0.61
26:c:101:TRP:NE1	37:o:61:GLU:O	2.27	0.61
11:L:156:LYS:O	12:M:51:GLN:NE2	2.33	0.61
6:X:124:ASP:OD1	38:p:25:ARG:NH2	2.33	0.61
39:r:11:LEU:HB3	39:r:100:ILE:HD13	1.82	0.61
1:A:364:VAL:HG12	1:A:400:VAL:HG12	1.81	0.61
1:A:392:MET:HG3	1:A:412:LEU:HD21	1.83	0.61
14:O:123:ASN:HD22	14:O:127:VAL:HG11	1.66	0.61
26:c:101:TRP:HD1	37:o:62:ASN:HD22	1.48	0.61
27:d:108:GLN:HG3	34:l:203:LEU:HD23	1.83	0.61
44:i:155:LEU:HD13	44:i:278:ILE:HD13	1.83	0.61
31:h:38:LYS:NZ	31:h:42:GLU:OE2	2.34	0.61
41:u:100:CYS:O	41:u:102:LYS:N	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:LEU:HB3	14:O:234:LEU:HD11	1.80	0.61
9:J:64:PHE:CE2	9:J:242:VAL:HG21	2.36	0.61
16:Q:255:LEU:HD11	16:Q:337:MET:HB3	1.82	0.61
42:v:114:ARG:HD3	42:v:117:LYS:HD2	1.83	0.61
5:F:69:TYR:HB2	5:F:73:GLN:HG3	1.83	0.60
9:J:125:VAL:HG12	9:J:163:LYS:HB2	1.83	0.60
34:l:417:SER:HB3	34:l:493:VAL:HG13	1.82	0.60
41:u:41:LYS:NZ	41:u:129:THR:OG1	2.34	0.60
8:I:30:GLU:HG2	8:I:31:ILE:H	1.64	0.60
11:L:90:GLY:HA2	12:M:59:GLN:HE22	1.65	0.60
20:V:40:ARG:NH1	20:V:44:ASN:O	2.34	0.60
32:j:86:LEU:HD21	35:m:150:ARG:HD3	1.83	0.60
6:G:74:LEU:HD22	6:G:154:VAL:HG21	1.83	0.60
6:G:101:ASN:HD22	6:G:140:CYS:HB3	1.67	0.60
8:I:33:LYS:NZ	8:I:35:THR:O	2.32	0.60
39:r:1:MET:HE2	39:r:52:CYS:HB3	1.83	0.60
39:r:382:LEU:HD21	39:r:393:LEU:HD13	1.82	0.60
3:C:87:ALA:HA	16:Q:141:TYR:CZ	2.37	0.60
40:s:289:LEU:HA	40:s:293:PHE:HB2	1.81	0.60
7:H:50:GLN:HE22	8:I:94:ALA:H	1.50	0.60
13:N:42:ASP:OD1	13:N:42:ASP:N	2.26	0.60
16:Q:174:PHE:O	16:Q:178:THR:OG1	2.20	0.60
34:l:387:THR:OG1	34:l:461:SER:O	2.20	0.60
12:M:66:HIS:HB3	12:M:69:LEU:HB2	1.82	0.60
39:r:403:THR:HA	39:r:406:TYR:CE2	2.37	0.60
7:H:24:LEU:HD21	7:H:80:VAL:HG13	1.82	0.60
16:Q:145:MET:HE1	16:Q:226:TYR:HB3	1.84	0.60
40:s:156:MET:HE3	40:s:307:MET:HE1	1.82	0.60
26:c:100:ASN:HB2	26:c:103:GLU:HB2	1.84	0.60
26:c:127:HIS:N	26:c:130:CYS:HG	2.00	0.60
35:m:72:ALA:HB1	40:s:129:LEU:HD11	1.83	0.60
13:N:51:ASP:N	13:N:51:ASP:OD1	2.33	0.60
32:j:6:ILE:HD12	40:s:84:LEU:HD23	1.82	0.60
21:W:57:ARG:HB3	40:s:316:PRO:HG3	1.83	0.59
34:l:142:ILE:HG12	39:r:370:PRO:HB2	1.83	0.59
1:A:112:TYR:HB2	1:A:240:THR:HG22	1.84	0.59
15:P:188:LEU:HD22	16:Q:462:ASP:HB3	1.83	0.59
34:l:359:MET:O	34:l:436:ARG:NH2	2.34	0.59
40:s:179:TRP:N	40:s:180:PRO:HD2	2.16	0.59
23:Z:69:LYS:HE2	34:l:371:THR:HG22	1.83	0.59
40:s:89:LEU:HA	40:s:162:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:383:SER:HB3	12:M:388:ASN:HD21	1.67	0.59
15:P:115:THR:HA	15:P:170:ILE:HD11	1.84	0.59
18:T:70:ASP:OD1	18:T:70:ASP:N	2.34	0.59
20:V:81:ARG:HG2	20:V:83:LYS:HG3	1.84	0.59
31:h:49:TYR:OH	44:i:89:THR:HB	2.02	0.59
34:l:526:LEU:HD12	34:l:530:PRO:HG3	1.83	0.59
3:C:186:THR:HG22	3:C:188:GLU:H	1.66	0.59
6:G:110:LEU:HD22	6:G:114:ASP:HB3	1.85	0.59
11:L:111:LEU:HD11	13:N:126:PRO:HG2	1.85	0.59
44:i:55:ALA:HB1	44:i:118:VAL:HG22	1.84	0.59
39:r:47:ASN:H	39:r:50:PHE:HD2	1.51	0.59
15:P:186:ARG:HD2	15:P:191:TYR:HA	1.85	0.59
23:Z:65:ASP:OD1	23:Z:65:ASP:N	2.34	0.59
24:a:95:GLN:HA	24:a:116:PRO:HD3	1.84	0.59
34:l:401:MET:HG3	34:l:479:GLN:HG2	1.84	0.59
44:i:142:MET:HB3	44:i:194:LEU:HD11	1.83	0.59
33:k:62:ALA:O	33:k:63:MET:C	2.46	0.59
41:u:88:CYS:SG	41:u:103:GLN:NE2	2.75	0.59
24:a:179:ILE:HG12	31:h:20:ILE:HD11	1.83	0.59
3:C:90:ALA:HA	3:C:93:MET:HE2	1.83	0.58
40:s:282:TYR:O	40:s:283:ASP:C	2.46	0.58
2:B:124:GLN:HB3	15:P:231:ARG:HH21	1.68	0.58
2:B:180:GLU:OE2	13:N:123:GLN:NE2	2.36	0.58
4:E:41:ARG:NH2	6:G:123:GLU:OE2	2.37	0.58
9:J:279:TYR:HB2	9:J:372:ALA:HB2	1.85	0.58
12:M:149:ASP:HB2	16:Q:361:ALA:HB3	1.86	0.58
12:M:173:MET:O	12:M:175:ARG:N	2.35	0.58
15:P:114:LEU:HB3	15:P:166:TYR:HB3	1.85	0.58
12:M:140:GLN:NE2	45:M:801:SF4:S3	2.77	0.58
12:M:186:ALA:HA	12:M:190:ALA:HB3	1.85	0.58
9:J:135:GLU:HG3	9:J:141:PHE:H	1.68	0.58
9:J:171:ASN:ND2	9:J:325:THR:O	2.36	0.58
11:L:173:SER:HB3	14:O:111:ARG:HE	1.68	0.58
44:i:269:GLU:O	44:i:273:ASN:ND2	2.36	0.58
1:A:423:THR:OG1	45:A:501:SF4:S4	2.61	0.58
2:B:133:ARG:CZ	2:B:139:ARG:HG3	2.33	0.58
6:G:83:VAL:HG21	6:G:145:VAL:HG22	1.85	0.58
12:M:223:ILE:HD13	12:M:233:SER:HB3	1.86	0.58
12:M:569:GLN:NE2	12:M:619:ASP:OD1	2.37	0.58
13:N:5:GLN:O	13:N:9:ARG:HG2	2.03	0.58
14:O:188:ILE:HB	14:O:193:TYR:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:l:193:SER:HB3	34:l:205:ASN:HD21	1.69	0.58
16:Q:268:TRP:HD1	40:s:278:PRO:HG3	1.69	0.58
17:S:37:ARG:HG3	17:S:60:TYR:HE2	1.67	0.58
44:i:99:MET:HE2	44:i:149:LEU:HG	1.84	0.58
9:J:270:ARG:HH12	9:J:326:ASP:HB2	1.69	0.58
25:b:26:GLN:HB3	38:p:175:ARG:HH21	1.69	0.58
31:h:65:GLU:OE2	31:h:71:LYS:N	2.37	0.58
39:r:213:HIS:HB2	39:r:291:ILE:HD13	1.86	0.58
12:M:540:ASN:HD21	12:M:560:LEU:HD13	1.68	0.57
34:l:18:PRO:HG3	34:l:39:ILE:HD12	1.84	0.57
4:E:25:MET:HE1	4:E:79:VAL:HG21	1.86	0.57
6:G:92:LYS:HE3	6:G:110:LEU:HB3	1.85	0.57
12:M:193:ASP:OD1	14:O:111:ARG:NH2	2.37	0.57
12:M:351:LEU:O	12:M:530:TYR:OH	2.23	0.57
16:Q:267:ILE:HB	40:s:278:PRO:HG2	1.87	0.57
34:l:174:TYR:CD2	34:l:232:TRP:HB3	2.38	0.57
44:i:33:LEU:HD21	44:i:102:MET:HE1	1.86	0.57
3:C:131:ALA:HB3	3:C:132:PRO:HD3	1.87	0.57
26:c:155:PRO:HD3	42:v:5:LEU:HD22	1.86	0.57
34:l:15:LEU:HB3	34:l:122:LEU:HD21	1.86	0.57
44:i:38:LEU:HA	44:i:41:ILE:HD12	1.85	0.57
44:i:159:ILE:HD11	44:i:278:ILE:HG23	1.86	0.57
15:P:83:GLU:OE1	15:P:142:ARG:NH1	2.37	0.57
15:P:140:ARG:NH2	16:Q:306:GLN:OE1	2.37	0.57
24:a:189:ASN:ND2	41:u:142:TYR:OH	2.38	0.57
34:l:51:THR:HG21	34:l:91:PRO:HG3	1.86	0.57
12:M:560:LEU:HD11	12:M:562:LYS:HB3	1.85	0.57
17:S:55:SER:O	17:S:64:LYS:NZ	2.37	0.57
24:a:120:TRP:HD1	24:a:123:ARG:HH21	1.51	0.57
36:n:35:LEU:HD11	39:r:54:PRO:HD3	1.86	0.57
40:s:24:GLU:HA	40:s:271:LEU:HD13	1.87	0.57
44:i:44:LEU:HD22	44:i:122:THR:HG21	1.87	0.57
9:J:192:ARG:NH1	9:J:198:ALA:O	2.38	0.57
16:Q:166:ARG:NH2	21:W:9:ASP:O	2.38	0.57
3:C:81:PRO:HG2	3:C:110:PHE:CD1	2.38	0.57
6:G:82:ARG:NH1	6:G:125:GLU:OE2	2.32	0.57
12:M:173:MET:C	12:M:175:ARG:N	2.63	0.57
9:J:125:VAL:HG11	9:J:253:VAL:HG13	1.87	0.57
12:M:342:ALA:HB3	12:M:368:THR:HA	1.87	0.57
39:r:208:PRO:HG3	39:r:216:LEU:HD12	1.86	0.57
24:a:180:ASP:OD1	24:a:184:LYS:NZ	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:e:115:LYS:NZ	39:r:452:ASP:OD2	2.38	0.56
34:l:102:GLU:HB3	34:l:453:PRO:HG3	1.86	0.56
4:E:20:ILE:HG12	15:P:152:PRO:HD3	1.86	0.56
9:J:228:LEU:HD11	9:J:277:VAL:HG21	1.86	0.56
11:L:84:ARG:NH1	11:L:88:GLN:O	2.39	0.56
12:M:114:GLU:O	12:M:118:GLU:HG2	2.04	0.56
14:O:197:THR:O	14:O:201:ILE:HG13	2.05	0.56
15:P:185:ARG:HH22	16:Q:110:ASP:HB2	1.69	0.56
34:l:553:LEU:HD22	39:r:271:MET:HE2	1.88	0.56
39:r:167:THR:HG23	39:r:174:LEU:HD21	1.88	0.56
40:s:65:THR:O	40:s:124:ASN:ND2	2.34	0.56
44:i:102:MET:HB2	44:i:142:MET:HE2	1.87	0.56
44:i:210:ILE:O	44:i:214:THR:OG1	2.22	0.56
41:u:24:VAL:HG13	41:u:86:TRP:CD1	2.40	0.56
44:i:36:ASN:ND2	44:i:134:GLN:OE1	2.39	0.56
16:Q:81:THR:HA	16:Q:100:GLU:HA	1.88	0.56
6:X:155:TYR:HA	25:b:20:ARG:HD3	1.86	0.56
12:M:405:THR:HG23	12:M:687:PRO:HD2	1.87	0.56
40:s:154:LEU:HD13	40:s:160:PHE:CD1	2.40	0.56
4:E:62:LYS:HE3	4:E:66:MET:HE2	1.87	0.56
12:M:36:VAL:HG11	12:M:56:VAL:HG11	1.87	0.56
14:O:38:LEU:O	14:O:124:ARG:NH2	2.39	0.56
14:O:213:ILE:HG22	14:O:215:LYS:H	1.71	0.56
40:s:149:ILE:HG21	40:s:185:TRP:HB2	1.88	0.56
1:A:379:CYS:SG	1:A:380:GLY:N	2.78	0.56
20:V:22:ALA:O	20:V:26:THR:HG23	2.06	0.56
35:m:10:VAL:HG13	35:m:99:GLU:HG3	1.88	0.56
34:l:342:CYS:HG	34:l:372:SER:HG	1.54	0.56
1:A:149:MET:HE3	1:A:241:THR:HG21	1.88	0.56
18:T:112:CYS:SG	18:T:115:CYS:N	2.75	0.55
39:r:120:ILE:O	39:r:124:THR:HG23	2.06	0.55
39:r:155:VAL:O	39:r:159:PRO:HG2	2.05	0.55
12:M:259:SER:HB2	12:M:282:ASN:HB3	1.87	0.55
44:i:33:LEU:HG	44:i:105:LYS:HE2	1.88	0.55
12:M:258:GLY:O	12:M:604:GLN:NE2	2.39	0.55
14:O:143:ARG:HB2	14:O:184:PRO:HD3	1.86	0.55
27:d:136:ARG:NH2	28:e:138:GLU:O	2.39	0.55
12:M:371:VAL:HG22	12:M:482:GLN:HG3	1.89	0.55
12:M:647:GLU:HA	12:M:651:PRO:HA	1.89	0.55
20:V:139:PRO:O	20:V:141:VAL:N	2.39	0.55
34:l:102:GLU:OE1	34:l:456:ARG:NH2	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:71:ASN:HD21	9:J:75:ARG:HH21	1.52	0.55
11:L:92:ASN:HB3	15:P:238:PRO:HA	1.89	0.55
30:g:46:LEU:HD13	30:g:52:ILE:HD11	1.88	0.55
34:l:380:LEU:O	34:l:392:LYS:NZ	2.39	0.55
42:v:39:MET:HE3	42:v:41:ALA:HB3	1.89	0.55
3:C:178:ILE:HD13	3:C:197:LEU:HB2	1.88	0.55
11:L:118:ALA:HA	15:P:225:GLU:HA	1.88	0.55
12:M:595:THR:HA	12:M:605:GLN:HA	1.87	0.55
15:P:129:VAL:HG22	15:P:144:LYS:HG2	1.89	0.55
25:b:86:MET:HE3	34:l:9:THR:HG21	1.89	0.55
11:L:89:SER:O	12:M:59:GLN:NE2	2.39	0.55
26:c:58:ARG:NH1	26:c:60:GLU:OE1	2.40	0.55
7:H:65:VAL:HG13	7:H:77:LEU:HD12	1.89	0.55
34:l:22:THR:HG21	34:l:119:LYS:HE2	1.89	0.55
2:B:63:GLU:HG2	2:B:64:LEU:HD12	1.88	0.55
3:C:175:PRO:HB2	9:J:92:MET:HG3	1.88	0.55
10:K:91:LEU:HB3	10:K:95:ARG:HH12	1.72	0.55
12:M:413:LEU:HD12	12:M:413:LEU:H	1.72	0.55
39:r:154:LEU:HD22	44:i:287:LEU:HD12	1.89	0.55
40:s:18:ALA:HB1	40:s:48:PRO:HB2	1.89	0.55
8:I:66:PRO:HB3	15:P:79:SER:HA	1.89	0.54
16:Q:182:ASN:HD22	16:Q:403:PRO:HB2	1.72	0.54
6:X:103:HIS:HB2	6:X:106:LYS:HB3	1.87	0.54
34:l:76:LEU:HD11	34:l:138:PHE:HB2	1.88	0.54
1:A:429:ASP:N	1:A:429:ASP:OD1	2.41	0.54
12:M:157:LYS:NZ	16:Q:375:MET:HB2	2.21	0.54
12:M:513:MET:HB3	12:M:665:PHE:HE1	1.72	0.54
14:O:82:VAL:HG21	14:O:105:LEU:HD11	1.90	0.54
14:O:164:THR:HG22	14:O:166:ASP:H	1.71	0.54
15:P:204:LEU:HB2	16:Q:126:TYR:HE2	1.71	0.54
19:U:59:ASP:HB2	41:u:132:LYS:HG2	1.88	0.54
33:k:19:MET:HE3	33:k:29:SER:HB2	1.89	0.54
36:n:10:ASP:HB3	39:r:19:LYS:HE2	1.90	0.54
44:i:54:GLU:OE2	44:i:58:LYS:NZ	2.39	0.54
2:B:129:GLU:HB2	2:B:142:ARG:HG2	1.88	0.54
6:G:87:LEU:HB3	6:G:93:ILE:HD13	1.89	0.54
16:Q:185:MET:HE3	16:Q:189:THR:HG21	1.90	0.54
17:S:19:PRO:HB3	40:s:9:LEU:HA	1.88	0.54
39:r:231:LEU:HG	39:r:235:LEU:HD12	1.89	0.54
40:s:169:GLN:HE21	40:s:174:LEU:H	1.53	0.54
12:M:355:LYS:HD2	12:M:530:TYR:HE1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:l:10:LEU:HD12	34:l:46:ILE:HG21	1.88	0.54
38:p:124:GLN:HA	38:p:127:LYS:HZ3	1.71	0.54
40:s:164:THR:O	40:s:168:THR:HG23	2.08	0.54
1:A:383:THR:HG22	12:M:75:CYS:HA	1.90	0.54
3:C:184:PRO:HD3	16:Q:223:HIS:CD2	2.42	0.54
6:G:120:MET:HA	6:G:123:GLU:HG2	1.90	0.54
9:J:77:GLY:O	9:J:102:GLN:NE2	2.41	0.54
16:Q:150:ALA:HA	16:Q:400:ILE:HG13	1.89	0.54
16:Q:251:PHE:HD2	16:Q:341:LEU:HD21	1.71	0.54
16:Q:260:GLU:HG3	21:W:25:LEU:HD22	1.89	0.54
26:c:36:MET:HB3	26:c:54:LYS:HG3	1.90	0.54
34:l:191:LEU:O	37:o:126:HIS:ND1	2.41	0.54
34:l:217:LEU:HD21	34:l:277:THR:HG22	1.89	0.54
12:M:497:ALA:HB3	12:M:666:GLN:HE22	1.72	0.54
13:N:50:GLU:HG3	13:N:89:TRP:HZ2	1.73	0.54
44:i:218:LEU:HD21	44:i:330:ILE:HD11	1.90	0.54
7:H:32:LEU:HD23	7:H:35:LEU:HD21	1.90	0.54
15:P:215:GLU:HG3	15:P:216:VAL:HG13	1.90	0.54
39:r:447:LEU:HD13	39:r:454:ILE:HD11	1.90	0.54
3:C:81:PRO:HD2	3:C:109:VAL:O	2.08	0.54
9:J:172:ALA:O	9:J:185:ALA:HB2	2.07	0.54
12:M:68:ARG:NH2	12:M:279:GLU:OE2	2.41	0.54
24:a:57:ILE:HG23	38:p:99:VAL:HB	1.90	0.54
2:B:35:THR:OG1	16:Q:304:LYS:NZ	2.41	0.54
2:B:99:HIS:HE1	2:B:150:CYS:SG	2.22	0.54
15:P:46:THR:HG21	16:Q:359:ASP:HB2	1.89	0.54
18:T:85:ILE:HD12	18:T:103:LEU:HD11	1.90	0.54
27:d:23:PRO:HA	27:d:26:TYR:CE2	2.42	0.54
5:F:23:LEU:HD13	5:F:33:VAL:HB	1.89	0.53
11:L:163:ASN:HB3	11:L:172:VAL:HB	1.88	0.53
19:U:82:LYS:HG2	41:u:122:LEU:HD21	1.89	0.53
20:V:22:ALA:O	20:V:25:THR:OG1	2.23	0.53
27:d:65:VAL:HG22	27:d:66:PRO:HD2	1.90	0.53
31:h:9:ARG:HH11	31:h:10:PHE:HE1	1.56	0.53
44:i:139:ILE:HD11	44:i:187:MET:HE1	1.91	0.53
4:E:37:ARG:NH2	6:G:123:GLU:OE2	2.37	0.53
18:T:37:GLU:HB3	18:T:45:VAL:HG23	1.89	0.53
34:l:69:ALA:HB2	39:r:376:LEU:HD11	1.90	0.53
34:l:233:LEU:HD21	34:l:253:VAL:HG21	1.90	0.53
4:E:110:THR:HG21	15:P:220:VAL:HG21	1.90	0.53
9:J:95:ARG:HG2	9:J:105:PHE:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:k:60:PRO:HA	33:k:63:MET:HE2	1.91	0.53
34:l:537:ILE:HB	34:l:538:PRO:HD3	1.90	0.53
12:M:478:SER:HB2	12:M:517:HIS:HA	1.90	0.53
12:M:517:HIS:HB2	12:M:599:THR:HG22	1.89	0.53
26:c:62:TYR:OH	26:c:74:ASP:O	2.23	0.53
12:M:482:GLN:O	12:M:483:ARG:C	2.51	0.53
14:O:205:ILE:HA	14:O:208:LEU:HD12	1.89	0.53
40:s:187:ILE:HD12	40:s:293:PHE:HZ	1.74	0.53
40:s:210:GLY:C	40:s:212:ASN:H	2.16	0.53
41:u:20:ILE:HG12	41:u:24:VAL:HG21	1.90	0.53
8:I:12:ARG:HH22	8:I:21:GLN:NE2	2.07	0.53
17:S:5:ILE:HA	40:s:26:LYS:HE2	1.91	0.53
3:C:203:ARG:NH2	13:N:76:ASP:OD1	2.42	0.53
12:M:531:LYS:O	12:M:533:GLY:N	2.42	0.53
14:O:96:SER:HA	14:O:99:ASN:HD21	1.74	0.53
16:Q:179:ARG:HG3	16:Q:403:PRO:HB3	1.91	0.53
21:W:50:ILE:HD11	40:s:174:LEU:HD22	1.90	0.53
40:s:85:LEU:HD13	40:s:233:MET:HE2	1.90	0.53
40:s:210:GLY:O	40:s:212:ASN:ND2	2.41	0.53
4:E:97:TRP:HB3	16:Q:96:ARG:HH22	1.73	0.53
12:M:126:LEU:CD1	16:Q:375:MET:HA	2.39	0.53
12:M:210:ILE:HD13	12:M:211:GLU:H	1.74	0.53
16:Q:451:ILE:HG23	16:Q:456:ILE:HD12	1.91	0.53
22:Y:72:ARG:HG2	34:l:385:PHE:HA	1.89	0.53
33:k:75:LEU:HD13	35:m:70:THR:HG21	1.90	0.53
42:v:73:SER:HB2	42:v:76:ASN:HB2	1.90	0.53
1:A:394:LYS:HB3	12:M:155:GLU:HG2	1.90	0.53
12:M:647:GLU:HG3	12:M:651:PRO:HB3	1.91	0.53
40:s:187:ILE:HG23	40:s:198:PHE:CE2	2.44	0.53
41:u:90:ASP:OD1	41:u:90:ASP:N	2.41	0.53
3:C:115:ARG:HA	3:C:142:PRO:HD3	1.91	0.53
6:X:90:TYR:CE2	6:X:92:LYS:HB2	2.44	0.53
34:l:71:THR:O	34:l:73:THR:N	2.41	0.53
34:l:132:VAL:O	34:l:262:ARG:NH2	2.41	0.53
34:l:552:LEU:O	34:l:557:TRP:HB3	2.09	0.53
16:Q:139:LEU:HD13	16:Q:424:ILE:HG21	1.90	0.52
30:g:63:TYR:HE1	44:i:328:THR:HG22	1.75	0.52
34:l:468:ILE:HG23	34:l:472:ILE:HD13	1.91	0.52
34:l:553:LEU:HD21	37:o:94:GLY:HA2	1.91	0.52
12:M:50:LEU:HG	12:M:60:ILE:HD13	1.91	0.52
25:b:86:MET:HA	25:b:90:VAL:HG12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:l:191:LEU:HD12	37:o:126:HIS:CE1	2.43	0.52
4:E:53:ASP:OD1	9:J:354:ARG:NH2	2.42	0.52
9:J:350:ILE:HD12	9:J:366:ILE:HG12	1.91	0.52
12:M:319:TRP:HZ3	12:M:584:LEU:HD22	1.73	0.52
12:M:432:ILE:HG23	12:M:451:ILE:HD11	1.90	0.52
13:N:68:MET:HG3	13:N:69:ASN:HD22	1.73	0.52
14:O:132:ILE:HA	14:O:188:ILE:HG12	1.91	0.52
23:Z:52:ARG:HD3	34:l:439:THR:HG22	1.92	0.52
29:f:42:LEU:HG	29:f:43:LYS:HG3	1.91	0.52
7:H:64:ASP:OD1	7:H:64:ASP:N	2.42	0.52
12:M:560:LEU:HD12	12:M:561:PRO:HD2	1.92	0.52
13:N:34:LYS:NZ	13:N:58:ARG:HG2	2.25	0.52
16:Q:143:SER:O	16:Q:147:ASN:ND2	2.42	0.52
34:l:246:LEU:HD13	34:l:340:PHE:CB	2.34	0.52
41:u:168:TYR:OH	44:i:268:GLU:OE1	2.26	0.52
16:Q:163:PRO:HD2	16:Q:168:GLN:HE21	1.74	0.52
25:b:104:ILE:HG23	27:d:18:PRO:HG3	1.91	0.52
40:s:209:SER:HB3	40:s:213:ILE:HG13	1.91	0.52
12:M:574:ASP:O	12:M:576:GLY:N	2.43	0.52
15:P:209:GLU:N	15:P:222:GLU:O	2.36	0.52
22:Y:88:ASP:N	22:Y:88:ASP:OD1	2.40	0.52
34:l:186:LEU:HB3	34:l:196:TRP:HE1	1.75	0.52
34:l:230:HIS:N	34:l:231:PRO:HD2	2.24	0.52
44:i:277:ILE:O	44:i:280:THR:OG1	2.27	0.52
5:F:59:SER:OG	12:M:655:ARG:NH1	2.42	0.52
21:W:27:ARG:C	21:W:29:GLY:N	2.68	0.52
27:d:63:ARG:NH2	36:n:46:LYS:O	2.40	0.52
31:h:47:ILE:HG22	31:h:51:ARG:HG3	1.91	0.52
12:M:335:GLY:O	12:M:363:SER:OG	2.27	0.52
33:k:59:VAL:HB	33:k:60:PRO:HD3	1.92	0.52
1:A:159:ARG:HH22	14:O:177:LEU:C	2.17	0.52
14:O:65:ALA:O	14:O:69:ASN:ND2	2.43	0.52
16:Q:93:GLY:HA3	16:Q:458:PHE:HD2	1.73	0.52
27:d:70:GLU:HG2	28:e:146:LYS:HE2	1.92	0.52
30:g:44:ASP:OD2	30:g:48:ARG:NH2	2.43	0.52
5:F:62:GLN:HB2	5:F:80:ASN:HB2	1.92	0.52
16:Q:94:VAL:HG12	16:Q:115:LEU:HD22	1.91	0.52
39:r:124:THR:HG22	44:i:256:PRO:HB3	1.92	0.52
22:Y:86:TYR:HA	22:Y:88:ASP:H	1.74	0.51
27:d:63:ARG:NH1	36:n:43:MET:O	2.41	0.51
30:g:10:LEU:HB2	31:h:9:ARG:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:k:73:VAL:HG21	44:i:38:LEU:HD22	1.92	0.51
34:l:188:TRP:HA	34:l:191:LEU:HD23	1.92	0.51
2:B:146:ASP:HB3	2:B:182:LEU:HG	1.92	0.51
3:C:166:VAL:O	3:C:168:ARG:NH1	2.44	0.51
6:G:140:CYS:HB2	6:G:143:GLU:HG3	1.91	0.51
13:N:29:ARG:HD2	13:N:74:PHE:HD2	1.76	0.51
34:l:315:VAL:O	34:l:319:ILE:HG13	2.11	0.51
34:l:549:PRO:HB3	39:r:271:MET:HE3	1.92	0.51
8:I:60:ARG:HD2	15:P:242:PHE:HE1	1.75	0.51
3:C:128:ASN:HB3	15:P:210:LEU:HD21	1.92	0.51
8:I:40:LYS:HB3	21:W:7:LYS:HG2	1.92	0.51
26:c:154:GLN:HB2	26:c:156:VAL:HG22	1.92	0.51
27:d:94:GLN:HB3	34:l:73:THR:HB	1.92	0.51
32:j:111:LEU:HD13	40:s:290:TRP:HB3	1.92	0.51
33:k:1:MET:HE2	35:m:46:PHE:CE2	2.46	0.51
36:n:50:GLN:HG3	36:n:51:PRO:HD2	1.93	0.51
39:r:122:PHE:O	39:r:125:THR:OG1	2.26	0.51
44:i:193:VAL:HG23	44:i:201:THR:HG22	1.93	0.51
5:F:20:ARG:HG2	5:F:66:TRP:HB2	1.91	0.51
9:J:217:PHE:HA	9:J:220:MET:HG2	1.91	0.51
16:Q:82:LEU:HD12	16:Q:101:LEU:HD21	1.93	0.51
16:Q:191:ALA:HB1	16:Q:196:ALA:HB3	1.92	0.51
16:Q:251:PHE:CE1	16:Q:255:LEU:HG	2.46	0.51
16:Q:301:ASP:O	16:Q:305:THR:OG1	2.24	0.51
19:U:68:SER:HA	41:u:130:LYS:HB2	1.92	0.51
39:r:52:CYS:HB2	39:r:57:SER:HA	1.93	0.51
16:Q:446:ASP:OD1	40:s:281:ARG:NH1	2.44	0.51
31:h:49:TYR:CZ	44:i:89:THR:HB	2.45	0.51
35:m:26:ILE:HD11	40:s:70:LEU:HD11	1.91	0.51
3:C:81:PRO:HA	3:C:119:VAL:HG13	1.93	0.51
16:Q:83:ASN:C	16:Q:85:GLY:H	2.17	0.51
6:X:132:ASP:OD2	38:p:18:ARG:NE	2.43	0.51
24:a:136:THR:HG21	39:r:50:PHE:HD1	1.76	0.51
1:A:192:ASP:N	1:A:192:ASP:OD1	2.43	0.51
11:L:130:THR:OG1	11:L:133:ASP:OD2	2.22	0.51
12:M:81:GLU:HB3	12:M:88:VAL:HG12	1.92	0.51
14:O:67:VAL:HG13	14:O:75:LYS:HD2	1.93	0.51
24:a:82:VAL:HG11	28:e:104:THR:HG21	1.93	0.51
35:m:1:MET:HA	35:m:122:GLY:H	1.75	0.51
2:B:86:PHE:CZ	13:N:30:THR:HA	2.46	0.51
6:G:99:SER:HB3	6:G:102:SER:HB3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:540:ASN:O	12:M:540:ASN:ND2	2.43	0.51
21:W:32:GLY:H	21:W:35:MET:HE3	1.76	0.51
34:l:522:PHE:HA	34:l:528:PHE:CE2	2.45	0.51
40:s:105:ILE:HG21	40:s:237:LEU:HD11	1.92	0.51
1:A:338:ASP:OD1	1:A:338:ASP:N	2.42	0.51
8:I:48:LYS:HG3	8:I:52:ASN:HB2	1.93	0.51
31:h:95:PRO:HD2	31:h:98:HIS:HB2	1.92	0.51
40:s:236:THR:HG22	40:s:263:THR:HG21	1.92	0.51
2:B:145:ILE:HG22	2:B:188:LEU:HD11	1.92	0.50
7:H:111:GLN:NE2	15:P:124:ASN:O	2.43	0.50
12:M:387:LEU:HD12	12:M:514:ASN:HB2	1.93	0.50
34:l:81:LYS:HB2	34:l:135:ASN:HB2	1.93	0.50
4:E:98:LYS:HE2	4:E:102:HIS:HB3	1.92	0.50
7:H:68:LEU:HD23	7:H:77:LEU:HD11	1.92	0.50
39:r:138:ASN:ND2	39:r:141:GLU:OE1	2.44	0.50
1:A:126:LYS:NZ	1:A:246:GLU:HG3	2.26	0.50
4:E:89:GLU:OE2	15:P:186:ARG:NH2	2.43	0.50
12:M:126:LEU:HD11	16:Q:375:MET:HA	1.94	0.50
14:O:95:ILE:O	14:O:99:ASN:ND2	2.44	0.50
19:U:58:ARG:NH1	41:u:135:ARG:O	2.37	0.50
22:Y:49:GLN:OE1	22:Y:49:GLN:N	2.42	0.50
24:a:130:GLU:OE2	27:d:60:ARG:NH2	2.44	0.50
32:j:51:PHE:HE2	35:m:74:ALA:HB2	1.75	0.50
2:B:57:ARG:HA	2:B:62:THR:HG23	1.94	0.50
2:B:144:ASP:OD1	2:B:144:ASP:N	2.45	0.50
12:M:281:ILE:HD11	12:M:602:ARG:HD2	1.93	0.50
13:N:74:PHE:HD1	13:N:74:PHE:H	1.57	0.50
14:O:58:GLU:O	14:O:62:ARG:HG3	2.11	0.50
16:Q:334:VAL:HA	16:Q:337:MET:HE3	1.92	0.50
24:a:97:GLU:OE1	27:d:54:ARG:NH2	2.44	0.50
24:a:136:THR:HG21	39:r:50:PHE:HA	1.93	0.50
26:c:155:PRO:HB3	42:v:5:LEU:HD13	1.92	0.50
33:k:9:MET:HG2	44:i:72:MET:HE1	1.93	0.50
16:Q:161:ILE:HD11	16:Q:363:VAL:HG21	1.94	0.50
40:s:307:MET:N	40:s:308:PRO:HD2	2.26	0.50
7:H:35:LEU:HD22	7:H:48:THR:HG23	1.93	0.50
9:J:67:ARG:NH1	9:J:210:GLU:OE2	2.44	0.50
16:Q:319:PRO:HG3	16:Q:336:GLU:HG3	1.92	0.50
21:W:137:SER:HB2	35:m:126:ILE:HG12	1.92	0.50
41:u:77:HIS:HB3	41:u:114:LYS:HE3	1.94	0.50
9:J:67:ARG:NE	15:P:214:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:210:ILE:HG13	14:O:95:ILE:HD12	1.93	0.50
14:O:60:TYR:O	14:O:63:ILE:HG13	2.12	0.50
14:O:70:TYR:O	14:O:75:LYS:NZ	2.44	0.50
27:d:98:ASN:HD21	34:l:74:THR:HA	1.76	0.50
34:l:368:LEU:HD13	34:l:451:LEU:HD22	1.94	0.50
39:r:373:ILE:HG23	39:r:448:SER:HA	1.93	0.50
9:J:354:ARG:HG2	9:J:362:LEU:HD12	1.94	0.50
11:L:106:ARG:HG2	11:L:117:THR:HG22	1.94	0.50
12:M:483:ARG:O	12:M:485:ASP:N	2.44	0.50
24:a:134:GLU:OE1	36:n:57:TRP:NE1	2.27	0.50
44:i:211:LEU:HD23	44:i:333:THR:HG22	1.94	0.50
1:A:211:ALA:HB2	1:A:223:PRO:HG3	1.93	0.50
3:C:97:ALA:HA	3:C:103:MET:HG2	1.94	0.50
12:M:512:VAL:O	12:M:514:ASN:ND2	2.44	0.50
15:P:61:PHE:O	15:P:65:VAL:HG23	2.12	0.50
18:T:68:ALA:O	18:T:72:ILE:HG12	2.11	0.50
27:d:80:TYR:HE1	39:r:49:LEU:HB3	1.77	0.50
33:k:37:MET:HE2	33:k:64:LEU:HA	1.94	0.50
33:k:37:MET:HE3	33:k:41:PHE:HB2	1.92	0.50
1:A:225:LEU:HG	1:A:227:PRO:HD3	1.94	0.49
3:C:80:TRP:HB3	3:C:111:ARG:HB2	1.93	0.49
26:c:101:TRP:CD1	37:o:62:ASN:HD22	2.28	0.49
39:r:94:LEU:O	39:r:98:MET:HG2	2.10	0.49
7:H:39:PRO:HG2	7:H:99:LEU:HD23	1.93	0.49
34:l:558:LEU:HD23	39:r:214:LEU:HD21	1.94	0.49
2:B:72:LEU:HB2	40:s:272:TRP:CZ2	2.47	0.49
16:Q:139:LEU:HD11	16:Q:424:ILE:HD13	1.95	0.49
16:Q:196:ALA:O	16:Q:198:THR:N	2.42	0.49
16:Q:198:THR:HA	40:s:32:GLN:OE1	2.11	0.49
16:Q:315:GLU:HB2	16:Q:346:GLN:HE22	1.78	0.49
25:b:16:ARG:O	25:b:20:ARG:HG2	2.12	0.49
25:b:54:LYS:HD2	25:b:58:ARG:HE	1.77	0.49
26:c:154:GLN:NE2	34:l:400:ASN:O	2.45	0.49
27:d:72:LYS:HB2	27:d:75:ASP:HB2	1.94	0.49
38:p:31:CYS:O	38:p:33:GLN:N	2.44	0.49
39:r:205:VAL:HG22	39:r:212:LEU:HD13	1.94	0.49
39:r:343:ILE:O	39:r:346:GLN:HG2	2.12	0.49
4:E:101:THR:O	4:E:105:ARG:HG3	2.12	0.49
12:M:68:ARG:NH1	12:M:284:GLU:OE1	2.45	0.49
12:M:394:VAL:HG11	12:M:418:ILE:HG12	1.94	0.49
16:Q:316:PHE:HB2	16:Q:339:GLN:HE21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:138:HIS:HB3	21:W:142:TRP:HD1	1.76	0.49
24:a:184:LYS:O	24:a:186:THR:N	2.46	0.49
34:l:53:MET:O	34:l:57:LEU:N	2.35	0.49
15:P:85:GLU:OE2	15:P:142:ARG:NH1	2.45	0.49
16:Q:102:SER:HB3	16:Q:107:ARG:HE	1.78	0.49
24:a:140:LEU:HD21	39:r:177:LEU:HB3	1.93	0.49
33:k:75:LEU:HD21	35:m:67:PHE:HD1	1.77	0.49
34:l:341:MET:HE2	34:l:457:LEU:HD12	1.93	0.49
5:F:25:GLN:NE2	12:M:655:ARG:HH12	2.11	0.49
9:J:219:SER:HA	9:J:222:ARG:HB2	1.94	0.49
9:J:279:TYR:O	9:J:283:VAL:HG22	2.13	0.49
11:L:120:PRO:HG2	11:L:121:LEU:HD12	1.93	0.49
34:l:366:MET:HG3	34:l:443:ILE:HG22	1.94	0.49
34:l:517:LEU:HD23	34:l:517:LEU:H	1.78	0.49
1:A:414:GLU:HB3	12:M:152:ARG:HH12	1.77	0.49
4:E:80:ASP:HA	4:E:83:VAL:HG22	1.93	0.49
12:M:58:MET:HE2	12:M:104:THR:HB	1.95	0.49
12:M:343:GLY:HA3	12:M:548:LEU:HB2	1.95	0.49
12:M:365:THR:HA	12:M:531:LYS:HD2	1.94	0.49
26:c:78:LEU:HB2	26:c:106:HIS:HD2	1.78	0.49
27:d:101:GLN:HE22	34:l:194:ASN:HD22	1.60	0.49
28:e:111:ASP:N	28:e:111:ASP:OD1	2.45	0.49
30:g:106:LYS:HB3	30:g:110:GLU:HB2	1.94	0.49
38:p:143:GLU:OE1	38:p:158:ARG:NH2	2.46	0.49
1:A:111:LYS:HG2	1:A:239:PRO:HB2	1.94	0.49
1:A:244:ASN:O	1:A:248:VAL:HG12	2.12	0.49
4:E:44:PRO:HG3	4:E:56:VAL:HG11	1.95	0.49
15:P:86:VAL:HB	15:P:143:VAL:HG12	1.94	0.49
16:Q:355:GLU:HG2	16:Q:357:LYS:H	1.77	0.49
27:d:79:MET:SD	30:g:108:TYR:OH	2.68	0.49
38:p:104:LEU:HB2	38:p:122:ARG:NH1	2.28	0.49
40:s:13:ILE:O	40:s:17:MET:HG2	2.12	0.49
40:s:172:LEU:HD21	40:s:176:LEU:HD12	1.94	0.49
1:A:99:TRP:HA	1:A:149:MET:HE1	1.95	0.49
3:C:141:MET:O	3:C:145:ARG:NH1	2.46	0.49
9:J:174:ILE:HG13	9:J:182:ARG:HD3	1.95	0.49
38:p:101:GLU:OE1	38:p:122:ARG:NH2	2.46	0.49
3:C:90:ALA:HB1	16:Q:91:ALA:HB1	1.94	0.49
12:M:278:HIS:N	12:M:282:ASN:OD1	2.46	0.49
12:M:382:ARG:HA	12:M:385:TYR:CZ	2.48	0.49
6:X:110:LEU:HB3	6:X:114:ASP:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:a:129:PRO:HG2	27:d:60:ARG:HH22	1.78	0.49
30:g:45:ASN:HD21	30:g:60:GLN:HE21	1.60	0.49
34:l:25:ASN:OD1	34:l:25:ASN:N	2.46	0.49
39:r:116:ILE:HG13	41:u:168:TYR:CE2	2.48	0.49
1:A:121:GLU:HG2	1:A:321:GLY:O	2.13	0.48
3:C:126:LEU:HD13	3:C:134:LEU:HD13	1.95	0.48
12:M:585:PRO:HB2	12:M:616:ALA:HB2	1.95	0.48
12:M:602:ARG:HB2	12:M:659:ILE:HG23	1.93	0.48
13:N:13:GLN:HB3	13:N:35:VAL:HG22	1.93	0.48
13:N:64:TYR:O	13:N:65:THR:OG1	2.30	0.48
16:Q:399:ALA:HB1	16:Q:406:GLU:HG3	1.95	0.48
32:j:66:ASP:O	32:j:69:ILE:HG22	2.13	0.48
1:A:208:GLU:OE1	1:A:210:THR:N	2.45	0.48
1:A:378:SER:O	12:M:201:GLY:N	2.46	0.48
3:C:95:HIS:HD1	16:Q:208:GLU:HG3	1.77	0.48
9:J:145:PHE:CZ	9:J:184:LYS:HE3	2.48	0.48
25:b:88:TYR:CE1	27:d:43:ARG:HG2	2.49	0.48
26:c:78:LEU:HB2	26:c:106:HIS:CD2	2.48	0.48
26:c:156:VAL:HG12	42:v:98:ARG:HD2	1.95	0.48
1:A:219:LYS:HB3	11:L:174:THR:HG22	1.95	0.48
2:B:113:ALA:O	2:B:115:LYS:NZ	2.46	0.48
9:J:316:ARG:O	9:J:320:GLU:HG2	2.12	0.48
25:b:83:HIS:HE1	25:b:87:LYS:HE3	1.79	0.48
34:l:213:LEU:HB3	34:l:273:ILE:HG12	1.95	0.48
34:l:383:MET:HB3	34:l:386:LEU:HD11	1.94	0.48
40:s:187:ILE:HG23	40:s:198:PHE:CZ	2.48	0.48
2:B:108:GLU:HB2	18:T:72:ILE:HG23	1.95	0.48
9:J:106:LEU:HD12	9:J:119:VAL:HG23	1.95	0.48
11:L:109:ASN:ND2	11:L:111:LEU:O	2.40	0.48
12:M:587:ALA:HB2	12:M:612:PRO:HG3	1.95	0.48
25:b:46:PHE:O	25:b:49:LYS:HG2	2.14	0.48
34:l:239:GLY:H	34:l:240:PRO:HD2	1.77	0.48
44:i:268:GLU:O	44:i:271:THR:OG1	2.29	0.48
12:M:557:ARG:NH1	13:N:144:TYR:O	2.47	0.48
14:O:198:ALA:O	14:O:202:GLU:HG2	2.13	0.48
44:i:172:GLN:OE1	44:i:172:GLN:N	2.47	0.48
1:A:317:VAL:O	1:A:327:ILE:N	2.46	0.48
2:B:158:GLU:O	16:Q:368:ARG:NH1	2.46	0.48
5:F:48:ASN:OD1	5:F:48:ASN:N	2.45	0.48
9:J:195:PHE:CE2	9:J:197:GLU:HG2	2.48	0.48
12:M:209:TYR:H	14:O:110:MET:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:591:GLU:N	12:M:591:GLU:OE1	2.46	0.48
17:S:69:ILE:O	41:u:75:LYS:NZ	2.46	0.48
34:l:548:LEU:HB2	34:l:549:PRO:HD3	1.95	0.48
35:m:121:VAL:HG12	35:m:123:SER:H	1.77	0.48
39:r:82:ARG:HH11	39:r:82:ARG:HA	1.77	0.48
39:r:138:ASN:HD22	39:r:140:PRO:HD2	1.77	0.48
39:r:303:ILE:HG22	39:r:305:THR:HG23	1.95	0.48
44:i:190:MET:HE3	44:i:205:LEU:HB2	1.95	0.48
34:l:172:ILE:HG21	39:r:408:LEU:HD12	1.95	0.48
2:B:84:TYR:CD1	2:B:85:PRO:HA	2.48	0.48
2:B:118:GLU:OE2	2:B:128:ILE:N	2.33	0.48
9:J:82:ILE:HD12	9:J:105:PHE:HE1	1.79	0.48
10:K:85:LEU:HD22	14:O:66:ILE:HD11	1.96	0.48
18:T:52:ARG:O	18:T:55:ARG:HG2	2.14	0.48
39:r:53:SER:HB2	39:r:54:PRO:HD2	1.96	0.48
39:r:73:LEU:HD12	39:r:103:GLN:HG2	1.95	0.48
39:r:386:PHE:HD1	39:r:393:LEU:HB2	1.79	0.48
2:B:107:GLY:HA3	18:T:71:LEU:HD23	1.96	0.48
3:C:95:HIS:ND1	16:Q:208:GLU:HG3	2.28	0.48
14:O:201:ILE:HG13	14:O:201:ILE:H	1.41	0.48
16:Q:174:PHE:CZ	16:Q:217:VAL:HG11	2.44	0.48
21:W:101:VAL:HG21	21:W:104:TRP:HB3	1.95	0.48
25:b:100:LYS:HD3	34:l:60:GLU:HB2	1.96	0.48
27:d:67:ASP:OD1	27:d:67:ASP:N	2.46	0.48
40:s:128:ALA:HB2	40:s:208:VAL:HG11	1.94	0.48
3:C:102:ASP:OD1	40:s:34:ARG:NH2	2.46	0.48
7:H:74:GLY:HA2	15:P:136:ARG:HE	1.79	0.48
9:J:180:TYR:HD1	9:J:181:LEU:HD12	1.78	0.48
19:U:58:ARG:NH2	41:u:49:GLU:OE1	2.43	0.48
27:d:127:THR:HG22	37:o:125:PHE:HZ	1.79	0.48
2:B:61:TRP:CH2	40:s:183:MET:HB3	2.48	0.47
3:C:79:LEU:O	3:C:108:VAL:HA	2.14	0.47
6:G:92:LYS:HB3	6:G:92:LYS:HZ2	1.78	0.47
7:H:112:TRP:CZ2	15:P:144:LYS:HB2	2.49	0.47
14:O:93:LEU:HD12	14:O:122:TYR:HB3	1.96	0.47
16:Q:329:ARG:HD2	16:Q:453:THR:CG2	2.43	0.47
18:T:83:ARG:NH1	18:T:102:ASN:OD1	2.46	0.47
22:Y:51:THR:HG21	34:l:446:ASN:OD1	2.14	0.47
33:k:3:LEU:HB2	35:m:117:ASN:HD21	1.78	0.47
9:J:209:ARG:NH2	9:J:351:GLU:OE1	2.47	0.47
11:L:69:GLU:HA	11:L:72:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:620:TRP:HZ3	12:M:624:ARG:HD2	1.79	0.47
15:P:133:LEU:HD22	15:P:140:ARG:HG2	1.96	0.47
27:d:109:GLN:HE22	34:l:199:GLN:CD	2.22	0.47
34:l:100:ILE:HD11	34:l:246:LEU:HG	1.96	0.47
34:l:156:SER:HA	34:l:164:ALA:HB1	1.95	0.47
34:l:516:PRO:HG2	34:l:520:PHE:HB2	1.95	0.47
39:r:136:TRP:HE3	39:r:138:ASN:HB2	1.79	0.47
40:s:17:MET:HG3	40:s:229:THR:HG23	1.95	0.47
1:A:279:SER:HB2	14:O:181:VAL:HA	1.95	0.47
1:A:446:LEU:O	1:A:450:MET:HG2	2.14	0.47
14:O:207:GLU:HB3	14:O:213:ILE:HG13	1.96	0.47
20:V:66:VAL:HG21	20:V:101:LEU:HD12	1.95	0.47
25:b:29:SER:OG	38:p:117:ASP:OD2	2.22	0.47
28:e:106:VAL:HA	28:e:109:LEU:HG	1.96	0.47
39:r:425:ASN:O	39:r:425:ASN:ND2	2.38	0.47
40:s:235:ASN:O	40:s:238:THR:OG1	2.25	0.47
40:s:273:ILE:HG23	40:s:277:TYR:CD2	2.49	0.47
40:s:280:PHE:O	40:s:281:ARG:HB3	2.13	0.47
7:H:59:VAL:HA	7:H:68:LEU:HD11	1.95	0.47
12:M:367:CYS:HB3	12:M:531:LYS:HB2	1.95	0.47
16:Q:357:LYS:HE3	16:Q:364:SER:HB2	1.95	0.47
20:V:89:ASN:N	20:V:89:ASN:OD1	2.47	0.47
34:l:184:LEU:HB2	39:r:393:LEU:HD21	1.95	0.47
39:r:63:THR:OG1	39:r:64:PRO:HD3	2.15	0.47
39:r:178:LEU:O	39:r:182:THR:OG1	2.30	0.47
2:B:78:GLU:HB3	8:I:26:LEU:HD11	1.97	0.47
9:J:111:ARG:NH1	9:J:148:ILE:HD11	2.24	0.47
15:P:73:VAL:HA	15:P:87:CYS:O	2.14	0.47
15:P:115:THR:OG1	15:P:116:ALA:N	2.47	0.47
15:P:181:HIS:ND1	15:P:183:ASP:O	2.47	0.47
21:W:138:HIS:HB3	21:W:142:TRP:CD1	2.49	0.47
34:l:367:PRO:O	34:l:370:SER:OG	2.27	0.47
39:r:68:LEU:HD22	39:r:317:ILE:HD13	1.96	0.47
41:u:23:ALA:HB1	41:u:90:ASP:OD1	2.14	0.47
8:I:46:SER:O	12:M:150:ARG:NH1	2.47	0.47
12:M:36:VAL:HG12	12:M:37:ASP:H	1.79	0.47
12:M:126:LEU:HD12	16:Q:378:LEU:HD22	1.96	0.47
12:M:483:ARG:O	12:M:484:ASN:C	2.58	0.47
16:Q:371:MET:HE3	16:Q:371:MET:HB2	1.72	0.47
39:r:42:PHE:HB3	39:r:63:THR:HG22	1.97	0.47
9:J:64:PHE:HE2	9:J:242:VAL:HG21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:J:66:GLY:HA2	9:J:69:VAL:HG22	1.97	0.47
9:J:132:ARG:NH2	48:J:401:NDP:O1X	2.45	0.47
11:L:62:THR:OG1	11:L:141:ASN:O	2.31	0.47
12:M:198:THR:HG21	12:M:209:TYR:HB2	1.96	0.47
15:P:147:THR:HG21	15:P:153:ILE:HB	1.97	0.47
15:P:165:TRP:CZ2	16:Q:111:PRO:HG2	2.49	0.47
16:Q:432:LEU:O	16:Q:435:LEU:HB3	2.15	0.47
19:U:33:PRO:HA	40:s:310:THR:HG22	1.97	0.47
25:b:87:LYS:O	25:b:91:SER:OG	2.32	0.47
33:k:40:LEU:HD12	44:i:68:MET:HE3	1.97	0.47
33:k:58:ILE:O	33:k:59:VAL:C	2.58	0.47
34:l:342:CYS:SG	34:l:372:SER:OG	2.64	0.47
37:o:28:GLU:HA	37:o:31:ARG:HD3	1.97	0.47
38:p:30:TRP:NE1	38:p:76:HIS:HB2	2.30	0.47
40:s:185:TRP:CD1	40:s:238:THR:HG22	2.49	0.47
2:B:182:LEU:HD23	11:L:112:MET:HG3	1.97	0.47
4:E:48:HIS:CE1	9:J:363:SER:HB2	2.50	0.47
5:F:23:LEU:HG	5:F:24:CYS:O	2.15	0.47
13:N:71:LYS:HG2	13:N:72:ASN:H	1.79	0.47
14:O:182:ASN:OD1	14:O:222:ARG:NH2	2.47	0.47
15:P:130:TYR:HB2	15:P:143:VAL:HG23	1.97	0.47
16:Q:329:ARG:HD2	16:Q:453:THR:HG22	1.96	0.47
16:Q:457:VAL:O	16:Q:460:GLU:HG2	2.15	0.47
31:h:37:GLU:HB2	31:h:63:PHE:CE1	2.50	0.47
38:p:136:GLU:HG2	38:p:165:PRO:HA	1.97	0.47
39:r:91:ARG:O	39:r:135:ARG:NH2	2.44	0.47
40:s:233:MET:HE3	40:s:233:MET:HB3	1.69	0.47
1:A:325:PRO:HB3	1:A:437:GLY:HA3	1.97	0.47
12:M:355:LYS:HD2	12:M:530:TYR:CE1	2.50	0.47
14:O:133:GLN:O	14:O:187:GLN:N	2.44	0.47
35:m:166:ILE:O	35:m:170:ILE:HG12	2.15	0.47
6:G:88:LYS:HE3	6:G:98:LEU:HD13	1.96	0.47
6:G:106:LYS:HD2	6:G:107:ASP:H	1.80	0.47
6:G:137:LYS:HG3	6:G:144:ILE:HG23	1.97	0.47
13:N:29:ARG:HH12	13:N:65:THR:HA	1.80	0.47
44:i:271:THR:HG22	44:i:276:LEU:HD21	1.95	0.47
3:C:180:ILE:HD13	3:C:190:LEU:HA	1.96	0.46
5:F:37:ILE:HA	5:F:41:TYR:HB2	1.96	0.46
18:T:102:ASN:HD21	18:T:104:ASP:HB2	1.80	0.46
26:c:136:PHE:O	26:c:140:MET:HG2	2.15	0.46
34:l:226:GLN:HG3	34:l:284:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:THR:N	8:I:105:GLU:O	2.48	0.46
9:J:272:LEU:HB3	9:J:275:HIS:HD2	1.81	0.46
12:M:128:CYS:N	12:M:129:PRO:HD2	2.30	0.46
15:P:108:PHE:HB3	15:P:132:LEU:HB3	1.97	0.46
31:h:95:PRO:HG2	31:h:98:HIS:ND1	2.31	0.46
33:k:27:MET:HG2	33:k:78:LEU:HD11	1.97	0.46
33:k:47:MET:HE2	44:i:79:MET:HB2	1.97	0.46
34:l:68:TRP:NE1	34:l:78:LEU:HB3	2.30	0.46
34:l:314:MET:HE3	34:l:314:MET:HB2	1.76	0.46
39:r:209:LEU:HD13	39:r:264:LEU:HD11	1.97	0.46
39:r:433:GLU:O	39:r:437:MET:HG2	2.16	0.46
42:v:56:ARG:O	42:v:60:ALA:HB2	2.15	0.46
1:A:205:ILE:HG12	1:A:379:CYS:HB3	1.97	0.46
1:A:382:CYS:HB2	1:A:384:PRO:HD2	1.97	0.46
6:G:115:GLN:O	6:G:118:ILE:HG13	2.15	0.46
8:I:35:THR:HG23	13:N:95:ASP:H	1.79	0.46
12:M:473:MET:HG3	12:M:514:ASN:HD21	1.79	0.46
15:P:154:GLU:HA	15:P:179:ALA:HB3	1.96	0.46
15:P:181:HIS:CD2	15:P:182:PRO:HD2	2.50	0.46
20:V:62:THR:HG22	20:V:104:ARG:HE	1.80	0.46
31:h:51:ARG:NH1	31:h:55:GLU:OE2	2.49	0.46
34:l:138:PHE:O	34:l:142:ILE:HG13	2.16	0.46
39:r:209:LEU:O	39:r:213:HIS:HB3	2.15	0.46
7:H:36:GLU:HA	7:H:45:ARG:HH21	1.80	0.46
15:P:135:LEU:HD22	16:Q:300:TRP:CD2	2.51	0.46
18:T:40:THR:OG1	18:T:42:THR:O	2.33	0.46
26:c:169:GLU:OE2	42:v:56:ARG:NH2	2.47	0.46
26:c:173:ASP:N	26:c:173:ASP:OD1	2.46	0.46
1:A:73:PRO:HD3	1:A:147:ARG:NH2	2.31	0.46
1:A:227:PRO:HB3	12:M:95:PRO:HD2	1.98	0.46
2:B:144:ASP:OD2	11:L:114:TRP:NE1	2.47	0.46
3:C:126:LEU:HD23	3:C:173:ILE:HD13	1.97	0.46
9:J:358:THR:O	9:J:362:LEU:N	2.49	0.46
11:L:78:ARG:HD3	12:M:607:LYS:NZ	2.30	0.46
30:g:6:ASN:OD1	30:g:6:ASN:N	2.48	0.46
32:j:77:TRP:HB3	35:m:140:ILE:HD13	1.97	0.46
34:l:306:THR:O	34:l:310:LEU:HG	2.16	0.46
37:o:108:GLU:OE2	39:r:390:ASN:N	2.48	0.46
44:i:106:LEU:HD21	44:i:138:PRO:HB2	1.97	0.46
2:B:129:GLU:HG2	12:M:266:ARG:HH22	1.81	0.46
4:E:87:LYS:O	4:E:91:GLU:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:18:GLU:HB3	5:F:68:ARG:HB3	1.97	0.46
5:F:68:ARG:HH11	12:M:359:ASN:HD21	1.63	0.46
8:I:12:ARG:HH22	8:I:21:GLN:HE21	1.63	0.46
9:J:117:ARG:HG2	9:J:155:LEU:HD13	1.97	0.46
16:Q:142:VAL:O	16:Q:144:MET:HE2	2.15	0.46
27:d:134:GLN:OE1	37:o:124:THR:HA	2.15	0.46
28:e:89:LEU:HD13	39:r:29:THR:HG21	1.98	0.46
39:r:192:ASN:HB3	39:r:253:LEU:HD11	1.97	0.46
39:r:452:ASP:O	39:r:455:THR:OG1	2.29	0.46
40:s:76:THR:O	40:s:80:THR:HG23	2.15	0.46
40:s:267:THR:O	40:s:271:LEU:HG	2.16	0.46
44:i:261:LEU:HD11	44:i:340:SER:HA	1.98	0.46
1:A:119:GLU:H	46:A:502:FMN:HM71	1.80	0.46
2:B:75:LEU:HB2	40:s:31:MET:SD	2.56	0.46
2:B:142:ARG:NH2	2:B:144:ASP:OD2	2.49	0.46
3:C:88:CYS:HG	45:C:301:SF4:FE3	1.28	0.46
20:V:81:ARG:HD3	20:V:83:LYS:HE2	1.98	0.46
21:W:43:LEU:HG	40:s:179:TRP:NE1	2.31	0.46
35:m:111:GLY:HA2	35:m:116:VAL:HA	1.97	0.46
44:i:96:LEU:HD22	44:i:153:LEU:HD13	1.96	0.46
44:i:250:SER:O	44:i:259:GLY:HA3	2.16	0.46
8:I:12:ARG:HG2	8:I:20:LEU:HD12	1.96	0.46
14:O:110:MET:O	14:O:114:GLU:HG3	2.15	0.46
16:Q:101:LEU:HA	16:Q:107:ARG:H	1.80	0.46
19:U:33:PRO:HB2	19:U:34:PRO:HD3	1.97	0.46
6:X:120:MET:HE1	38:p:24:LEU:HB2	1.98	0.46
29:f:43:LYS:HA	29:f:46:PHE:HD1	1.81	0.46
31:h:74:ARG:NH1	35:m:111:GLY:O	2.46	0.46
35:m:50:TYR:HB3	35:m:138:ASP:HB3	1.97	0.46
39:r:67:MET:HE1	39:r:453:ILE:HD11	1.98	0.46
39:r:150:LEU:HD23	44:i:291:TYR:HB2	1.98	0.46
1:A:307:VAL:HG11	1:A:314:LEU:HG	1.98	0.46
11:L:75:ARG:HH11	11:L:121:LEU:HB2	1.81	0.46
12:M:708:ALA:O	12:M:711:VAL:HG12	2.16	0.46
23:Z:36:LEU:HD11	38:p:39:TYR:HA	1.97	0.46
25:b:42:PRO:HA	25:b:45:LYS:HB2	1.98	0.46
25:b:58:ARG:HA	25:b:61:VAL:HG22	1.98	0.46
26:c:110:ASP:OD1	26:c:110:ASP:N	2.49	0.46
30:g:16:GLU:HB3	41:u:158:LEU:HD12	1.97	0.46
33:k:33:LEU:HD11	44:i:64:ALA:HB1	1.98	0.46
38:p:20:TYR:CZ	38:p:24:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:r:106:LEU:O	39:r:109:THR:OG1	2.31	0.46
1:A:347:THR:HG22	1:A:348:GLY:H	1.80	0.46
3:C:160:TYR:HE1	16:Q:120:THR:HG22	1.81	0.46
4:E:122:PHE:HD1	12:M:621:LYS:HG2	1.81	0.46
12:M:80:VAL:HG22	12:M:91:ALA:HB2	1.98	0.46
14:O:39:PHE:HD1	14:O:124:ARG:HH22	1.64	0.46
15:P:165:TRP:HZ2	16:Q:111:PRO:HG2	1.81	0.46
21:W:73:PRO:HG3	41:u:40:ASN:HB3	1.98	0.46
6:X:132:ASP:HA	6:X:135:ALA:HB3	1.97	0.46
22:Y:85:PRO:O	22:Y:86:TYR:HB2	2.17	0.46
25:b:51:LEU:HD23	25:b:58:ARG:HG3	1.97	0.46
33:k:1:MET:HE2	35:m:46:PHE:HE2	1.81	0.46
33:k:35:GLY:HA3	35:m:19:PHE:HZ	1.81	0.46
34:l:341:MET:CE	34:l:457:LEU:HD12	2.47	0.46
44:i:139:ILE:HG21	44:i:205:LEU:HD22	1.98	0.46
44:i:323:THR:HB	44:i:326:LEU:HD12	1.98	0.46
1:A:62:TRP:HE3	1:A:65:THR:HG21	1.81	0.45
2:B:118:GLU:HG3	2:B:128:ILE:HD12	1.98	0.45
12:M:144:MET:HG3	16:Q:383:LYS:HG3	1.98	0.45
12:M:598:ASN:OD1	12:M:599:THR:N	2.47	0.45
15:P:243:PRO:HB3	15:P:246:ARG:HH21	1.80	0.45
16:Q:180:LEU:HD23	16:Q:337:MET:HG2	1.97	0.45
16:Q:432:LEU:HG	16:Q:456:ILE:HD13	1.97	0.45
34:l:357:ARG:HG2	38:p:32:VAL:HG22	1.98	0.45
1:A:379:CYS:SG	1:A:381:GLN:HG2	2.56	0.45
4:E:110:THR:O	9:J:75:ARG:NH1	2.49	0.45
8:I:96:THR:OG1	8:I:98:ALA:O	2.27	0.45
9:J:81:ILE:HD13	18:T:54:ILE:HG12	1.97	0.45
9:J:206:ILE:HA	9:J:240:VAL:O	2.16	0.45
9:J:212:ARG:O	9:J:216:SER:CB	2.64	0.45
12:M:177:ILE:HG13	12:M:179:CYS:HB3	1.97	0.45
14:O:123:ASN:OD1	14:O:123:ASN:N	2.49	0.45
15:P:149:GLU:H	15:P:149:GLU:HG2	1.54	0.45
16:Q:372:LYS:HA	18:T:97:PRO:HA	1.98	0.45
25:b:107:GLY:H	25:b:115:GLU:HB2	1.80	0.45
27:d:93:ASP:OD2	27:d:136:ARG:NH1	2.49	0.45
40:s:184:MET:HE1	40:s:293:PHE:HA	1.98	0.45
1:A:132:ARG:HA	1:A:165:GLU:OE1	2.16	0.45
8:I:71:SER:HA	15:P:75:GLN:HG2	1.99	0.45
9:J:89:TYR:HA	9:J:92:MET:HE2	1.97	0.45
12:M:401:LEU:HD22	12:M:462:PHE:HE2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:M:405:THR:HA	12:M:686:PRO:HB3	1.98	0.45
15:P:167:GLU:HG2	15:P:184:LEU:HD21	1.99	0.45
15:P:237:SER:HB3	16:Q:387:GLU:OE1	2.15	0.45
16:Q:95:LEU:HB2	16:Q:458:PHE:CZ	2.51	0.45
16:Q:159:LEU:HG	16:Q:391:VAL:HG22	1.97	0.45
27:d:140:LEU:HD22	27:d:148:LYS:HB3	1.99	0.45
34:l:555:LEU:H	34:l:555:LEU:HD23	1.81	0.45
35:m:166:ILE:HG22	44:i:42:PRO:HG2	1.99	0.45
39:r:156:GLY:HA3	39:r:202:ALA:HA	1.98	0.45
9:J:359:TYR:HB2	40:s:65:THR:HB	1.99	0.45
12:M:188:GLU:O	12:M:419:ARG:NE	2.39	0.45
16:Q:83:ASN:C	16:Q:85:GLY:N	2.74	0.45
16:Q:87:GLN:O	16:Q:88:HIS:C	2.60	0.45
23:Z:29:LEU:HD21	23:Z:49:GLU:HB3	1.99	0.45
26:c:44:THR:HB	26:c:47:GLU:HB2	1.98	0.45
27:d:21:PRO:HD2	42:v:74:PHE:CZ	2.51	0.45
30:g:51:PRO:HB2	30:g:54:THR:OG1	2.16	0.45
38:p:34:ARG:HD3	38:p:37:TYR:HD2	1.80	0.45
4:E:50:PHE:HB2	4:E:52:LEU:HD12	1.97	0.45
5:F:57:GLU:HG2	12:M:662:ALA:HB3	1.98	0.45
12:M:372:PHE:HD1	12:M:481:LEU:HD13	1.80	0.45
22:Y:58:SER:HB2	34:l:371:THR:HG21	1.98	0.45
23:Z:57:PHE:CG	34:l:435:PRO:HG3	2.51	0.45
24:a:179:ILE:HD13	31:h:38:LYS:HG3	1.98	0.45
26:c:38:PRO:HD2	37:o:70:TYR:CD2	2.51	0.45
44:i:18:LEU:O	44:i:22:LEU:HG	2.17	0.45
1:A:248:VAL:O	1:A:251:SER:OG	2.29	0.45
2:B:149:LYS:HA	3:C:158:GLY:HA2	1.99	0.45
2:B:169:PRO:HG3	2:B:198:GLU:HG2	1.98	0.45
4:E:97:TRP:CD2	16:Q:112:HIS:HE1	2.35	0.45
6:G:117:GLU:O	6:G:120:MET:HG2	2.17	0.45
13:N:34:LYS:HZ3	13:N:58:ARG:HG2	1.82	0.45
13:N:55:PHE:CE1	13:N:58:ARG:HD2	2.52	0.45
16:Q:289:SER:H	16:Q:431:HIS:HE1	1.63	0.45
23:Z:62:SER:OG	23:Z:65:ASP:OD1	2.34	0.45
27:d:45:PHE:HA	27:d:48:ARG:HE	1.81	0.45
35:m:40:CYS:O	35:m:44:LEU:HG	2.16	0.45
1:A:303:HIS:HA	14:O:232:THR:HG21	1.99	0.45
12:M:449:PRO:HB2	12:M:680:LEU:HD23	1.99	0.45
15:P:72:TYR:HD1	15:P:89:HIS:HB3	1.81	0.45
16:Q:206:GLU:HB2	16:Q:254:ARG:NH1	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:317:ASP:OD1	16:Q:317:ASP:N	2.47	0.45
32:j:62:PHE:CG	40:s:140:ILE:HG23	2.51	0.45
34:l:221:ALA:HA	34:l:226:GLN:HE21	1.81	0.45
40:s:86:TRP:HA	40:s:89:LEU:HD21	1.99	0.45
42:v:63:LEU:HB2	42:v:87:TRP:CZ3	2.51	0.45
2:B:146:ASP:HB2	2:B:148:THR:HG22	1.99	0.45
12:M:347:ASP:OD1	12:M:347:ASP:N	2.43	0.45
12:M:697:THR:O	12:M:702:ARG:NH2	2.50	0.45
32:j:84:LEU:HD13	40:s:309:ILE:HG23	1.99	0.45
39:r:141:GLU:OE1	39:r:141:GLU:N	2.50	0.45
40:s:136:VAL:O	40:s:140:ILE:HB	2.17	0.45
10:K:96:MET:HE3	10:K:97:PRO:HD2	1.98	0.45
16:Q:235:ASP:OD1	16:Q:235:ASP:N	2.50	0.45
19:U:45:ILE:HG23	21:W:58:ARG:HG2	1.98	0.45
25:b:77:VAL:HB	25:b:78:PRO:HD3	1.99	0.45
34:l:248:HIS:O	34:l:253:VAL:HG23	2.16	0.45
1:A:390:ASP:O	1:A:394:LYS:HG2	2.16	0.45
5:F:23:LEU:HD21	5:F:34:ARG:HG2	1.99	0.45
12:M:624:ARG:NE	12:M:636:TYR:O	2.50	0.45
13:N:84:PRO:HD3	13:N:113:HIS:CD2	2.52	0.45
15:P:140:ARG:NH2	16:Q:399:ALA:HB3	2.31	0.45
15:P:204:LEU:HB2	16:Q:126:TYR:CE2	2.51	0.45
16:Q:159:LEU:HD23	16:Q:392:PRO:HD3	1.99	0.45
6:X:137:LYS:HB3	25:b:4:TYR:CE2	2.51	0.45
25:b:13:GLN:O	25:b:17:GLU:HG2	2.17	0.45
32:j:84:LEU:HD22	40:s:309:ILE:HD13	1.99	0.45
39:r:305:THR:O	39:r:308:SER:OG	2.25	0.45
40:s:77:LEU:O	40:s:80:THR:OG1	2.29	0.45
1:A:56:SER:HB2	1:A:61:ASP:HB2	1.99	0.44
2:B:74:TYR:HA	2:B:77:ARG:HH11	1.83	0.44
11:L:169:ARG:HH21	12:M:426:ASP:HA	1.82	0.44
12:M:351:LEU:HD12	12:M:351:LEU:HA	1.84	0.44
12:M:591:GLU:HG3	12:M:610:VAL:HG23	1.98	0.44
13:N:44:TYR:HE2	13:N:83:PRO:HB3	1.82	0.44
15:P:69:LEU:N	15:P:70:PRO:HD3	2.31	0.44
21:W:43:LEU:HG	40:s:179:TRP:HE1	1.82	0.44
24:a:146:LYS:HZ1	41:u:171:THR:HA	1.81	0.44
26:c:41:TYR:O	26:c:43:ARG:N	2.50	0.44
44:i:99:MET:HG3	44:i:142:MET:HE1	1.98	0.44
1:A:44:ASN:CG	1:A:49:HIS:HB2	2.41	0.44
1:A:387:GLU:HG2	12:M:119:PHE:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:184:ASN:OD1	13:N:129:THR:OG1	2.35	0.44
19:U:33:PRO:HB2	19:U:34:PRO:CD	2.46	0.44
22:Y:89:PRO:O	42:v:107:ARG:NH2	2.50	0.44
24:a:133:TYR:CZ	36:n:44:LEU:HD12	2.52	0.44
33:k:27:MET:HE3	33:k:27:MET:HB3	1.85	0.44
34:l:152:PHE:CD1	34:l:168:ALA:HB1	2.52	0.44
34:l:331:THR:HB	34:l:387:THR:HG23	1.98	0.44
35:m:16:PHE:HA	35:m:19:PHE:CD1	2.52	0.44
5:F:23:LEU:HD11	5:F:34:ARG:HG3	1.99	0.44
10:K:81:THR:HB	14:O:88:ARG:HD2	1.99	0.44
13:N:28:PHE:HB3	13:N:75:TRP:HH2	1.83	0.44
16:Q:100:GLU:O	16:Q:107:ARG:HB2	2.17	0.44
16:Q:180:LEU:HB3	16:Q:210:MET:HE1	1.99	0.44
22:Y:96:GLU:HA	42:v:111:ARG:HD2	1.98	0.44
34:l:407:TRP:NE1	34:l:411:ILE:HD11	2.32	0.44
39:r:75:LEU:HD13	39:r:440:HIS:CD2	2.53	0.44
40:s:77:LEU:HD22	40:s:77:LEU:HA	1.80	0.44
40:s:210:GLY:C	40:s:212:ASN:N	2.74	0.44
1:A:415:ILE:O	1:A:419:ILE:HG13	2.17	0.44
4:E:118:PHE:CE2	12:M:624:ARG:HD3	2.53	0.44
22:Y:51:THR:OG1	34:l:446:ASN:ND2	2.51	0.44
24:a:176:LYS:HE2	31:h:42:GLU:HG2	2.00	0.44
34:l:389:PHE:HA	34:l:393:ASP:HB2	1.99	0.44
35:m:99:GLU:O	35:m:103:VAL:HG23	2.17	0.44
38:p:119:PHE:O	38:p:123:GLU:HG2	2.17	0.44
44:i:197:ASN:ND2	44:i:269:GLU:OE2	2.43	0.44
1:A:141:GLY:HA2	1:A:252:PRO:HD3	2.00	0.44
12:M:666:GLN:HB2	12:M:670:GLU:HB2	1.98	0.44
39:r:165:ILE:HG22	44:i:271:THR:HG21	1.99	0.44
39:r:209:LEU:HD21	39:r:298:VAL:HG11	1.99	0.44
39:r:270:ILE:HD11	39:r:395:LEU:HB3	1.99	0.44
2:B:42:GLN:HE21	8:I:112:TYR:HB3	1.81	0.44
2:B:63:GLU:CD	2:B:63:GLU:H	2.25	0.44
4:E:79:VAL:O	4:E:83:VAL:HG13	2.17	0.44
12:M:257:VAL:HG12	12:M:281:ILE:HG23	1.99	0.44
14:O:55:PHE:HB3	14:O:59:ASN:HB2	2.00	0.44
14:O:138:THR:HG23	14:O:139:PRO:HD3	1.98	0.44
20:V:51:GLU:O	20:V:55:LYS:HG2	2.18	0.44
34:l:194:ASN:O	34:l:194:ASN:ND2	2.50	0.44
38:p:64:LEU:HD23	38:p:64:LEU:HA	1.86	0.44
39:r:233:ALA:O	39:r:237:LYS:HD3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:u:41:LYS:HG3	41:u:129:THR:HG21	1.99	0.44
41:u:142:TYR:O	41:u:144:SER:N	2.50	0.44
1:A:340:ASP:O	1:A:344:GLN:HG2	2.18	0.44
2:B:71:THR:HG23	40:s:272:TRP:HE1	1.83	0.44
12:M:145:MET:HG3	15:P:239:TRP:O	2.17	0.44
12:M:350:ALA:HB2	12:M:619:ASP:HB3	1.99	0.44
17:S:66:LEU:HD23	41:u:20:ILE:HD11	1.99	0.44
27:d:68:ILE:HG22	27:d:150:LEU:HD12	1.99	0.44
41:u:85:TYR:OH	41:u:104:GLN:NE2	2.51	0.44
4:E:118:PHE:CZ	12:M:624:ARG:HD3	2.52	0.44
12:M:395:GLU:HA	12:M:421:SER:HB2	2.00	0.44
14:O:205:ILE:HD13	14:O:208:LEU:HD12	1.99	0.44
15:P:210:LEU:HA	15:P:221:ALA:HA	1.99	0.44
21:W:115:ARG:NH1	31:h:35:ALA:HB1	2.33	0.44
34:l:237:MET:C	34:l:239:GLY:H	2.26	0.44
39:r:210:TYR:HB2	39:r:268:GLY:HA3	2.00	0.44
39:r:328:CYS:HB3	39:r:437:MET:HE1	1.99	0.44
39:r:370:PRO:HD3	39:r:375:LEU:HD13	2.00	0.44
4:E:22:SER:HB3	4:E:27:GLU:HB2	1.99	0.44
12:M:381:LEU:HD11	12:M:668:ALA:HB3	1.99	0.44
21:W:51:MET:HG2	40:s:313:SER:HB3	1.99	0.44
24:a:95:GLN:HB3	24:a:96:ALA:H	1.58	0.44
27:d:115:TYR:HD2	34:l:203:LEU:HD22	1.83	0.44
30:g:9:PRO:HG3	31:h:5:ASP:HB2	1.98	0.44
40:s:210:GLY:O	40:s:212:ASN:N	2.51	0.44
44:i:64:ALA:O	44:i:68:MET:HG2	2.18	0.44
44:i:255:PRO:HA	44:i:260:PHE:CG	2.52	0.44
1:A:288:VAL:HG11	1:A:303:HIS:CD2	2.53	0.43
2:B:145:ILE:HD11	2:B:150:CYS:SG	2.58	0.43
9:J:135:GLU:HG3	9:J:141:PHE:N	2.33	0.43
11:L:146:ASP:OD1	11:L:146:ASP:N	2.49	0.43
12:M:346:VAL:HB	12:M:548:LEU:HD13	2.00	0.43
15:P:111:LEU:HD12	15:P:131:ASN:O	2.18	0.43
20:V:26:THR:HG22	20:V:68:ALA:HB2	2.00	0.43
24:a:164:GLY:HA3	31:h:50:THR:HB	1.99	0.43
25:b:78:PRO:HB2	34:l:10:LEU:HD21	1.99	0.43
34:l:10:LEU:O	34:l:11:THR:C	2.61	0.43
34:l:298:ILE:HG21	34:l:359:MET:HE1	2.00	0.43
34:l:306:THR:HA	34:l:336:LYS:NZ	2.33	0.43
34:l:382:GLY:HA2	34:l:388:GLY:HA3	2.00	0.43
40:s:137:ALA:HB3	40:s:282:TYR:OH	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:u:42:GLU:HG3	41:u:133:THR:HG22	2.00	0.43
1:A:132:ARG:HH22	14:O:224:SER:HA	1.82	0.43
2:B:189:LEU:HB3	18:T:64:ASN:HD22	1.82	0.43
6:G:137:LYS:HB3	6:G:144:ILE:HG12	2.00	0.43
8:I:34:ARG:NH1	16:Q:216:ARG:HH11	2.16	0.43
9:J:117:ARG:HG2	9:J:155:LEU:HD22	1.99	0.43
9:J:318:LYS:O	9:J:322:MET:HG2	2.18	0.43
12:M:266:ARG:HG2	12:M:267:THR:HG23	2.01	0.43
13:N:41:GLU:HB3	13:N:86:TRP:HZ2	1.83	0.43
15:P:148:ASP:N	15:P:148:ASP:OD1	2.51	0.43
16:Q:345:ALA:HB2	21:W:19:ILE:HD11	2.00	0.43
25:b:110:ILE:HG23	25:b:111:LEU:HG	2.00	0.43
34:l:59:GLN:HE21	34:l:59:GLN:HA	1.82	0.43
34:l:231:PRO:HD3	34:l:529:TYR:HE2	1.79	0.43
34:l:254:VAL:HG21	34:l:329:ILE:HG23	2.00	0.43
36:n:30:LYS:HE2	36:n:34:ARG:HH21	1.83	0.43
40:s:161:ASN:HB3	40:s:164:THR:HG23	1.99	0.43
40:s:227:GLU:O	40:s:231:ILE:HG13	2.17	0.43
3:C:89:CYS:HG	45:C:301:SF4:FE2	1.33	0.43
16:Q:458:PHE:O	16:Q:459:GLY:C	2.61	0.43
34:l:111:ASP:OD1	38:p:97:TYR:OH	2.25	0.43
34:l:332:HIS:HA	34:l:335:PHE:CE2	2.53	0.43
39:r:134:THR:HB	39:r:142:ARG:HD2	1.99	0.43
39:r:204:MET:HE3	39:r:261:PHE:CD2	2.53	0.43
39:r:324:SER:HB2	39:r:440:HIS:HE1	1.84	0.43
40:s:196:THR:N	40:s:197:PRO:HD2	2.33	0.43
1:A:88:ARG:HB2	1:A:244:ASN:HD22	1.82	0.43
1:A:315:LEU:HB2	1:A:359:ARG:HA	2.01	0.43
12:M:649:VAL:HG13	12:M:650:SER:H	1.84	0.43
15:P:162:ALA:HB2	16:Q:286:TYR:C	2.43	0.43
15:P:195:GLY:HA3	15:P:202:PHE:CE1	2.54	0.43
19:U:59:ASP:OD1	41:u:131:VAL:N	2.51	0.43
26:c:68:ASP:OD1	26:c:69:GLY:N	2.50	0.43
38:p:129:ARG:HD2	38:p:168:TRP:CD2	2.53	0.43
1:A:165:GLU:HA	1:A:168:ASN:HD22	1.84	0.43
12:M:443:ASP:OD1	12:M:443:ASP:N	2.50	0.43
6:X:118:ILE:O	6:X:122:MET:HG2	2.18	0.43
6:X:137:LYS:O	6:X:138:LEU:HB2	2.18	0.43
39:r:307:TRP:HZ3	39:r:383:VAL:HB	1.83	0.43
40:s:86:TRP:O	40:s:89:LEU:HG	2.18	0.43
40:s:150:LEU:HG	40:s:185:TRP:CZ3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:u:24:VAL:HG13	41:u:86:TRP:HD1	1.83	0.43
2:B:186:GLU:HG2	18:T:62:GLU:O	2.19	0.43
4:E:127:ASP:OD1	4:E:127:ASP:N	2.52	0.43
9:J:88:LYS:HE3	9:J:95:ARG:HH22	1.84	0.43
12:M:266:ARG:HB3	12:M:271:MET:HE3	2.01	0.43
14:O:78:ALA:C	14:O:81:PRO:HD2	2.43	0.43
19:U:53:TYR:HD2	21:W:72:LEU:HD12	1.82	0.43
23:Z:66:VAL:HG21	34:l:432:THR:HG22	2.01	0.43
34:l:233:LEU:HD22	34:l:237:MET:HE2	2.00	0.43
35:m:140:ILE:HD13	35:m:140:ILE:HA	1.86	0.43
38:p:103:CYS:HB3	39:r:426:MET:HE3	2.01	0.43
39:r:188:ASN:OD1	39:r:188:ASN:N	2.52	0.43
40:s:288:LEU:HD22	40:s:288:LEU:HA	1.86	0.43
41:u:30:HIS:CG	41:u:119:ARG:HH21	2.36	0.43
5:F:55:ILE:HD12	12:M:381:LEU:HD23	2.00	0.43
9:J:360:ARG:O	9:J:360:ARG:NH1	2.38	0.43
12:M:460:HIS:O	12:M:463:SER:OG	2.36	0.43
16:Q:329:ARG:HH11	16:Q:453:THR:HG21	1.84	0.43
23:Z:28:PRO:HD2	23:Z:53:TYR:CD2	2.53	0.43
24:a:94:GLY:HA3	27:d:50:HIS:CE1	2.54	0.43
30:g:11:ARG:O	30:g:13:LEU:N	2.51	0.43
31:h:6:ILE:HB	44:i:22:LEU:HD22	2.01	0.43
35:m:51:MET:HB2	35:m:138:ASP:OD2	2.18	0.43
35:m:159:THR:O	35:m:163:GLY:N	2.47	0.43
41:u:100:CYS:SG	41:u:101:ARG:N	2.91	0.43
11:L:121:LEU:HG	15:P:203:PRO:HG3	2.01	0.43
13:N:127:TYR:HE2	18:T:44:GLN:HE21	1.67	0.43
14:O:207:GLU:HG2	14:O:213:ILE:HA	2.01	0.43
17:S:25:TYR:OH	40:s:253:GLU:OE2	2.29	0.43
31:h:67:LEU:HD23	31:h:67:LEU:HA	1.84	0.43
34:l:338:MET:HB2	34:l:457:LEU:HB3	2.01	0.43
40:s:92:PRO:HB3	40:s:255:TYR:CD1	2.53	0.43
40:s:196:THR:OG1	40:s:274:ARG:HG3	2.18	0.43
44:i:172:GLN:HG2	44:i:177:LYS:HD3	1.99	0.43
1:A:284:HIS:ND1	14:O:228:ALA:HB3	2.34	0.43
1:A:386:ARG:NH1	12:M:178:GLN:OE1	2.50	0.43
3:C:116:GLN:HE21	40:s:216:ALA:HA	1.84	0.43
5:F:45:LYS:HE2	5:F:45:LYS:HB3	1.79	0.43
12:M:151:SER:HB3	16:Q:376:GLU:HG3	2.00	0.43
12:M:637:ASP:N	12:M:641:GLN:OE1	2.51	0.43
14:O:82:VAL:HG12	14:O:101:VAL:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:57:VAL:HG23	17:S:59:ARG:HB2	2.01	0.43
24:a:160:MET:HE3	24:a:167:PRO:HD2	2.00	0.43
38:p:47:ARG:O	38:p:50:GLU:HG2	2.19	0.43
41:u:140:ASN:ND2	41:u:144:SER:OG	2.49	0.43
1:A:383:THR:N	1:A:384:PRO:HD2	2.34	0.43
3:C:106:PHE:HA	40:s:39:VAL:HB	2.00	0.43
6:G:104:PHE:HB2	6:G:138:LEU:HD12	2.01	0.43
34:l:246:LEU:HD21	34:l:337:ALA:O	2.19	0.43
44:i:115:VAL:HB	44:i:116:PRO:HD3	2.00	0.43
3:C:91:VAL:HG21	16:Q:222:MET:SD	2.59	0.42
16:Q:435:LEU:HA	16:Q:438:MET:HE3	2.01	0.42
18:T:40:THR:HG22	18:T:63:VAL:HG12	2.00	0.42
24:a:52:LYS:N	25:b:27:GLU:OE1	2.51	0.42
26:c:108:HIS:HE1	34:l:546:GLN:HG2	1.84	0.42
33:k:66:PHE:HE1	35:m:156:THR:HG22	1.84	0.42
34:l:100:ILE:CD1	34:l:246:LEU:HG	2.49	0.42
34:l:174:TYR:CD1	34:l:229:LEU:HD22	2.54	0.42
39:r:299:THR:O	39:r:303:ILE:HG13	2.18	0.42
1:A:369:ARG:HH21	14:O:136:THR:HB	1.84	0.42
4:E:29:LYS:HG2	47:E:201:ZMP:H19B	2.01	0.42
4:E:122:PHE:CD1	12:M:621:LYS:HG2	2.54	0.42
12:M:322:ALA:O	12:M:326:VAL:HG22	2.18	0.42
12:M:545:LEU:HD22	12:M:567:ILE:HD13	2.01	0.42
14:O:182:ASN:ND2	14:O:225:CYS:SG	2.93	0.42
15:P:183:ASP:OD1	15:P:183:ASP:N	2.51	0.42
21:W:24:ASN:O	21:W:26:PRO:HD3	2.19	0.42
25:b:120:MET:SD	42:v:65:ARG:NH2	2.92	0.42
26:c:75:TYR:OH	26:c:105:MET:O	2.25	0.42
27:d:111:GLU:O	27:d:114:ASN:ND2	2.52	0.42
33:k:27:MET:SD	35:m:71:THR:HG22	2.59	0.42
34:l:39:ILE:O	34:l:43:THR:HG23	2.18	0.42
34:l:55:MET:HE2	34:l:55:MET:HA	2.01	0.42
40:s:145:THR:HG21	40:s:289:LEU:HD22	2.00	0.42
44:i:336:LEU:HD12	44:i:339:ILE:HD11	2.00	0.42
3:C:177:ASP:OD1	3:C:177:ASP:N	2.52	0.42
5:F:23:LEU:HD22	5:F:37:ILE:HD13	2.01	0.42
16:Q:293:LEU:HD22	16:Q:298:ILE:HD12	2.01	0.42
17:S:37:ARG:HG3	17:S:60:TYR:CE2	2.50	0.42
34:l:451:LEU:HB3	34:l:455:LYS:HZ2	1.85	0.42
37:o:71:ALA:HA	37:o:75:ASN:HB3	2.01	0.42
44:i:37:MET:HE2	44:i:63:GLN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:PHE:O	1:A:456:GLN:HB3	2.20	0.42
2:B:84:TYR:OH	3:C:192:TYR:HB2	2.19	0.42
3:C:99:PRO:HG2	16:Q:205:GLU:HB2	2.01	0.42
3:C:153:CYS:HA	3:C:157:GLY:C	2.45	0.42
12:M:260:ASN:OD1	12:M:260:ASN:N	2.53	0.42
12:M:414:PHE:CE2	12:M:418:ILE:HD11	2.54	0.42
12:M:693:ASP:OD1	12:M:693:ASP:N	2.51	0.42
16:Q:86:PRO:HB3	16:Q:94:VAL:HG13	2.02	0.42
16:Q:110:ASP:OD1	16:Q:110:ASP:N	2.51	0.42
20:V:46:PRO:HG2	20:V:52:GLY:HA2	2.00	0.42
26:c:88:PRO:HB3	26:c:98:ARG:NH2	2.35	0.42
34:l:89:PHE:O	34:l:90:ILE:C	2.63	0.42
34:l:182:PHE:O	34:l:186:LEU:HG	2.18	0.42
34:l:312:LEU:O	34:l:316:THR:HG23	2.19	0.42
38:p:76:HIS:O	38:p:78:GLN:N	2.52	0.42
39:r:370:PRO:HB3	39:r:375:LEU:HD22	2.02	0.42
1:A:275:LEU:HA	1:A:289:GLU:HA	2.01	0.42
2:B:115:LYS:HD3	12:M:241:ARG:HB2	2.01	0.42
12:M:607:LYS:HD3	12:M:607:LYS:HA	1.84	0.42
20:V:43:LEU:HD21	44:i:113:PHE:CZ	2.54	0.42
34:l:71:THR:HA	39:r:307:TRP:HE1	1.84	0.42
34:l:264:HIS:O	34:l:268:GLU:HG3	2.19	0.42
42:v:44:GLN:NE2	42:v:48:ASP:OD2	2.52	0.42
7:H:94:MET:HE3	7:H:94:MET:HB3	1.87	0.42
9:J:168:SER:O	9:J:203:PRO:HD2	2.19	0.42
12:M:355:LYS:HB2	12:M:530:TYR:OH	2.20	0.42
15:P:198:PHE:CE1	16:Q:122:LYS:HB2	2.54	0.42
19:U:42:SER:HB2	40:s:314:ILE:HD11	2.02	0.42
26:c:42:PRO:HG3	26:c:51:ALA:HB2	2.02	0.42
34:l:33:PRO:HB2	34:l:105:LEU:HD21	2.01	0.42
34:l:393:ASP:O	34:l:397:GLU:HG3	2.20	0.42
34:l:452:ASN:HB2	34:l:453:PRO:HD3	2.02	0.42
39:r:151:PHE:HZ	39:r:212:LEU:HD22	1.84	0.42
40:s:150:LEU:HD23	40:s:150:LEU:HA	1.80	0.42
40:s:237:LEU:HD23	40:s:237:LEU:HA	1.90	0.42
44:i:145:ILE:H	44:i:145:ILE:HG13	1.68	0.42
44:i:255:PRO:N	44:i:256:PRO:HD2	2.35	0.42
2:B:146:ASP:OD1	2:B:146:ASP:N	2.52	0.42
3:C:144:PRO:HA	9:J:89:TYR:OH	2.20	0.42
4:E:97:TRP:CB	16:Q:96:ARG:HH22	2.33	0.42
6:G:102:SER:O	6:G:141:PRO:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:100:TRP:HA	7:H:100:TRP:CE3	2.55	0.42
7:H:100:TRP:CZ2	15:P:68:ILE:HG23	2.55	0.42
24:a:168:TRP:NE1	30:g:88:GLU:OE1	2.52	0.42
31:h:6:ILE:HG23	31:h:10:PHE:CD2	2.54	0.42
37:o:72:ARG:HH22	39:r:278:ARG:CZ	2.33	0.42
39:r:12:LEU:HB2	39:r:13:PRO:HD3	2.01	0.42
39:r:174:LEU:HA	39:r:179:LEU:HD11	2.02	0.42
44:i:176:ARG:HH11	44:i:219:LEU:HD21	1.85	0.42
4:E:105:ARG:HH11	15:P:221:ALA:HB2	1.85	0.42
5:F:21:ILE:HG12	5:F:65:LEU:HD13	2.01	0.42
11:L:105:GLU:OE2	11:L:107:TRP:HB3	2.20	0.42
12:M:217:GLU:O	12:M:288:ASP:HB2	2.19	0.42
12:M:251:ILE:HG22	12:M:260:ASN:HA	2.02	0.42
12:M:370:GLU:O	12:M:533:GLY:HA3	2.20	0.42
12:M:597:VAL:HA	12:M:603:ALA:HA	2.02	0.42
20:V:128:GLY:HA2	20:V:133:TRP:CD2	2.55	0.42
21:W:115:ARG:HH21	31:h:36:PHE:HD1	1.68	0.42
6:X:123:GLU:OE2	38:p:25:ARG:NH2	2.53	0.42
27:d:64:ARG:HD3	27:d:64:ARG:HA	1.94	0.42
39:r:10:MET:O	39:r:13:PRO:HD2	2.20	0.42
39:r:398:LEU:O	39:r:402:VAL:HG23	2.19	0.42
40:s:107:ALA:O	40:s:111:LEU:HG	2.20	0.42
44:i:112:HIS:HB2	44:i:184:ILE:HD13	2.02	0.42
12:M:82:ILE:HG22	12:M:83:GLU:H	1.85	0.42
31:h:97:HIS:HD2	31:h:98:HIS:CD2	2.38	0.42
34:l:158:TRP:CD2	38:p:93:ARG:HG3	2.55	0.42
34:l:362:LEU:HB2	34:l:431:LEU:HD23	2.01	0.42
34:l:547:ASN:HA	34:l:551:LEU:HD12	2.01	0.42
38:p:48:PHE:HD1	38:p:48:PHE:HA	1.75	0.42
39:r:87:GLU:O	39:r:92:LYS:HE3	2.20	0.42
39:r:139:GLN:HG3	39:r:142:ARG:NH2	2.34	0.42
40:s:231:ILE:HG23	40:s:270:PHE:HD2	1.85	0.42
44:i:163:MET:HG2	44:i:285:ILE:HD13	2.02	0.42
1:A:223:PRO:O	1:A:381:GLN:NE2	2.29	0.42
2:B:138:ARG:HG2	12:M:238:PHE:CG	2.55	0.42
9:J:247:LYS:HD2	9:J:340:ILE:HD12	2.01	0.42
12:M:60:ILE:HD12	12:M:60:ILE:H	1.84	0.42
12:M:339:ALA:HB3	12:M:544:VAL:HG22	2.02	0.42
16:Q:105:MET:HE3	16:Q:105:MET:HB3	1.82	0.42
28:e:97:ILE:O	28:e:101:LEU:HB2	2.20	0.42
35:m:57:LEU:HD23	35:m:57:LEU:HA	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:u:96:LEU:HD11	41:u:99:HIS:HD2	1.84	0.42
44:i:251:LEU:O	44:i:263:LYS:NZ	2.44	0.42
1:A:156:ILE:N	1:A:196:PHE:O	2.50	0.41
1:A:163:TYR:HB3	14:O:190:ASP:HB3	2.02	0.41
1:A:386:ARG:HH12	1:A:387:GLU:HB2	1.85	0.41
1:A:386:ARG:HD3	12:M:178:GLN:CD	2.45	0.41
5:F:35:ASP:HB3	5:F:39:LYS:NZ	2.35	0.41
7:H:62:GLU:HB2	7:H:68:LEU:HD13	2.02	0.41
8:I:23:LYS:HB3	16:Q:250:ASN:HB3	2.02	0.41
9:J:92:MET:O	9:J:96:PRO:HD3	2.20	0.41
15:P:134:SER:O	15:P:138:ASN:N	2.53	0.41
34:l:48:LEU:HD23	34:l:48:LEU:HA	1.84	0.41
39:r:203:PHE:O	39:r:207:MET:N	2.48	0.41
40:s:156:MET:HE1	40:s:177:PRO:HB2	2.02	0.41
2:B:209:TYR:CZ	8:I:39:PRO:HG3	2.55	0.41
4:E:33:ARG:NH1	6:G:136:GLU:OE2	2.54	0.41
4:E:77:ARG:HB2	15:P:150:LEU:HD13	2.01	0.41
12:M:540:ASN:ND2	12:M:560:LEU:HD13	2.34	0.41
32:j:95:ILE:HG21	40:s:302:MET:HG3	2.02	0.41
34:l:549:PRO:HA	34:l:553:LEU:HB2	2.02	0.41
40:s:6:LEU:HA	40:s:6:LEU:HD23	1.77	0.41
40:s:18:ALA:O	40:s:21:MET:HG2	2.19	0.41
2:B:201:ALA:HB1	13:N:88:ARG:CZ	2.50	0.41
3:C:160:TYR:CE1	16:Q:120:THR:HG22	2.55	0.41
9:J:208:GLY:H	9:J:211:ASP:HB3	1.83	0.41
9:J:235:THR:HG21	9:J:323:HIS:HA	2.02	0.41
11:L:169:ARG:HD2	12:M:422:TRP:CZ2	2.56	0.41
20:V:17:ASP:HB3	20:V:20:ARG:HD2	2.02	0.41
34:l:159:TYR:CE2	38:p:96:CYS:HB2	2.55	0.41
35:m:114:VAL:HG13	35:m:115:VAL:O	2.20	0.41
39:r:153:THR:HA	39:r:157:SER:HB3	2.01	0.41
39:r:164:LEU:HA	39:r:167:THR:HG22	2.03	0.41
1:A:158:ILE:O	1:A:200:GLY:N	2.48	0.41
1:A:203:ALA:HA	12:M:200:ARG:HH12	1.85	0.41
12:M:321:ASP:OD1	12:M:321:ASP:N	2.53	0.41
12:M:414:PHE:CD2	12:M:516:LEU:HD11	2.55	0.41
16:Q:148:GLU:OE2	16:Q:225:ALA:HA	2.20	0.41
16:Q:206:GLU:HG3	16:Q:247:PHE:CE1	2.55	0.41
26:c:164:ASN:HD22	26:c:180:ARG:H	1.68	0.41
26:c:166:LEU:HD22	42:v:56:ARG:HG3	2.01	0.41
33:k:54:LEU:O	33:k:55:LEU:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:o:112:LYS:HZ1	39:r:390:ASN:H	1.66	0.41
39:r:377:GLY:O	39:r:381:VAL:HG23	2.21	0.41
1:A:270:ASN:HD21	1:A:340:ASP:HB2	1.85	0.41
2:B:178:HIS:HB2	3:C:179:TYR:CZ	2.54	0.41
4:E:106:PHE:O	4:E:108:HIS:ND1	2.53	0.41
8:I:31:ILE:HB	8:I:32:SER:H	1.61	0.41
11:L:123:ASN:OD1	12:M:246:ARG:NH2	2.53	0.41
12:M:349:GLU:OE1	12:M:349:GLU:N	2.50	0.41
12:M:529:GLY:C	12:M:530:TYR:HD1	2.28	0.41
16:Q:130:LEU:HD11	16:Q:228:ARG:HD3	2.02	0.41
19:U:32:LEU:O	19:U:33:PRO:C	2.64	0.41
19:U:82:LYS:NZ	41:u:121:ASP:OD1	2.37	0.41
32:j:51:PHE:HZ	33:k:79:VAL:HG22	1.85	0.41
33:k:66:PHE:O	33:k:70:GLU:HG3	2.20	0.41
33:k:75:LEU:HD21	35:m:67:PHE:CD1	2.54	0.41
34:l:74:THR:HG22	34:l:75:GLN:H	1.86	0.41
41:u:158:LEU:HD23	41:u:158:LEU:HA	1.76	0.41
1:A:60:GLY:CA	14:O:241:PRO:HA	2.50	0.41
1:A:295:PRO:HA	1:A:336:LEU:HA	2.01	0.41
1:A:406:PRO:O	1:A:409:ILE:HG12	2.21	0.41
2:B:76:PHE:HB3	8:I:8:ILE:HG23	2.01	0.41
9:J:61:ALA:HA	9:J:66:GLY:HA3	2.03	0.41
9:J:217:PHE:HZ	9:J:273:LEU:HD11	1.86	0.41
11:L:70:GLU:O	11:L:74:THR:HG22	2.20	0.41
20:V:10:TRP:CZ3	20:V:129:ARG:HG2	2.56	0.41
25:b:86:MET:CE	34:l:9:THR:HG21	2.49	0.41
32:j:14:ALA:HB2	40:s:76:THR:HG21	2.03	0.41
32:j:77:TRP:CE2	35:m:139:PRO:HB2	2.56	0.41
39:r:116:ILE:HG22	41:u:169:PHE:HE2	1.85	0.41
42:v:49:ALA:O	42:v:51:LEU:N	2.53	0.41
1:A:102:MET:HE2	1:A:102:MET:HB3	1.96	0.41
1:A:293:SER:HB3	1:A:338:ASP:HB3	2.02	0.41
1:A:426:ALA:HB3	46:A:502:FMN:O2	2.20	0.41
9:J:41:MET:HE1	12:M:615:LEU:HD12	2.03	0.41
12:M:233:SER:OG	12:M:236:TYR:HB3	2.20	0.41
12:M:304:GLU:HB2	12:M:316:TYR:CD1	2.55	0.41
16:Q:145:MET:HE3	16:Q:145:MET:HB3	1.89	0.41
19:U:13:TRP:HD1	19:U:17:PRO:HA	1.84	0.41
20:V:95:CYS:HA	20:V:115:CYS:HA	2.01	0.41
20:V:141:VAL:HG12	24:a:157:ARG:HD3	2.02	0.41
25:b:105:PHE:HB2	42:v:68:LYS:HD3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:58:ARG:HB3	26:c:61:ASP:HB3	2.03	0.41
26:c:166:LEU:HD21	42:v:53:LEU:HD22	2.02	0.41
30:g:47:ILE:HD12	44:i:327:PRO:HG3	2.03	0.41
39:r:2:LEU:HG	39:r:6:VAL:HG23	2.01	0.41
40:s:81:ILE:HG23	40:s:108:THR:HB	2.02	0.41
40:s:185:TRP:O	40:s:189:THR:HG23	2.20	0.41
44:i:242:PRO:C	44:i:245:PRO:HD2	2.46	0.41
1:A:187:CYS:HG	1:A:189:SER:HG	1.67	0.41
3:C:102:ASP:OD2	40:s:34:ARG:HB2	2.21	0.41
9:J:83:PRO:HB2	9:J:108:TRP:CD1	2.55	0.41
12:M:353:ALA:HA	12:M:636:TYR:OH	2.20	0.41
12:M:406:ASN:OD1	12:M:406:ASN:N	2.52	0.41
15:P:69:LEU:HD13	15:P:96:VAL:HG22	2.03	0.41
20:V:17:ASP:OD1	20:V:17:ASP:N	2.54	0.41
34:l:249:SER:HB3	34:l:306:THR:HG21	2.01	0.41
34:l:366:MET:HG2	34:l:445:GLU:CD	2.46	0.41
38:p:14:GLN:O	38:p:18:ARG:HG3	2.21	0.41
38:p:108:HIS:CD2	38:p:109:PRO:HD2	2.56	0.41
39:r:216:LEU:HD22	39:r:220:HIS:CD2	2.56	0.41
2:B:138:ARG:HH12	12:M:241:ARG:HH12	1.68	0.41
3:C:148:VAL:HG13	3:C:178:ILE:HG13	2.02	0.41
4:E:81:LEU:HD12	4:E:81:LEU:HA	1.92	0.41
7:H:21:HIS:NE2	7:H:68:LEU:HD22	2.36	0.41
8:I:30:GLU:HG2	8:I:31:ILE:N	2.31	0.41
9:J:57:THR:HB	9:J:126:VAL:HG22	2.01	0.41
9:J:67:ARG:HD2	9:J:93:HIS:CE1	2.56	0.41
9:J:195:PHE:HB3	9:J:198:ALA:HB2	2.02	0.41
12:M:81:GLU:OE2	12:M:106:SER:HB3	2.21	0.41
12:M:149:ASP:HA	16:Q:380:HIS:NE2	2.35	0.41
12:M:246:ARG:HH21	15:P:232:LYS:HG2	1.86	0.41
12:M:301:ARG:NH1	12:M:591:GLU:OE2	2.54	0.41
12:M:319:TRP:CZ2	12:M:622:ILE:HD12	2.55	0.41
16:Q:82:LEU:HA	16:Q:82:LEU:HD23	1.74	0.41
16:Q:88:HIS:N	16:Q:89:PRO:HD3	2.36	0.41
17:S:39:ALA:C	17:S:41:PHE:H	2.28	0.41
20:V:37:ALA:HB1	20:V:56:VAL:HA	2.03	0.41
6:X:90:TYR:CE1	23:Z:44:PRO:HB2	2.56	0.41
22:Y:84:PHE:HE1	34:l:483:PRO:HA	1.86	0.41
25:b:11:ARG:HB2	38:p:156:PRO:HB3	2.03	0.41
25:b:23:LEU:HA	25:b:26:GLN:HG2	2.01	0.41
25:b:79:VAL:HG11	27:d:35:VAL:HG11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:c:71:GLY:HA3	37:o:76:VAL:HG13	2.03	0.41
28:e:87:MET:HB3	28:e:87:MET:HE3	1.81	0.41
32:j:24:LEU:HD23	32:j:24:LEU:HA	1.85	0.41
34:l:132:VAL:HA	34:l:258:PHE:CE2	2.55	0.41
34:l:194:ASN:OD1	37:o:128:SER:N	2.54	0.41
34:l:197:ASP:OD1	34:l:198:PRO:HD2	2.21	0.41
34:l:233:LEU:HA	34:l:233:LEU:HD23	1.75	0.41
34:l:356:ILE:HG22	34:l:429:LEU:HB3	2.02	0.41
34:l:417:SER:O	34:l:420:SER:OG	2.33	0.41
34:l:481:THR:O	34:l:481:THR:OG1	2.27	0.41
35:m:113:VAL:HG13	35:m:114:VAL:H	1.86	0.41
40:s:87:THR:HG22	40:s:95:LEU:HD23	2.03	0.41
41:u:131:VAL:HG12	41:u:133:THR:HG23	2.03	0.41
42:v:42:THR:O	42:v:46:MET:HG2	2.20	0.41
44:i:37:MET:CE	44:i:60:PHE:HA	2.50	0.41
44:i:108:MET:SD	44:i:191:MET:HG3	2.60	0.41
44:i:142:MET:HA	44:i:145:ILE:HD11	2.03	0.41
44:i:203:LEU:HD22	44:i:344:LEU:HD23	2.03	0.41
1:A:224:ARG:HD2	11:L:164:PHE:CZ	2.56	0.41
8:I:58:ASP:OD1	8:I:58:ASP:N	2.54	0.41
8:I:97:PRO:HG3	15:P:61:PHE:CE2	2.56	0.41
9:J:128:ASN:HD22	9:J:166:HIS:HD2	1.69	0.41
9:J:274:PHE:CD2	9:J:278:LYS:HE2	2.56	0.41
12:M:68:ARG:HE	12:M:283:GLU:HG2	1.86	0.41
12:M:282:ASN:OD1	12:M:283:GLU:N	2.54	0.41
12:M:314:LEU:H	12:M:314:LEU:HG	1.71	0.41
12:M:516:LEU:HD23	12:M:516:LEU:HA	1.94	0.41
12:M:531:LYS:HA	12:M:532:PRO:HD3	1.93	0.41
14:O:138:THR:HA	14:O:141:MET:HB3	2.03	0.41
20:V:90:TYR:HB3	20:V:122:ALA:HB1	2.03	0.41
21:W:111:PHE:HE1	31:h:65:GLU:HB3	1.86	0.41
39:r:203:PHE:HE2	39:r:246:LEU:HD12	1.86	0.41
39:r:346:GLN:HB3	39:r:418:SER:O	2.21	0.41
40:s:152:SER:O	40:s:155:LEU:HB2	2.21	0.41
1:A:329:LYS:HE3	1:A:329:LYS:HB2	1.92	0.40
3:C:181:PRO:O	3:C:185:PRO:HB3	2.21	0.40
4:E:115:PRO:HB2	4:E:120:SER:OG	2.21	0.40
7:H:43:ALA:H	7:H:100:TRP:HD1	1.69	0.40
9:J:212:ARG:O	9:J:216:SER:OG	2.31	0.40
10:K:100:SER:HA	14:O:72:GLU:HB3	2.02	0.40
11:L:86:ASN:ND2	12:M:224:ASP:OD2	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:Q:334:VAL:HA	16:Q:337:MET:CE	2.52	0.40
6:X:83:VAL:HA	6:X:122:MET:HE1	2.03	0.40
6:X:88:LYS:HD2	6:X:95:PRO:HB3	2.03	0.40
30:g:6:ASN:ND2	30:g:9:PRO:HA	2.36	0.40
34:l:367:PRO:O	34:l:371:THR:HG23	2.21	0.40
35:m:10:VAL:O	35:m:13:VAL:HG12	2.21	0.40
4:E:77:ARG:HA	4:E:80:ASP:OD2	2.22	0.40
6:G:77:GLU:CD	6:G:77:GLU:H	2.29	0.40
9:J:213:PHE:HZ	9:J:276:LEU:HD21	1.85	0.40
12:M:351:LEU:HG	12:M:530:TYR:CE2	2.57	0.40
14:O:96:SER:HA	14:O:99:ASN:ND2	2.36	0.40
21:W:82:ARG:HG2	21:W:86:MET:HE2	2.03	0.40
25:b:113:THR:HB	25:b:114:GLY:H	1.67	0.40
33:k:33:LEU:HA	33:k:36:MET:HE2	2.02	0.40
33:k:59:VAL:O	33:k:60:PRO:C	2.64	0.40
34:l:246:LEU:CD1	34:l:340:PHE:HB2	2.41	0.40
37:o:113:GLU:O	37:o:117:GLN:HG2	2.22	0.40
44:i:132:THR:HG23	44:i:209:ILE:HG23	2.03	0.40
1:A:126:LYS:HZ2	1:A:246:GLU:HG3	1.86	0.40
2:B:208:LEU:HD13	8:I:38:PRO:HB3	2.02	0.40
11:L:121:LEU:HD11	15:P:207:TYR:HE1	1.86	0.40
12:M:358:LEU:HB3	12:M:363:SER:O	2.21	0.40
13:N:129:THR:HG23	18:T:44:GLN:HE22	1.86	0.40
16:Q:362:LYS:O	16:Q:384:LEU:HD21	2.20	0.40
25:b:80:TRP:HE1	27:d:35:VAL:HA	1.86	0.40
34:l:135:ASN:ND2	34:l:197:ASP:OD1	2.54	0.40
34:l:151:SER:HB3	34:l:252:MET:SD	2.61	0.40
34:l:457:LEU:HD23	34:l:457:LEU:HA	1.88	0.40
39:r:35:SER:HA	39:r:70:THR:HB	2.03	0.40
39:r:290:SER:HA	39:r:319:HIS:CE1	2.56	0.40
40:s:207:LEU:HD12	40:s:208:VAL:HG23	2.03	0.40
2:B:89:GLY:HA2	2:B:90:PRO:HD3	1.96	0.40
2:B:169:PRO:HG3	2:B:198:GLU:CG	2.51	0.40
2:B:201:ALA:HB1	13:N:88:ARG:NH1	2.36	0.40
11:L:128:PHE:HB3	11:L:133:ASP:OD1	2.22	0.40
12:M:304:GLU:HB2	12:M:316:TYR:HD1	1.87	0.40
12:M:483:ARG:NH1	12:M:682:ASP:O	2.54	0.40
16:Q:133:LEU:HD11	16:Q:227:ILE:O	2.22	0.40
17:S:4:GLU:O	17:S:7:PRO:HD2	2.21	0.40
18:T:92:GLY:O	18:T:94:LEU:HD12	2.22	0.40
20:V:12:ILE:HB	20:V:21:LYS:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:b:12:LEU:HB3	25:b:16:ARG:NH1	2.37	0.40
34:l:407:TRP:O	34:l:411:ILE:HG13	2.21	0.40
39:r:177:LEU:HD23	39:r:177:LEU:HA	1.89	0.40
39:r:206:LYS:HE2	39:r:206:LYS:HB2	1.86	0.40
40:s:32:GLN:HB3	40:s:34:ARG:HG2	2.02	0.40
40:s:282:TYR:O	40:s:285:LEU:N	2.55	0.40
44:i:154:LEU:HD21	44:i:191:MET:O	2.21	0.40
2:B:99:HIS:HD2	45:B:302:SF4:S4	2.21	0.40
3:C:81:PRO:HD3	3:C:108:VAL:HG12	2.04	0.40
12:M:50:LEU:HA	12:M:60:ILE:HD13	2.03	0.40
12:M:161:GLU:H	12:M:161:GLU:CD	2.29	0.40
21:W:27:ARG:O	21:W:29:GLY:N	2.55	0.40
21:W:72:LEU:HD23	21:W:72:LEU:HA	1.85	0.40
27:d:48:ARG:O	27:d:52:LYS:HG3	2.22	0.40
38:p:91:TYR:CD2	38:p:92:GLU:HG3	2.57	0.40
44:i:124:LEU:HD12	44:i:125:THR:H	1.86	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	429/464 (92%)	413 (96%)	16 (4%)	0	100	100
2	B	174/210 (83%)	168 (97%)	6 (3%)	0	100	100
3	C	154/213 (72%)	141 (92%)	12 (8%)	1 (1%)	22	54
4	E	111/128 (87%)	103 (93%)	7 (6%)	1 (1%)	14	46
5	F	81/99 (82%)	77 (95%)	4 (5%)	0	100	100
6	G	81/156 (52%)	77 (95%)	4 (5%)	0	100	100
6	X	83/156 (53%)	76 (92%)	7 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	H	110/116 (95%)	102 (93%)	8 (7%)	0	100	100
8	I	91/113 (80%)	82 (90%)	7 (8%)	2 (2%)	5	29
9	J	309/377 (82%)	288 (93%)	20 (6%)	1 (0%)	37	68
10	K	28/108 (26%)	27 (96%)	1 (4%)	0	100	100
11	L	115/175 (66%)	105 (91%)	9 (8%)	1 (1%)	14	46
12	M	684/727 (94%)	630 (92%)	47 (7%)	7 (1%)	13	44
13	N	141/145 (97%)	126 (89%)	13 (9%)	2 (1%)	9	37
14	O	210/249 (84%)	198 (94%)	11 (5%)	1 (0%)	25	58
15	P	205/264 (78%)	179 (87%)	24 (12%)	2 (1%)	13	44
16	Q	382/463 (82%)	354 (93%)	26 (7%)	2 (0%)	25	58
17	S	68/70 (97%)	64 (94%)	4 (6%)	0	100	100
18	T	93/124 (75%)	91 (98%)	2 (2%)	0	100	100
19	U	81/84 (96%)	76 (94%)	5 (6%)	0	100	100
20	V	138/141 (98%)	131 (95%)	6 (4%)	1 (1%)	19	52
21	W	136/144 (94%)	132 (97%)	3 (2%)	1 (1%)	19	52
22	Y	56/105 (53%)	46 (82%)	9 (16%)	1 (2%)	7	32
23	Z	70/98 (71%)	69 (99%)	1 (1%)	0	100	100
24	a	136/189 (72%)	132 (97%)	3 (2%)	1 (1%)	19	52
25	b	116/128 (91%)	108 (93%)	8 (7%)	0	100	100
26	c	134/186 (72%)	123 (92%)	11 (8%)	0	100	100
27	d	164/172 (95%)	161 (98%)	3 (2%)	0	100	100
28	e	86/153 (56%)	77 (90%)	9 (10%)	0	100	100
29	f	45/76 (59%)	43 (96%)	2 (4%)	0	100	100
30	g	117/119 (98%)	108 (92%)	6 (5%)	3 (3%)	4	26
31	h	102/106 (96%)	94 (92%)	6 (6%)	2 (2%)	6	30
32	j	88/115 (76%)	85 (97%)	3 (3%)	0	100	100
33	k	82/98 (84%)	76 (93%)	6 (7%)	0	100	100
34	l	561/603 (93%)	528 (94%)	32 (6%)	1 (0%)	44	74
35	m	162/174 (93%)	151 (93%)	11 (7%)	0	100	100
36	n	54/58 (93%)	53 (98%)	0	1 (2%)	6	31
37	o	100/129 (78%)	98 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
38	p	169/179 (94%)	163 (96%)	5 (3%)	1 (1%)	22	54
39	r	457/459 (100%)	439 (96%)	17 (4%)	1 (0%)	44	74
40	s	316/318 (99%)	298 (94%)	17 (5%)	1 (0%)	37	68
41	u	167/172 (97%)	158 (95%)	8 (5%)	1 (1%)	22	54
42	v	108/137 (79%)	101 (94%)	6 (6%)	1 (1%)	14	46
44	i	300/347 (86%)	289 (96%)	11 (4%)	0	100	100
All	All	7494/8847 (85%)	7040 (94%)	418 (6%)	36 (0%)	27	58

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	98	LYS
12	M	210	ILE
13	N	115	PHE
31	h	20	ILE
36	n	55	VAL
41	u	101	ARG
42	v	23	PRO
8	I	31	ILE
12	M	482	GLN
12	M	484	ASN
14	O	160	VAL
24	a	185	ALA
40	s	211	PHE
12	M	174	THR
12	M	548	LEU
15	P	44	ARG
16	Q	89	PRO
21	W	28	ARG
30	g	12	PHE
3	C	113	SER
13	N	130	THR
20	V	135	VAL
12	M	47	THR
39	r	251	ASN
8	I	70	MET
11	L	96	LYS
16	Q	84	PHE
30	g	49	ARG
34	l	239	GLY

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Mol	Chain	Res	Type
15	P	224	VAL
30	g	50	ARG
22	Y	86	TYR
31	h	94	PRO
38	p	32	VAL
9	J	370	LYS
12	M	582	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	345/371 (93%)	322 (93%)	23 (7%)	13	40
2	B	151/174 (87%)	145 (96%)	6 (4%)	27	55
3	C	132/174 (76%)	121 (92%)	11 (8%)	9	32
4	E	106/116 (91%)	104 (98%)	2 (2%)	52	73
5	F	74/80 (92%)	69 (93%)	5 (7%)	13	40
6	G	71/136 (52%)	67 (94%)	4 (6%)	17	45
6	X	78/136 (57%)	76 (97%)	2 (3%)	41	67
7	H	100/102 (98%)	99 (99%)	1 (1%)	73	84
8	I	87/98 (89%)	83 (95%)	4 (5%)	23	51
9	J	268/323 (83%)	251 (94%)	17 (6%)	15	42
10	K	28/93 (30%)	28 (100%)	0	100	100
11	L	106/157 (68%)	99 (93%)	7 (7%)	14	41
12	M	574/608 (94%)	525 (92%)	49 (8%)	8	31
13	N	128/131 (98%)	115 (90%)	13 (10%)	6	25
14	O	180/206 (87%)	166 (92%)	14 (8%)	10	34
15	P	189/229 (82%)	174 (92%)	15 (8%)	10	34
16	Q	329/393 (84%)	308 (94%)	21 (6%)	14	41
17	S	59/59 (100%)	56 (95%)	3 (5%)	20	48

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	T	79/100 (79%)	72 (91%)	7 (9%)	8	30
19	U	72/73 (99%)	66 (92%)	6 (8%)	9	32
20	V	102/103 (99%)	97 (95%)	5 (5%)	21	49
21	W	115/123 (94%)	112 (97%)	3 (3%)	41	67
22	Y	54/87 (62%)	52 (96%)	2 (4%)	29	57
23	Z	56/79 (71%)	52 (93%)	4 (7%)	12	38
24	a	124/159 (78%)	122 (98%)	2 (2%)	58	76
25	b	113/122 (93%)	109 (96%)	4 (4%)	31	59
26	c	106/161 (66%)	100 (94%)	6 (6%)	17	45
27	d	145/155 (94%)	132 (91%)	13 (9%)	8	29
28	e	81/130 (62%)	79 (98%)	2 (2%)	42	67
29	f	43/67 (64%)	42 (98%)	1 (2%)	45	69
30	g	105/105 (100%)	102 (97%)	3 (3%)	37	64
31	h	86/92 (94%)	80 (93%)	6 (7%)	12	39
32	j	81/104 (78%)	76 (94%)	5 (6%)	15	42
33	k	72/85 (85%)	65 (90%)	7 (10%)	6	26
34	l	491/533 (92%)	458 (93%)	33 (7%)	13	40
35	m	130/137 (95%)	118 (91%)	12 (9%)	7	28
36	n	53/55 (96%)	47 (89%)	6 (11%)	4	21
37	o	86/115 (75%)	83 (96%)	3 (4%)	31	59
38	p	155/161 (96%)	151 (97%)	4 (3%)	41	67
39	r	416/416 (100%)	385 (92%)	31 (8%)	11	36
40	s	276/279 (99%)	254 (92%)	22 (8%)	10	33
41	u	153/155 (99%)	140 (92%)	13 (8%)	8	31
42	v	81/121 (67%)	79 (98%)	2 (2%)	42	67
44	i	271/314 (86%)	253 (93%)	18 (7%)	14	41
All	All	6551/7617 (86%)	6134 (94%)	417 (6%)	17	41

All (417) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	104	LYS
1	A	126	LYS

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Mol	Chain	Res	Type
1	A	175	GLU
1	A	192	ASP
1	A	241	THR
1	A	245	VAL
1	A	248	VAL
1	A	270	ASN
1	A	278	ILE
1	A	296	LEU
1	A	313	ASN
1	A	314	LEU
1	A	326	LEU
1	A	331	VAL
1	A	339	PHE
1	A	347	THR
1	A	379	CYS
1	A	386	ARG
1	A	390	ASP
1	A	412	LEU
1	A	423	THR
1	A	424	ILE
1	A	429	ASP
2	B	68	LEU
2	B	116	LEU
2	B	126	ILE
2	B	146	ASP
2	B	167	GLU
2	B	198	GLU
3	C	67	LEU
3	C	83	THR
3	C	84	PHE
3	C	88	CYS
3	C	93	MET
3	C	103	MET
3	C	108	VAL
3	C	110	PHE
3	C	119	VAL
3	C	166	VAL
3	C	203	ARG
4	E	17	VAL
4	E	82	LEU
5	F	20	ARG
5	F	25	GLN

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Mol	Chain	Res	Type
5	F	37	ILE
5	F	48	ASN
5	F	79	LEU
6	G	92	LYS
6	G	93	ILE
6	G	106	LYS
6	G	110	LEU
7	H	16	VAL
8	I	24	LEU
8	I	62	GLU
8	I	96	THR
8	I	106	LEU
9	J	85	ARG
9	J	94	LEU
9	J	111	ARG
9	J	134	TRP
9	J	145	PHE
9	J	174	ILE
9	J	211	ASP
9	J	214	LEU
9	J	226	ILE
9	J	235	THR
9	J	240	VAL
9	J	266	VAL
9	J	283	VAL
9	J	329	LEU
9	J	340	ILE
9	J	350	ILE
9	J	366	ILE
11	L	60	ASP
11	L	72	ILE
11	L	81	VAL
11	L	91	VAL
11	L	119	ASP
11	L	125	VAL
11	L	164	PHE
12	M	32	ILE
12	M	36	VAL
12	M	67	GLU
12	M	71	VAL
12	M	139	LEU
12	M	146	PHE

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Mol	Chain	Res	Type
12	M	155	GLU
12	M	179	CYS
12	M	204	MET
12	M	205	GLN
12	M	208	THR
12	M	210	ILE
12	M	215	MET
12	M	225	ILE
12	M	299	ARG
12	M	302	LEU
12	M	314	LEU
12	M	319	TRP
12	M	321	ASP
12	M	323	LEU
12	M	351	LEU
12	M	358	LEU
12	M	366	LEU
12	M	368	THR
12	M	384	ASN
12	M	389	THR
12	M	405	THR
12	M	443	ASP
12	M	453	GLN
12	M	466	LEU
12	M	490	LEU
12	M	499	LYS
12	M	506	VAL
12	M	515	ILE
12	M	519	ILE
12	M	523	VAL
12	M	537	ILE
12	M	543	LYS
12	M	545	LEU
12	M	547	LEU
12	M	566	ILE
12	M	610	VAL
12	M	634	LEU
12	M	648	GLU
12	M	649	VAL
12	M	659	ILE
12	M	665	PHE
12	M	691	ILE

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Mol	Chain	Res	Type
12	M	693	ASP
13	N	17	HIS
13	N	39	VAL
13	N	42	ASP
13	N	51	ASP
13	N	59	HIS
13	N	61	TRP
13	N	73	THR
13	N	74	PHE
13	N	90	LEU
13	N	94	THR
13	N	117	VAL
13	N	129	THR
13	N	134	ILE
14	O	40	VAL
14	O	51	THR
14	O	95	ILE
14	O	121	MET
14	O	123	ASN
14	O	134	VAL
14	O	136	THR
14	O	137	THR
14	O	138	THR
14	O	149	LEU
14	O	174	VAL
14	O	201	ILE
14	O	225	CYS
14	O	231	LEU
15	P	65	VAL
15	P	81	PHE
15	P	84	LEU
15	P	104	THR
15	P	133	LEU
15	P	148	ASP
15	P	149	GLU
15	P	171	TRP
15	P	180	ASN
15	P	187	ILE
15	P	200	LYS
15	P	208	VAL
15	P	210	LEU
15	P	224	VAL

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Mol	Chain	Res	Type
15	P	232	LYS
16	Q	82	LEU
16	Q	95	LEU
16	Q	97	LEU
16	Q	101	LEU
16	Q	113	ILE
16	Q	173	LEU
16	Q	178	THR
16	Q	235	ASP
16	Q	258	LEU
16	Q	261	LEU
16	Q	268	TRP
16	Q	309	ASP
16	Q	310	VAL
16	Q	356	ILE
16	Q	371	MET
16	Q	374	SER
16	Q	432	LEU
16	Q	435	LEU
16	Q	443	MET
16	Q	444	LEU
16	Q	463	ARG
17	S	50	ARG
17	S	54	ILE
17	S	60	TYR
18	T	48	ASP
18	T	60	GLN
18	T	69	ILE
18	T	70	ASP
18	T	85	ILE
18	T	115	CYS
18	T	117	LEU
19	U	11	ASN
19	U	14	ASP
19	U	40	LYS
19	U	59	ASP
19	U	63	MET
19	U	69	HIS
20	V	17	ASP
20	V	89	ASN
20	V	105	THR
20	V	115	CYS

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Mol	Chain	Res	Type
20	V	130	LEU
21	W	50	ILE
21	W	74	LEU
21	W	110	VAL
6	X	91	ASP
6	X	113	LEU
22	Y	43	ARG
22	Y	88	ASP
23	Z	42	ARG
23	Z	48	ASN
23	Z	53	TYR
23	Z	65	ASP
24	a	98	LEU
24	a	106	VAL
25	b	28	LEU
25	b	92	GLU
25	b	101	LYS
25	b	113	THR
26	c	63	GLU
26	c	67	ASP
26	c	110	ASP
26	c	144	CYS
26	c	156	VAL
26	c	173	ASP
27	d	24	ILE
27	d	33	LEU
27	d	49	GLN
27	d	65	VAL
27	d	67	ASP
27	d	68	ILE
27	d	97	ILE
27	d	104	LEU
27	d	107	CYS
27	d	108	GLN
27	d	109	GLN
27	d	137	TYR
27	d	150	LEU
28	e	137	MET
28	e	141	CYS
29	f	58	LEU
30	g	8	GLU
30	g	29	ARG

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Mol	Chain	Res	Type
30	g	111	ILE
31	h	5	ASP
31	h	20	ILE
31	h	37	GLU
31	h	47	ILE
31	h	93	THR
31	h	99	ILE
32	j	18	MET
32	j	63	LEU
32	j	67	LEU
32	j	98	LEU
32	j	111	LEU
33	k	1	MET
33	k	10	LEU
33	k	16	LEU
33	k	33	LEU
33	k	61	ILE
33	k	64	LEU
33	k	78	LEU
34	l	10	LEU
34	l	12	LEU
34	l	37	LYS
34	l	39	ILE
34	l	67	HIS
34	l	71	THR
34	l	78	LEU
34	l	114	ILE
34	l	122	LEU
34	l	125	LEU
34	l	139	GLN
34	l	191	LEU
34	l	196	TRP
34	l	203	LEU
34	l	205	ASN
34	l	213	LEU
34	l	217	LEU
34	l	233	LEU
34	l	243	VAL
34	l	246	LEU
34	l	252	MET
34	l	253	VAL
34	l	254	VAL

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Mol	Chain	Res	Type
34	l	301	ILE
34	l	314	MET
34	l	324	LEU
34	l	332	HIS
34	l	368	LEU
34	l	373	LEU
34	l	442	ASN
34	l	481	THR
34	l	482	ILE
34	l	514	LYS
35	m	26	ILE
35	m	51	MET
35	m	56	PHE
35	m	57	LEU
35	m	65	VAL
35	m	96	LEU
35	m	113	VAL
35	m	118	PHE
35	m	134	LEU
35	m	135	ILE
35	m	140	ILE
35	m	172	ARG
36	n	11	HIS
36	n	15	VAL
36	n	16	LEU
36	n	38	PHE
36	n	50	GLN
36	n	55	VAL
37	o	37	LEU
37	o	55	ASN
37	o	123	ARG
38	p	19	LEU
38	p	48	PHE
38	p	81	ILE
38	p	150	LEU
39	r	14	LEU
39	r	61	LEU
39	r	73	LEU
39	r	82	ARG
39	r	102	LEU
39	r	114	GLU
39	r	116	ILE

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Mol	Chain	Res	Type
39	r	138	ASN
39	r	150	LEU
39	r	154	LEU
39	r	201	MET
39	r	213	HIS
39	r	215	TRP
39	r	216	LEU
39	r	231	LEU
39	r	247	THR
39	r	294	MET
39	r	307	TRP
39	r	315	LEU
39	r	325	LEU
39	r	369	LEU
39	r	375	LEU
39	r	376	LEU
39	r	379	LEU
39	r	419	LEU
39	r	420	THR
39	r	424	ASN
39	r	425	ASN
39	r	431	THR
39	r	441	LEU
39	r	454	ILE
40	s	6	LEU
40	s	28	LEU
40	s	33	LEU
40	s	77	LEU
40	s	79	LEU
40	s	87	THR
40	s	89	LEU
40	s	91	MET
40	s	103	LEU
40	s	129	LEU
40	s	140	ILE
40	s	150	LEU
40	s	151	LEU
40	s	165	LEU
40	s	172	LEU
40	s	224	PHE
40	s	285	LEU
40	s	287	HIS

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Mol	Chain	Res	Type
40	s	288	LEU
40	s	294	LEU
40	s	296	LEU
40	s	311	ILE
41	u	20	ILE
41	u	24	VAL
41	u	30	HIS
41	u	37	ASP
41	u	42	GLU
41	u	48	TRP
41	u	89	ILE
41	u	90	ASP
41	u	103	GLN
41	u	111	VAL
41	u	124	GLU
41	u	128	VAL
41	u	172	LYS
42	v	5	LEU
42	v	63	LEU
44	i	29	THR
44	i	33	LEU
44	i	70	LEU
44	i	71	LEU
44	i	85	THR
44	i	124	LEU
44	i	154	LEU
44	i	171	ASN
44	i	193	VAL
44	i	194	LEU
44	i	214	THR
44	i	241	THR
44	i	261	LEU
44	i	273	ASN
44	i	286	THR
44	i	328	THR
44	i	330	ILE
44	i	339	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN

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Mol	Chain	Res	Type
1	A	220	GLN
1	A	270	ASN
1	A	393	ASN
1	A	456	GLN
2	B	157	GLN
2	B	190	ASN
2	B	204	GLN
3	C	196	GLN
4	E	48	HIS
4	E	49	GLN
4	E	51	GLN
5	F	81	ASN
6	G	101	ASN
7	H	71	GLN
7	H	73	GLN
7	H	86	HIS
8	I	21	GLN
9	J	71	ASN
9	J	102	GLN
9	J	122	HIS
9	J	166	HIS
9	J	183	ASN
9	J	221	HIS
9	J	275	HIS
10	K	98	GLN
11	L	86	ASN
12	M	59	GLN
12	M	101	ASN
12	M	140	GLN
12	M	205	GLN
12	M	359	ASN
12	M	388	ASN
12	M	425	ASN
12	M	514	ASN
12	M	652	ASN
12	M	663	ASN
12	M	666	GLN
12	M	688	GLN
13	N	12	GLN
13	N	31	ASN
13	N	69	ASN
13	N	113	HIS

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Mol	Chain	Res	Type
13	N	135	GLN
14	O	41	HIS
14	O	69	ASN
14	O	74	HIS
14	O	99	ASN
14	O	191	ASN
15	P	196	HIS
16	Q	147	ASN
16	Q	168	GLN
16	Q	182	ASN
16	Q	190	HIS
16	Q	246	GLN
16	Q	339	GLN
16	Q	431	HIS
17	S	68	ASN
18	T	75	GLN
19	U	52	ASN
21	W	24	ASN
21	W	61	GLN
21	W	76	GLN
6	X	142	GLN
23	Z	12	HIS
24	a	181	HIS
24	a	189	ASN
25	b	83	HIS
26	c	56	ASN
26	c	132	GLN
26	c	154	GLN
26	c	164	ASN
27	d	20	GLN
27	d	50	HIS
27	d	59	HIS
27	d	101	GLN
27	d	109	GLN
27	d	113	GLN
27	d	116	GLN
29	f	61	GLN
30	g	45	ASN
31	h	82	GLN
31	h	97	HIS
32	j	10	ASN
33	k	25	HIS

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Mol	Chain	Res	Type
34	l	59	GLN
34	l	139	GLN
34	l	192	HIS
34	l	199	GLN
34	l	207	ASN
34	l	226	GLN
34	l	230	HIS
34	l	505	ASN
35	m	45	ASN
36	n	40	ASN
36	n	50	GLN
37	o	62	ASN
37	o	79	ASN
38	p	12	HIS
39	r	83	HIS
39	r	138	ASN
39	r	168	HIS
39	r	175	ASN
39	r	319	HIS
39	r	415	GLN
39	r	422	HIS
40	s	99	ASN
40	s	169	GLN
40	s	230	ASN
40	s	235	ASN
41	u	95	GLN
41	u	99	HIS
41	u	103	GLN
41	u	104	GLN
41	u	140	ASN
41	u	143	HIS
42	v	50	GLN
42	v	85	HIS
44	i	36	ASN
44	i	134	GLN
44	i	273	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
46	FMN	A	502	-	33,33,33	1.07	2 (6%)	48,50,50	1.25	7 (14%)
45	SF4	M	802	12	0,12,12	-	-	-		
49	FES	O	301	14	0,4,4	-	-	-		
45	SF4	B	302	2	0,12,12	-	-	-		
45	SF4	C	301	3	0,12,12	-	-	-		
47	ZMP	E	201	-	27,29,36	1.76	6 (22%)	34,38,45	1.66	6 (17%)
45	SF4	B	301	2	0,12,12	-	-	-		
45	SF4	A	501	1	0,12,12	-	-	-		
48	NDP	J	401	-	47,52,52	0.65	0	61,80,80	0.81	3 (4%)
49	FES	M	803	12	0,4,4	-	-	-		
45	SF4	M	801	12	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
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
45	SF4	M	802	12	-	-	0/6/5/5
49	FES	O	301	14	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	SF4	B	302	2	-	-	0/6/5/5
45	SF4	C	301	3	-	-	0/6/5/5
47	ZMP	E	201	-	-	13/36/36/43	-
45	SF4	B	301	2	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
48	NDP	J	401	-	-	2/30/77/77	0/5/5/5
49	FES	M	803	12	-	-	0/1/1/1
45	SF4	M	801	12	-	-	0/6/5/5

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	E	201	ZMP	C16-N2	5.22	1.45	1.33
47	E	201	ZMP	C13-N1	5.11	1.45	1.33
46	A	502	FMN	C4A-N5	3.46	1.38	1.30
46	A	502	FMN	C10-N1	2.53	1.38	1.33
47	E	201	ZMP	C10-S1	2.44	1.82	1.76
47	E	201	ZMP	O3-C16	-2.22	1.19	1.23
47	E	201	ZMP	O2-C13	-2.19	1.18	1.23
47	E	201	ZMP	C9-C10	2.15	1.53	1.50

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	E	201	ZMP	C9-C10-S1	5.82	120.34	113.40
48	J	401	NDP	P2B-O2B-C2B	-3.66	113.66	123.43
47	E	201	ZMP	O1-C10-C9	-3.61	119.81	123.98
46	A	502	FMN	C4-N3-C2	-3.18	120.00	125.64
46	A	502	FMN	C5A-C9A-N10	2.85	120.55	117.97
46	A	502	FMN	C4A-C4-N3	2.58	119.82	113.25
46	A	502	FMN	C9A-C5A-N5	-2.49	119.82	122.45
46	A	502	FMN	O4-C4-C4A	-2.48	119.99	126.53
48	J	401	NDP	O4D-C1D-C2D	-2.41	101.45	106.62
47	E	201	ZMP	C11-S1-C10	2.40	108.95	101.84
46	A	502	FMN	C4A-C10-N10	2.34	119.83	116.48
47	E	201	ZMP	O1-C10-S1	-2.23	119.85	122.68
48	J	401	NDP	C5A-C6A-N6A	2.21	123.68	120.31
47	E	201	ZMP	C14-C13-N1	2.15	120.26	116.34
46	A	502	FMN	C10-C4A-N5	-2.09	120.53	124.81
47	E	201	ZMP	C20-C18-C17	2.08	112.31	108.77

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	C3'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O2P
46	A	502	FMN	C5'-O5'-P-O3P
47	E	201	ZMP	O4-C17-C18-C21
47	E	201	ZMP	C16-C17-C18-C21
47	E	201	ZMP	O4-C17-C18-C19
47	E	201	ZMP	C16-C17-C18-C19
47	E	201	ZMP	C16-C17-C18-C20
47	E	201	ZMP	C13-C14-C15-N2
48	J	401	NDP	C5D-O5D-PN-O1N
48	J	401	NDP	O4D-C1D-N1N-C6N
47	E	201	ZMP	C6-C7-C8-C9
46	A	502	FMN	O4'-C4'-C5'-O5'
46	A	502	FMN	C5'-O5'-P-O1P
47	E	201	ZMP	O4-C17-C18-C20
47	E	201	ZMP	C7-C8-C9-C10
47	E	201	ZMP	O3-C16-C17-O4
47	E	201	ZMP	O3-C16-C17-C18
47	E	201	ZMP	N2-C16-C17-C18
47	E	201	ZMP	N2-C16-C17-O4
46	A	502	FMN	N10-C1'-C2'-O2'

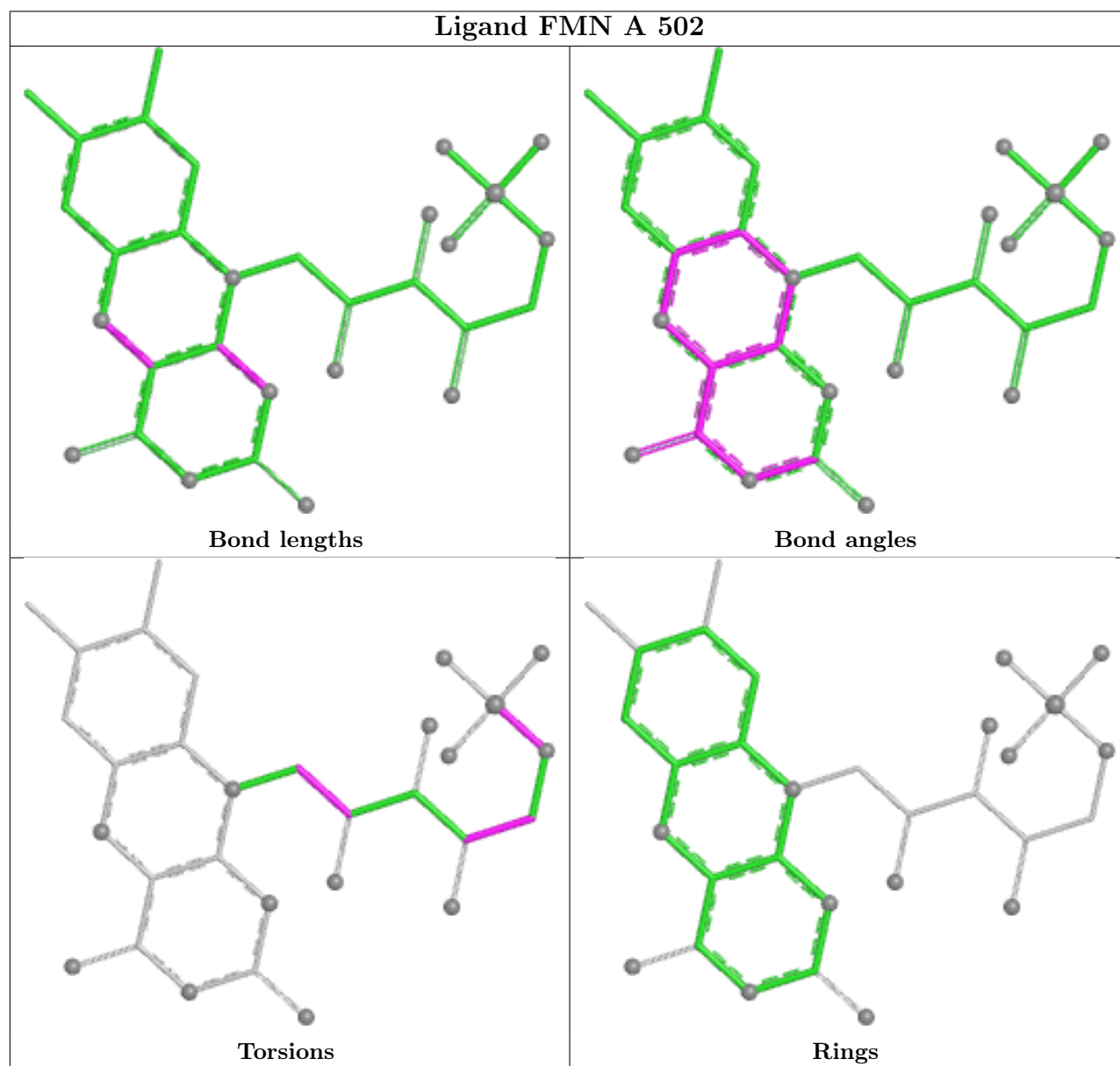
There are no ring outliers.

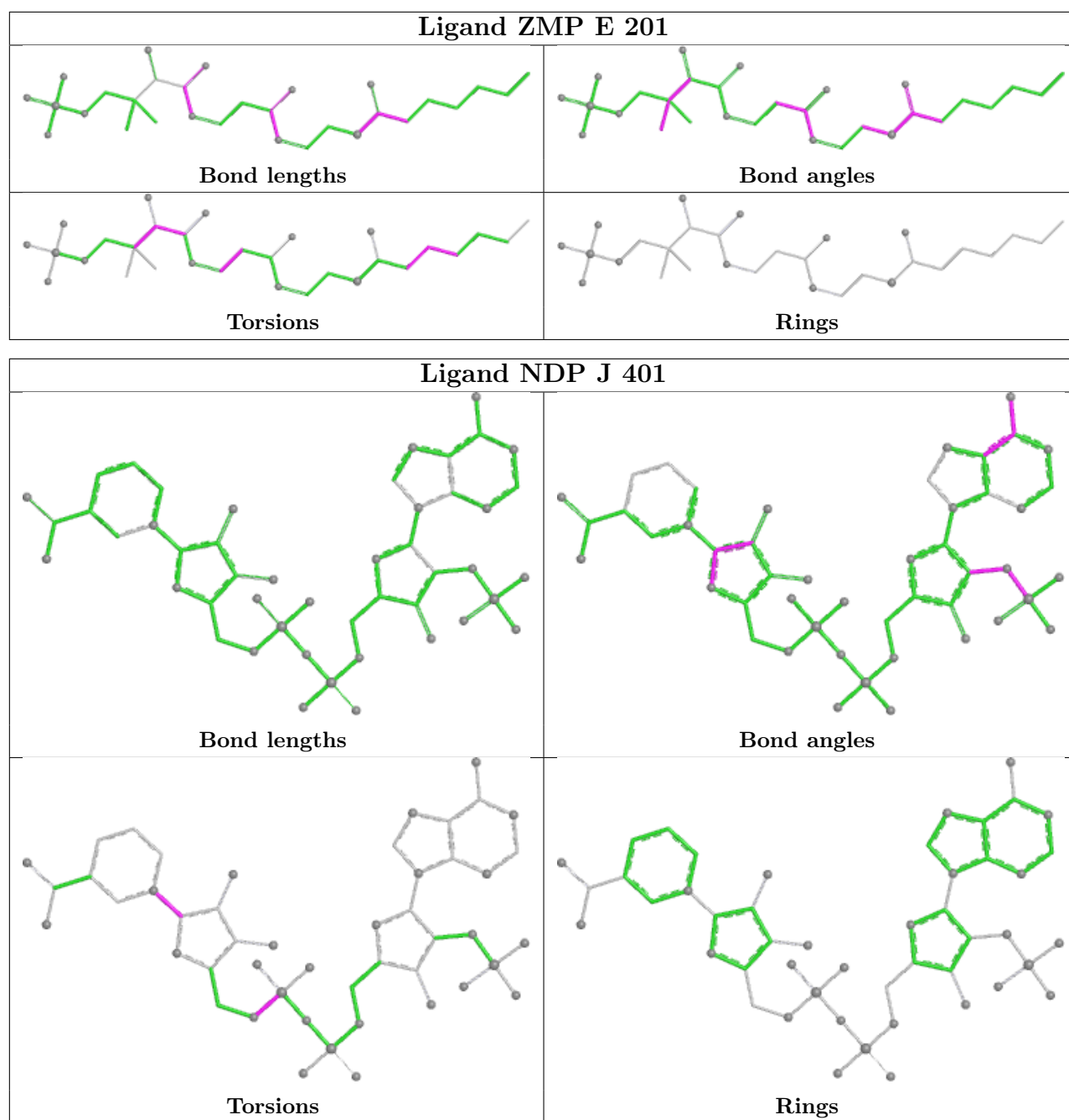
8 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	A	502	FMN	2	0
45	B	302	SF4	3	0
45	C	301	SF4	4	0
47	E	201	ZMP	1	0
45	B	301	SF4	1	0
45	A	501	SF4	2	0
48	J	401	NDP	1	0
45	M	801	SF4	1	0

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

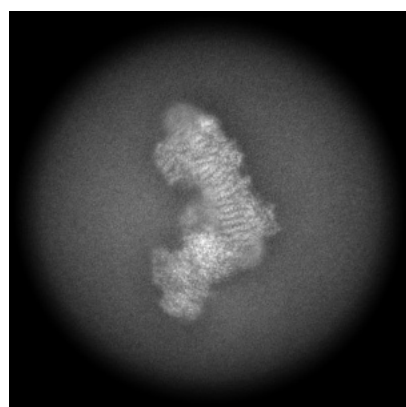
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-45974. These allow visual inspection of the internal detail of the map and identification of artifacts.

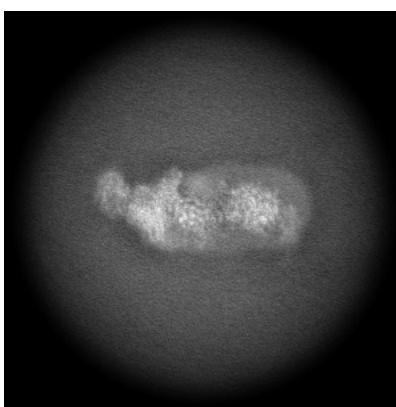
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

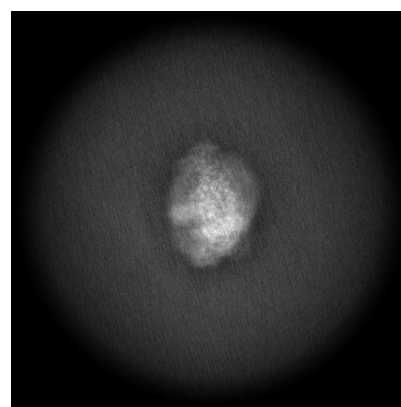
6.1.1 Primary map



X



Y

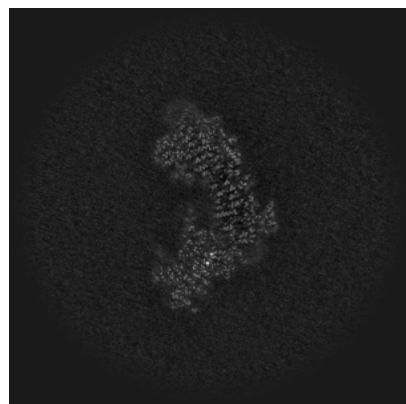


Z

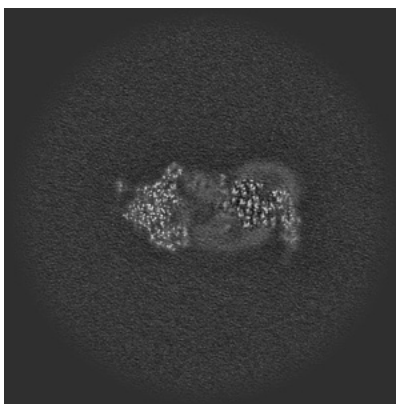
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

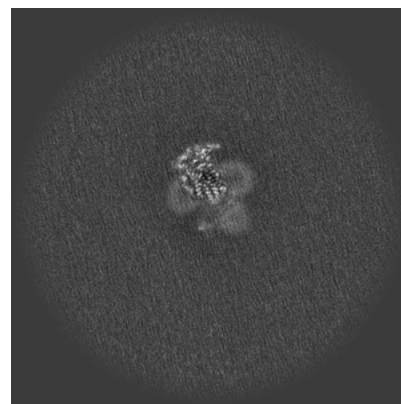
6.2.1 Primary map



X Index: 256



Y Index: 256

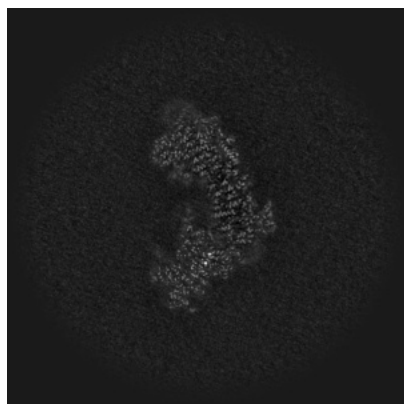


Z Index: 256

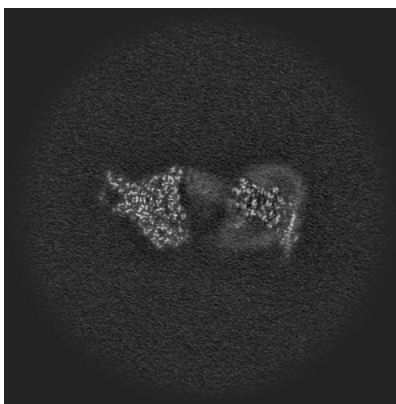
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

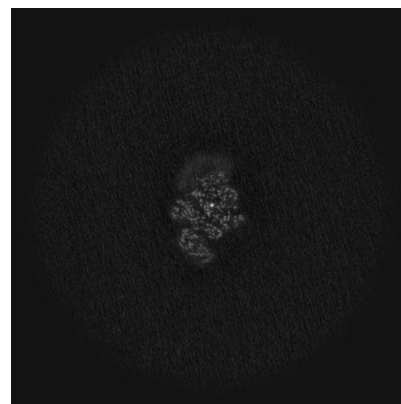
6.3.1 Primary map



X Index: 256



Y Index: 246

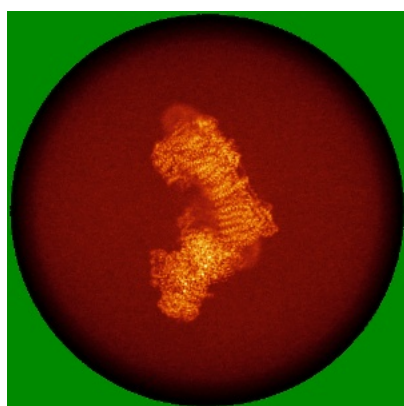


Z Index: 196

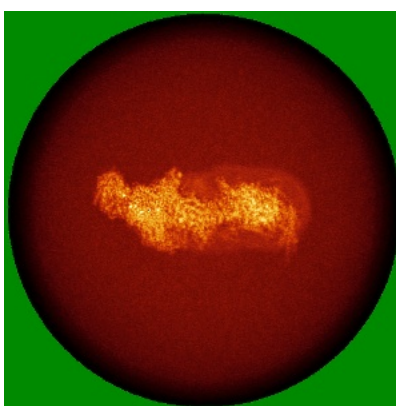
The images above show the largest variance slices of the map in three orthogonal directions.

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

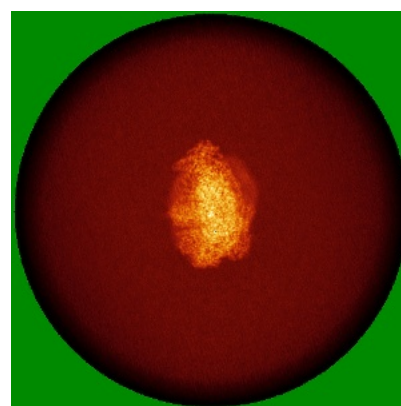
6.4.1 Primary map



X



Y

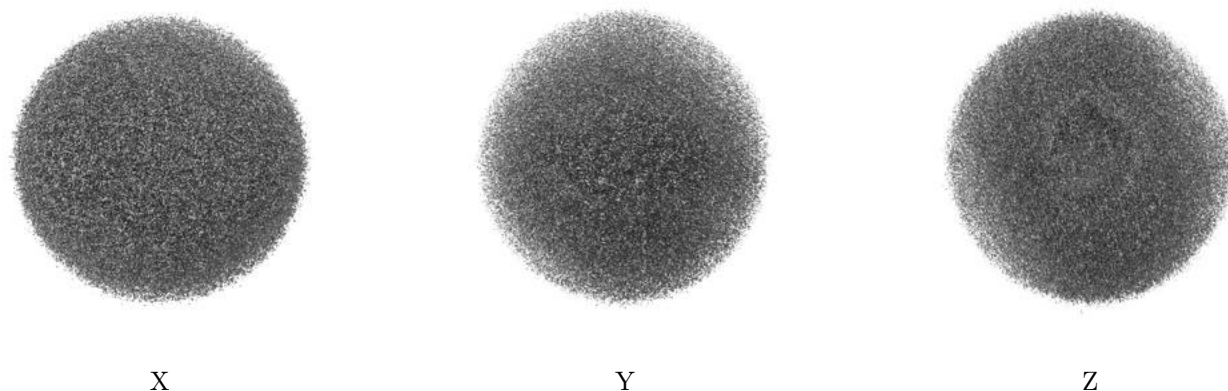


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.135. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

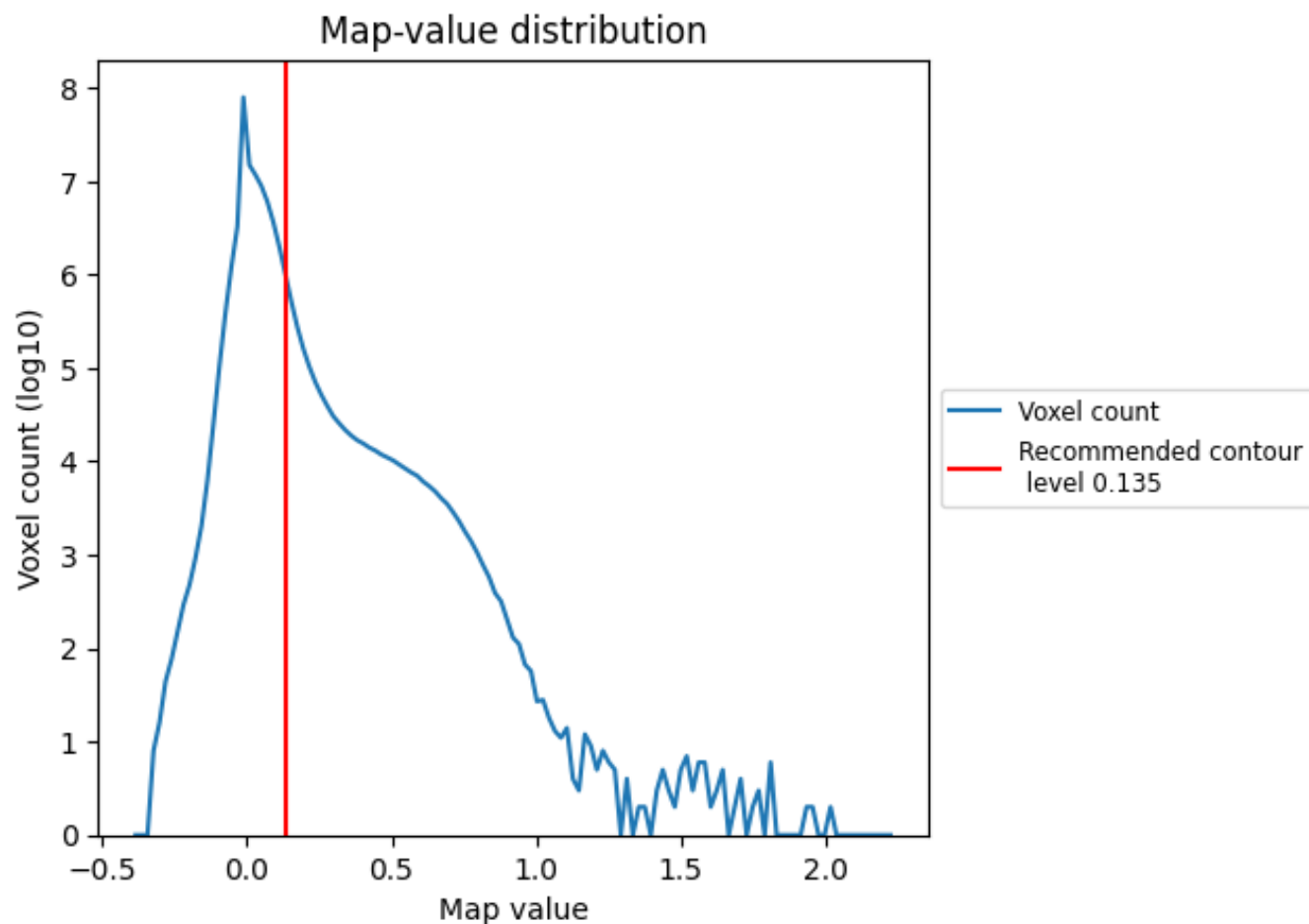
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

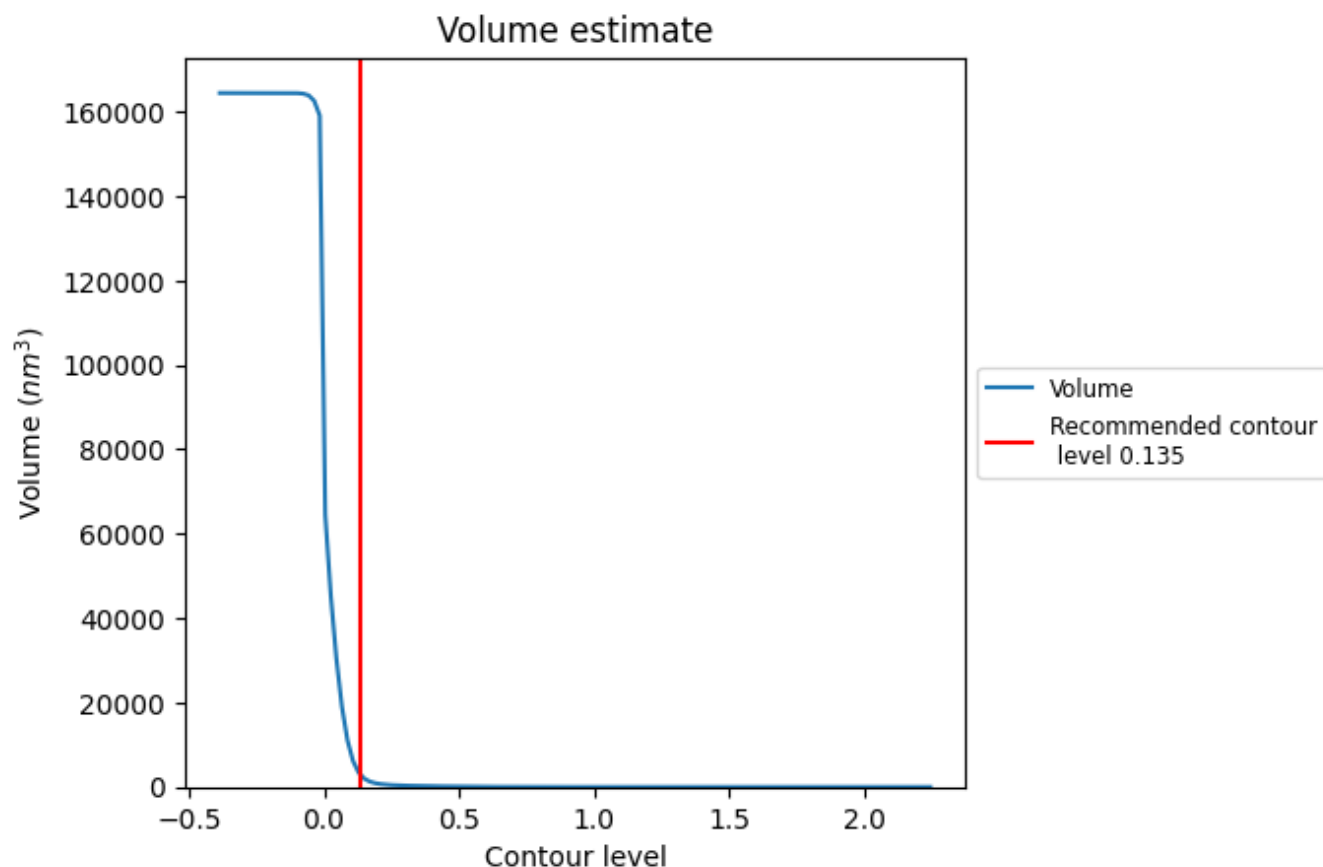
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

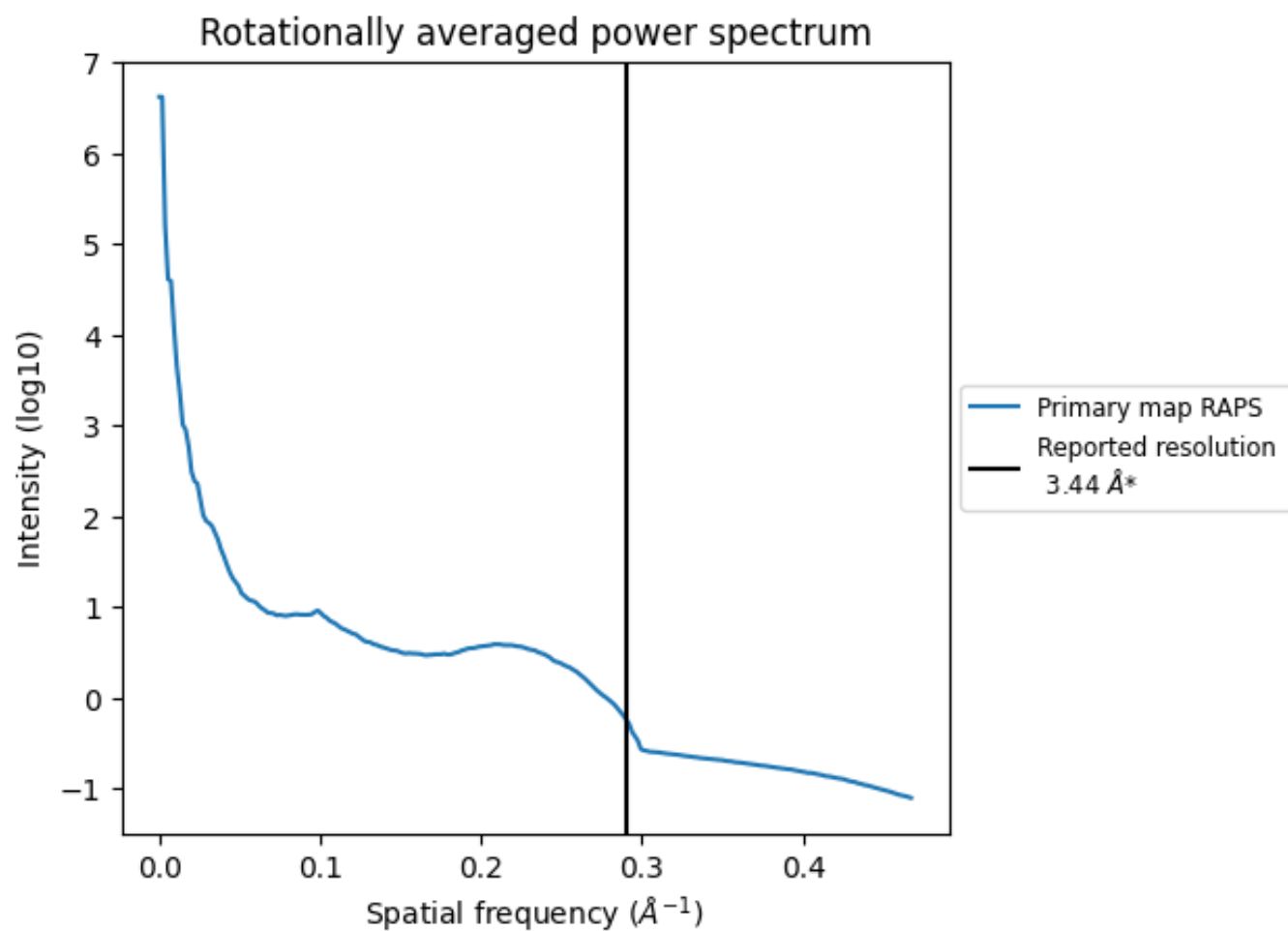
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2955 nm^3 ; this corresponds to an approximate mass of 2670 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 0.291 Å⁻¹

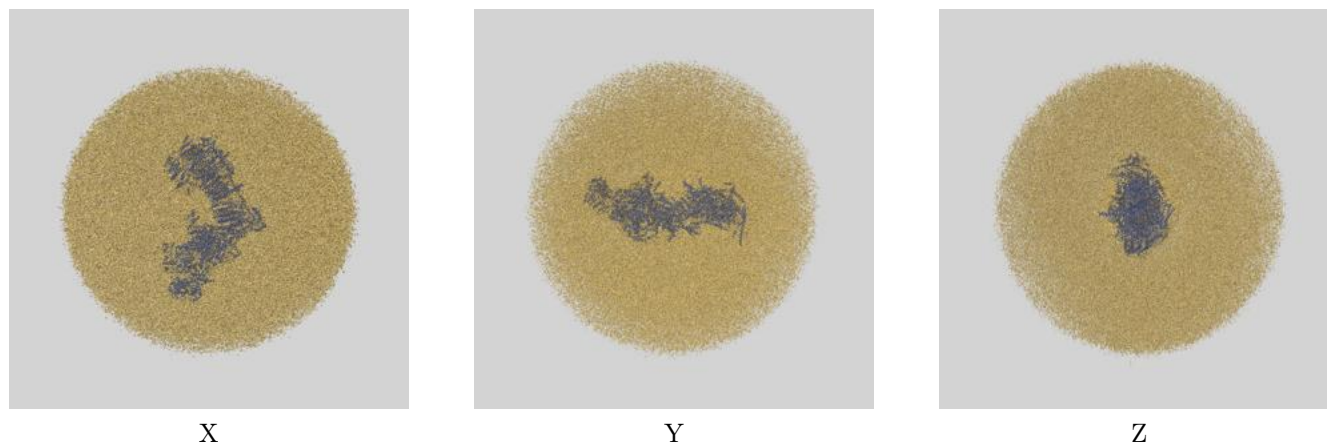
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-45974 and PDB model 9CWT. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



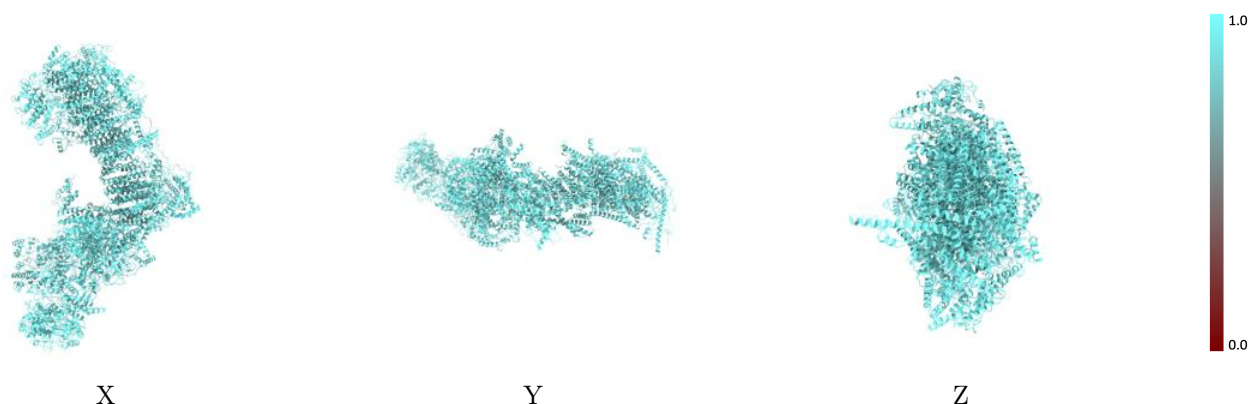
The images above show the 3D surface view of the map at the recommended contour level 0.135 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



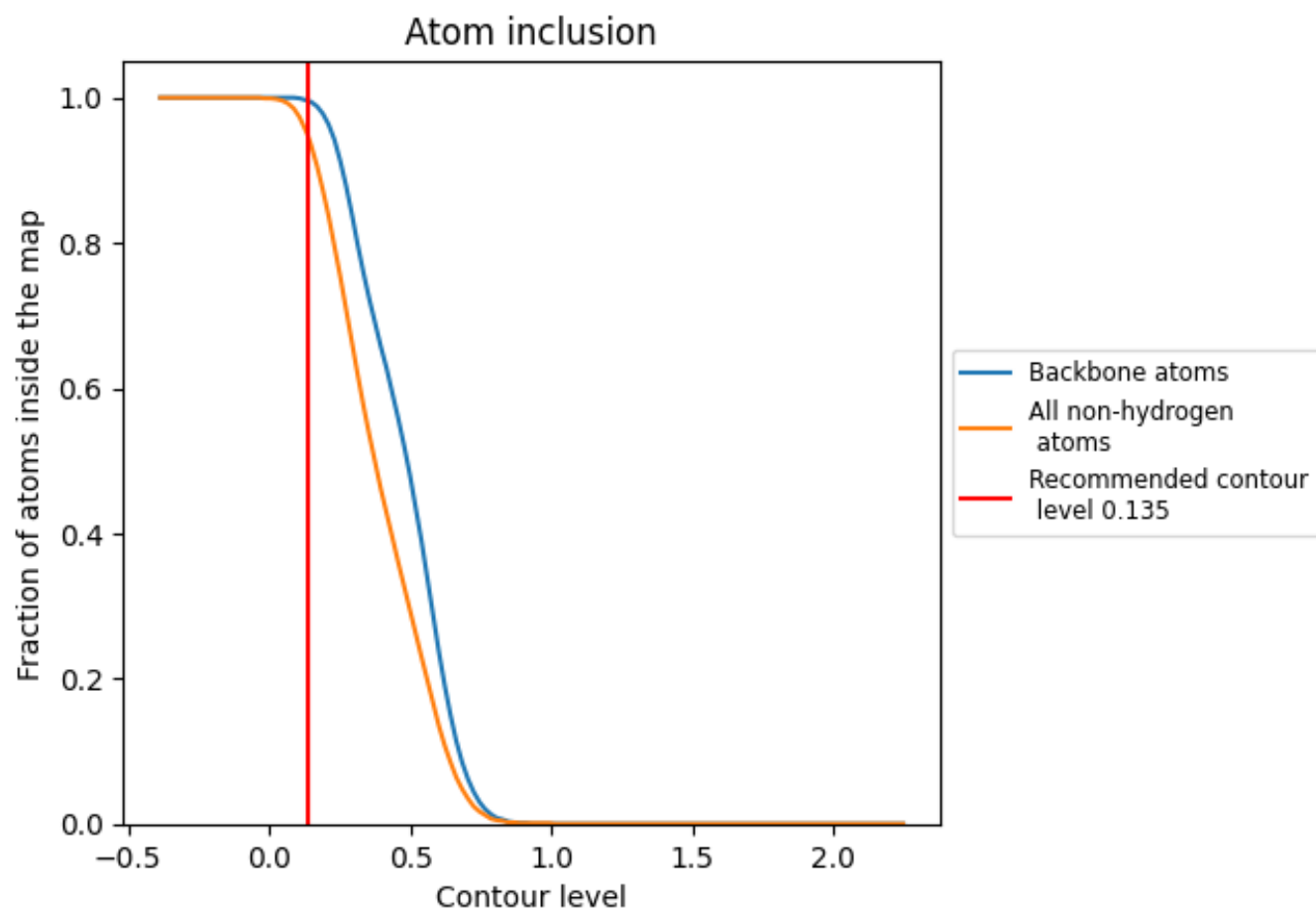
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.135).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 95% 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 (0.135) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9500	 0.4190
A	 0.9710	 0.4220
B	 0.9700	 0.4590
C	 0.9570	 0.4600
D	 0.9910	 0.4220
E	 0.9390	 0.4200
F	 0.9290	 0.3780
G	 0.9170	 0.3100
H	 0.9390	 0.3980
I	 0.9300	 0.4290
J	 0.9480	 0.3920
K	 0.9500	 0.4140
L	 0.9540	 0.4610
M	 0.9560	 0.4230
N	 0.9460	 0.4350
O	 0.9590	 0.4160
P	 0.9730	 0.4580
Q	 0.9590	 0.4460
S	 0.9580	 0.4500
T	 0.9570	 0.4510
U	 0.9550	 0.4240
V	 0.9150	 0.2990
W	 0.9620	 0.4340
X	 0.9620	 0.4040
Y	 0.9820	 0.3810
Z	 0.9680	 0.4220
a	 0.9580	 0.4550
b	 0.9650	 0.3730
c	 0.9500	 0.3490
d	 0.9690	 0.4370
e	 0.9590	 0.4380
f	 0.9210	 0.3270
g	 0.9510	 0.4400
h	 0.9440	 0.4350
i	 0.9330	 0.4560



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Chain	Atom inclusion	Q-score
j	 0.9020	 0.4140
k	 0.9310	 0.4430
l	 0.9400	 0.3910
m	 0.9350	 0.4160
n	 0.9410	 0.3930
o	 0.9470	 0.3650
p	 0.9520	 0.4040
r	 0.9470	 0.4430
s	 0.9240	 0.4310
u	 0.9430	 0.4210
v	 0.9660	 0.3720