



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:17 PM UTC

PDB ID : 7ZDJ / pdb_00007zdj
EMDB ID : EMD-14651
Title : Complex I from *Ovis aries* at pH5.5, Open state
Authors : Petrova, O.; Sazanov, L.
Deposited on : 2022-03-29
Resolution : 3.25 Å (reported)
Based on initial model : 6ZKE

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

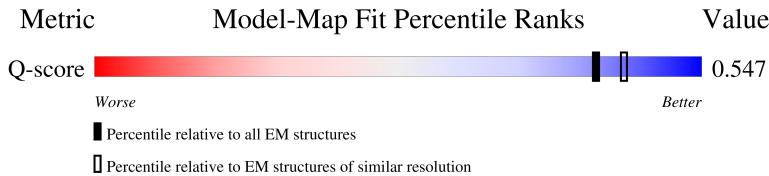
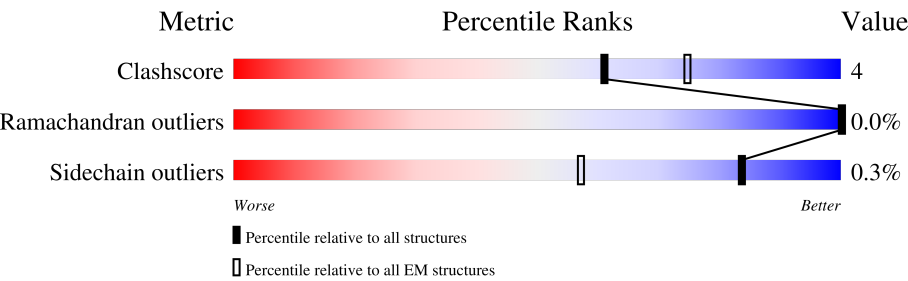
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.25 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



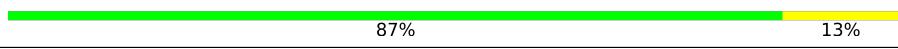
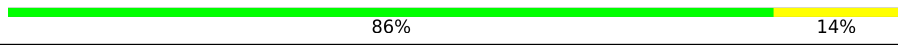
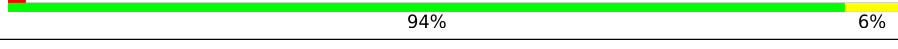
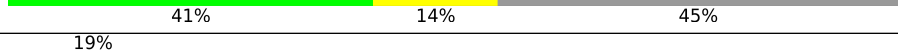
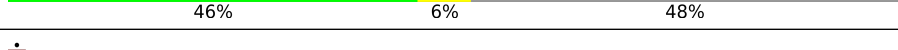
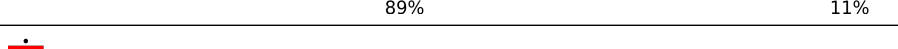
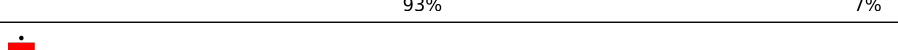
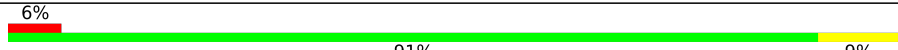
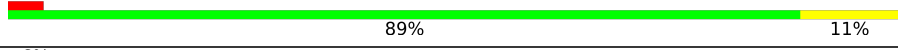
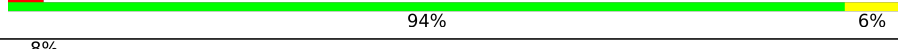
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14599 (2.75 - 3.75)

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	4	463	 78% 13% 9%
2	A	115	 9% 85% 10% .
3	H	318	 85% 14% .
4	J	175	 79% 17% .

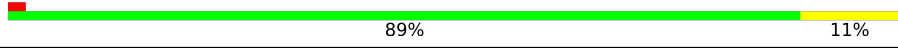
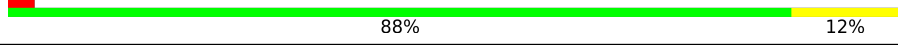
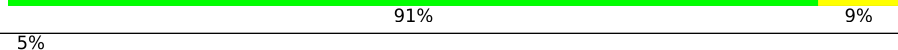
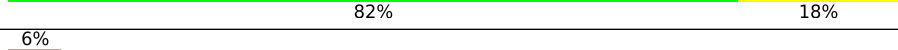
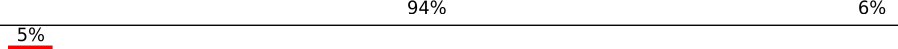
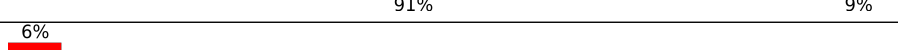
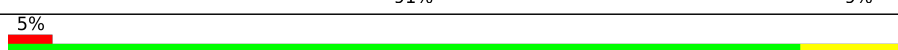
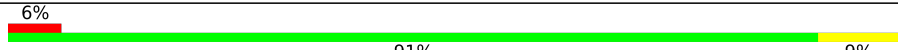
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Mol	Chain	Length	Quality of chain
5	K	98	
6	L	606	
7	M	459	
8	N	347	
9	V	140	
10	W	139	
11	X	157	
11	j	157	
12	Y	171	
13	Z	171	
14	k	320	
15	l	105	
16	m	80	
17	n	79	
18	o	120	
19	p	128	
20	q	144	
21	r	128	
22	s	122	
23	t	177	
24	u	65	
25	v	155	
26	w	101	
27	x	49	
28	y	50	

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Mol	Chain	Length	Quality of chain
29	z	70	
30	1	430	
31	2	213	
32	3	688	
33	5	208	
34	6	156	
35	9	176	
36	a	44	
37	b	95	
38	c	126	
39	d	380	
40	e	86	
41	f	113	
42	g	114	
43	h	114	
44	i	145	

2 Entry composition

There are 53 unique types of molecules in this entry. The entry contains 65812 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 Complex I-49kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	4	421	Total	C	N	O	S	0	0
			3390	2165	581	619	25		

- Molecule 2 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	110	Total	C	N	O	S	0	0
			880	593	128	153	6		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	314	Total	C	N	O	S	0	0
			2498	1685	380	414	19		

- Molecule 4 is a protein called NADH-ubiquinone oxidoreductase chain 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	169	Total	C	N	O	S	0	0
			1294	870	185	226	13		

- Molecule 5 is a protein called NADH-ubiquinone oxidoreductase chain 4L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	98	Total	C	N	O	S	0	0
			749	490	112	132	15		

- Molecule 6 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	606	Total	C	N	O	S	0	0
			4806	3187	746	829	44		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	459	Total	C	N	O	S	0	0
			3647	2429	571	607	40		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	347	Total	C	N	O	S	0	0
			2723	1808	416	459	40		

- Molecule 9 is a protein called Complex I-B14.7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	140	Total	C	N	O	S	0	0
			1028	656	175	191	6		

- Molecule 10 is a protein called Complex I-SGDH.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	139	Total	C	N	O	S	0	0
			1155	761	194	198	2		

- Molecule 11 is a protein called Acyl carrier protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	87	Total	C	N	O	S	0	0
			701	451	103	142	5		
11	j	82	Total	C	N	O	S	0	0
			660	425	98	132	5		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	171	Total	C	N	O	S	0	0
			1403	889	253	251	10		

- Molecule 13 is a protein called Complex I-PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	171	Total	C	N	O	S	0	0
			1441	905	266	262	8		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	k	320	Total	C	N	O	P	S	0	0
			2596	1659	432	494	1	10		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	l	105	Total	C	N	O	S	0	0
			874	551	164	153	6		

- Molecule 16 is a protein called Complex I-B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	m	80	Total	C	N	O	S	0	0
			626	411	103	110	2		

- Molecule 17 is a protein called Complex I-B12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	n	79	Total	C	N	O	S	0	0
			634	415	106	111	2		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	o	120	Total	C	N	O	S	0	0
			1004	652	175	172	5		

- Molecule 19 is a protein called NADH:ubiquinone oxidoreductase subunit B4.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	p	128	Total	C	N	O	S	0	0
			1059	675	189	194	1		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	q	139	Total	C	N	O	S	0	0
			1142	733	200	200	9		

- Molecule 21 is a protein called Mitochondrial complex I, B17 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	r	99	Total	C	N	O	S	0	0
			846	554	149	142	1		

- Molecule 22 is a protein called Complex I-B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	s	122	Total	C	N	O	S	0	0
			1047	653	199	186	9		

- Molecule 23 is a protein called Complex I-B22.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	t	177	Total	C	N	O	S	0	0
			1520	973	279	262	6		

- Molecule 24 is a protein called Complex I-AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	u	65	Total	C	N	O	S	0	0
			563	372	93	97	1		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	v	155	Total	C	N	O	S	0	0
			1307	846	213	239	9		

- Molecule 26 is a protein called Complex I-ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	w	101	Total	C	N	O	S	0	0
			846	542	140	160	4		

- Molecule 27 is a protein called Complex I-KFYI.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	x	49	Total	C	N	O	0	0
			412	271	70	71		

- Molecule 28 is a protein called Complex I-MNLL.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	y	50	Total	C	N	O	0	0
			436	287	77	72		

- Molecule 29 is a protein called Complex I-MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	z	70	Total	C	N	O	S	0	0
			576	369	106	96	5		

- Molecule 30 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	1	430	Total	C	N	O	S	0	0
			3312	2086	593	613	20		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	2	213	Total	C	N	O	S	0	0
			1655	1058	278	309	10		

- Molecule 32 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	3	688	Total	C	N	O	S	0	0
			5275	3301	922	1011	41		

- Molecule 33 is a protein called Complex I-30kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	5	208	Total	C	N	O	S	0	0
			1726	1112	296	315	3		

- Molecule 34 is a protein called Complex I-20kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	6	156	Total	C	N	O	S	0	0
			1247	795	225	213	14		

- Molecule 35 is a protein called Complex I-23kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	176	Total	C	N	O	S	0	0
			1414	889	243	270	12		

- Molecule 36 is a protein called Complex I-9kD.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	a	44	Total	C	N	O	S	0	0
			371	233	66	71	1		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	b	95	Total	C	N	O	S	0	0
			737	451	139	144	3		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	c	126	Total	C	N	O	S	0	0
			1024	646	182	193	3		

- Molecule 39 is a protein called NADH:ubiquinone oxidoreductase subunit A9.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	d	297	Total	C	N	O	S	0	0
			2372	1516	432	419	5		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	e	86	Total	C	N	O	S	0	0
			691	434	129	126	2		

- Molecule 41 is a protein called Complex I subunit B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	f	113	Total	C	N	O	S	0	0
			917	595	153	167	2		

- Molecule 42 is a protein called Complex I-B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	g	114	Total	C	N	O	S	0	0
			969	619	180	166	4		

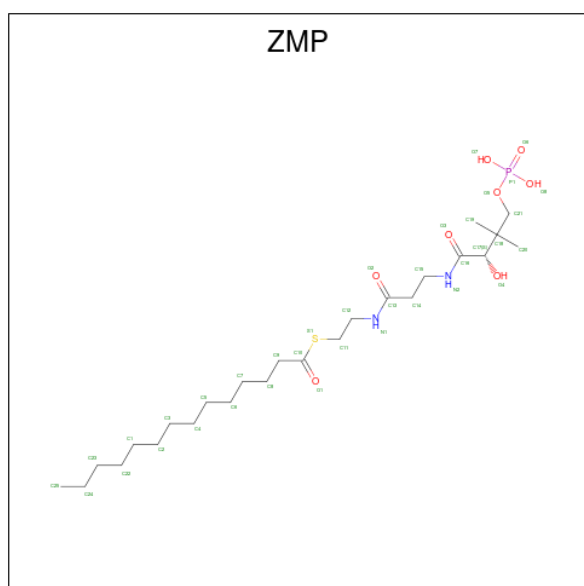
- Molecule 43 is a protein called Mitochondrial complex I, B14.5a subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	h	96	Total	C	N	O	S	0	0
			769	480	146	140	3		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

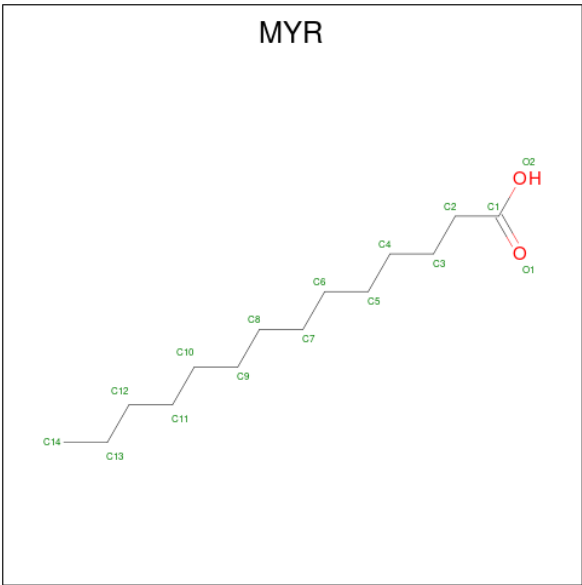
Mol	Chain	Residues	Atoms					AltConf	Trace
44	i	145	Total	C	N	O	S	0	0
			1209	778	216	210	5		

- Molecule 45 is S-[2-({N-[(2S)-2-hydroxy-3,3-dimethyl-4-(phosphonooxy)butanoyl]-beta-alanyl}amino)ethyl] tetradecanethioate (CCD ID: ZMP) (formula: C₂₅H₄₉N₂O₈PS).



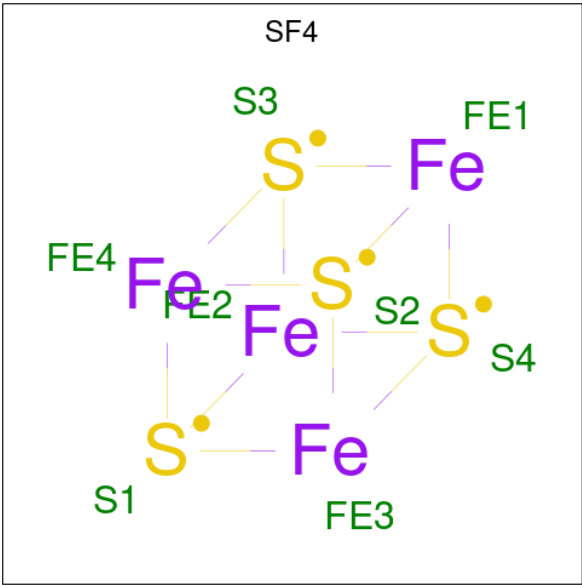
Mol	Chain	Residues	Atoms						AltConf
45	X	1	Total	C	N	O	P	S	0
			31	20	2	7	1	1	
45	j	1	Total	C	N	O	P	S	0
			34	23	2	7	1	1	

- Molecule 46 is MYRISTIC ACID (CCD ID: MYR) (formula: C₁₄H₂₈O₂).



Mol	Chain	Residues	Atoms			AltConf
46	s	1	Total	C	O	0
			15	14	1	

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



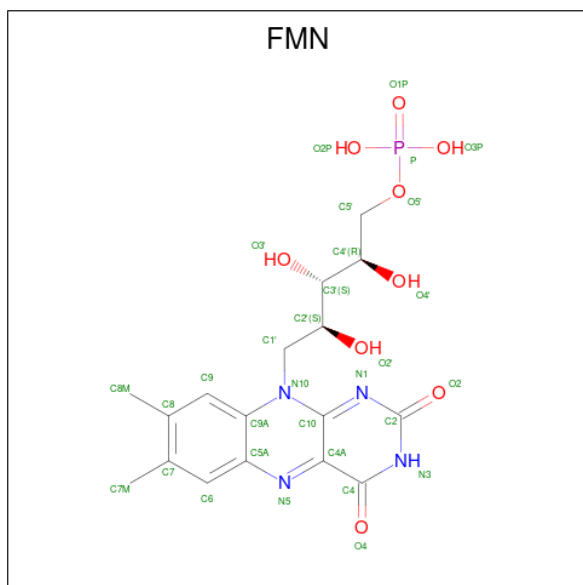
Mol	Chain	Residues	Atoms			AltConf
47	1	1	Total	Fe	S	0
			8	4	4	
47	3	1	Total	Fe	S	0
			8	4	4	
47	3	1	Total	Fe	S	0
			8	4	4	

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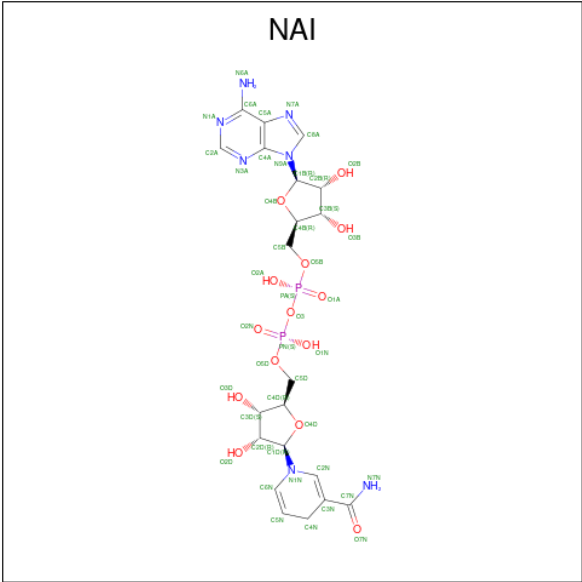
Mol	Chain	Residues	Atoms			AltConf
47	6	1	Total	Fe	S	0
			8	4	4	
47	9	1	Total	Fe	S	0
			8	4	4	
47	9	1	Total	Fe	S	0
			8	4	4	

- Molecule 48 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



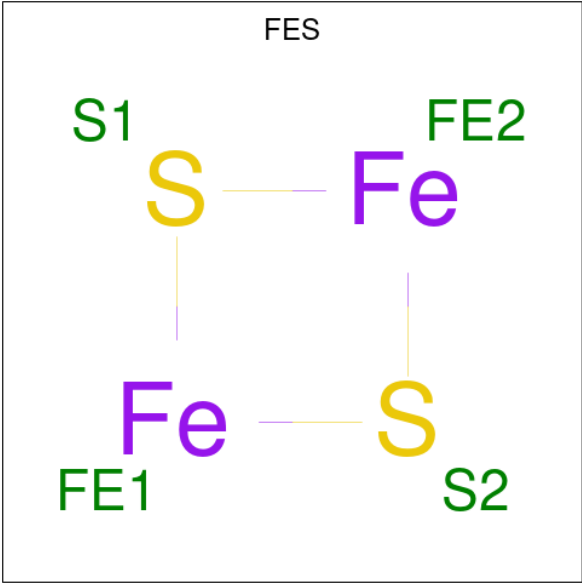
Mol	Chain	Residues	Atoms					AltConf
48	1	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 49 is 1,4-DIHYDRONICOTINAMIDE ADENINE DINUCLEOTIDE (CCD ID: NAI) (formula: $C_{21}H_{29}N_7O_{14}P_2$).



Mol	Chain	Residues	Atoms					AltConf
49	1	1	Total	C	N	O	P	0
			44	21	7	14	2	

- Molecule 50 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂).



Mol	Chain	Residues	Atoms			AltConf
50	2	1	Total	Fe	S	0
			4	2	2	
50	3	1	Total	Fe	S	0
			4	2	2	

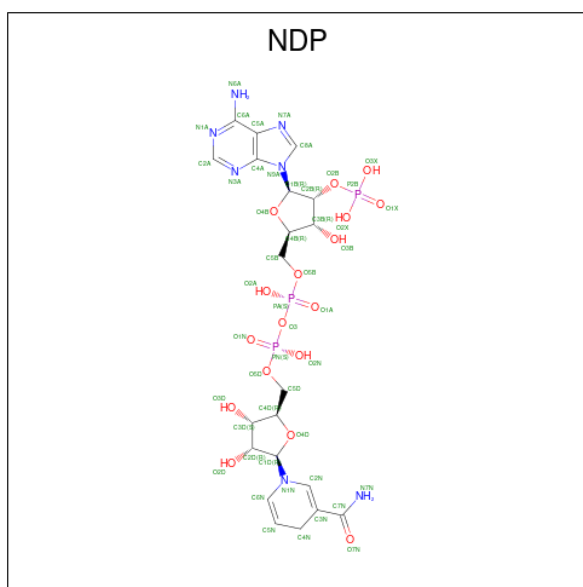
- Molecule 51 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	AltConf
51	3	1	Total K 1 1	0

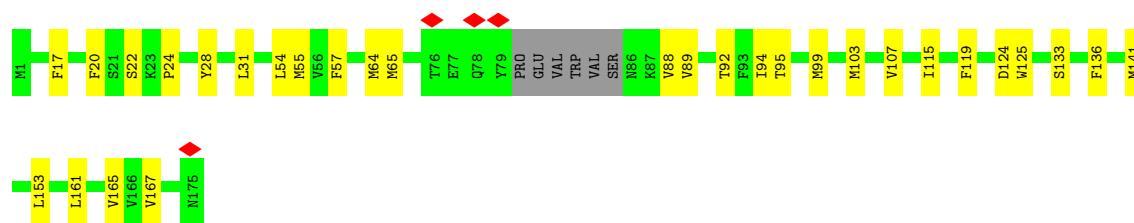
- Molecule 52 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
52	b	1	Total Zn 1 1	0

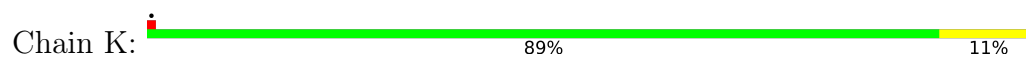
- Molecule 53 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $\text{C}_{21}\text{H}_{30}\text{N}_7\text{O}_{17}\text{P}_3$).



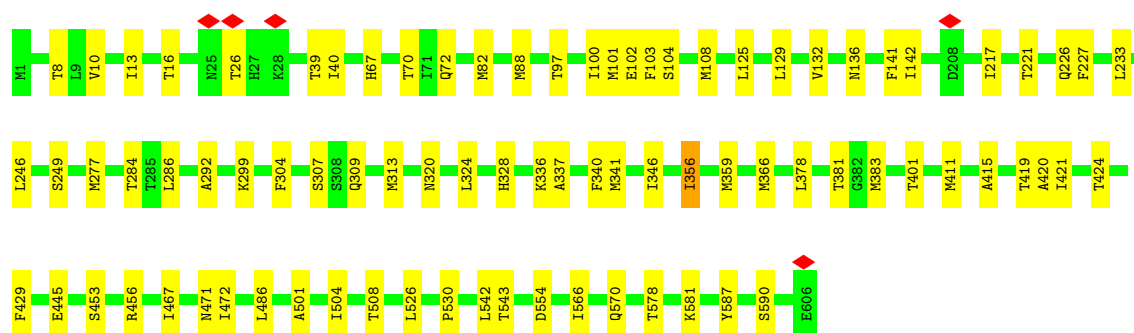
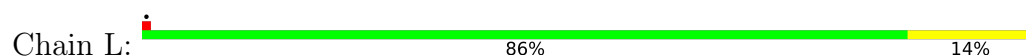
Mol	Chain	Residues	Atoms					AltConf
53	d	1	Total 48	C 21	N 7	O 17	P 3	0



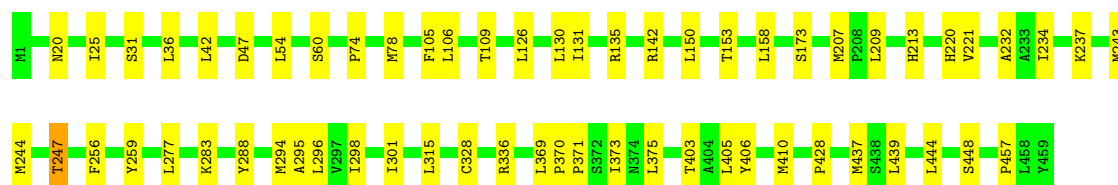
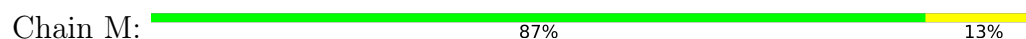
- Molecule 5: NADH-ubiquinone oxidoreductase chain 4L



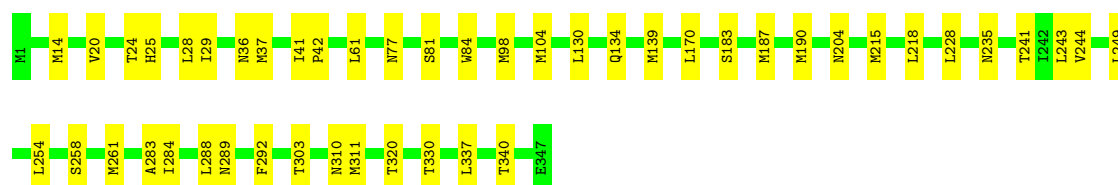
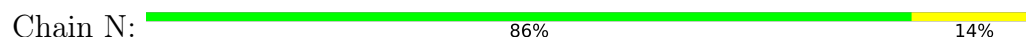
- Molecule 6: NADH-ubiquinone oxidoreductase chain 5



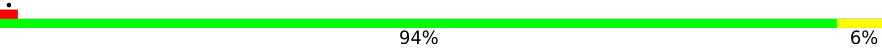
- Molecule 7: NADH-ubiquinone oxidoreductase chain 4

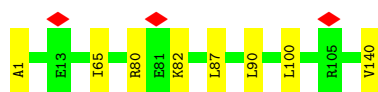


- Molecule 8: NADH-ubiquinone oxidoreductase chain 2



- Molecule 9: Complex I-B14.7

Chain V:  94% 6%

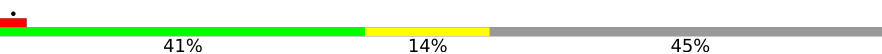


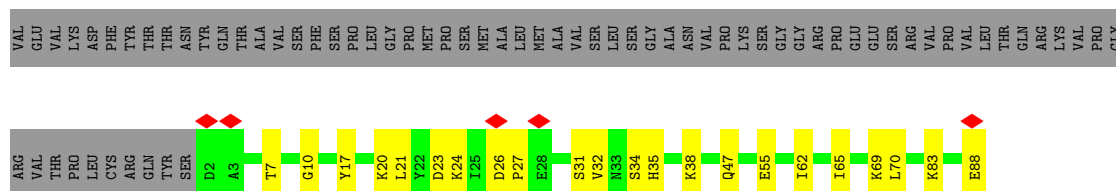
- Molecule 10: Complex I-SGDH

Chain W:  89% 11%

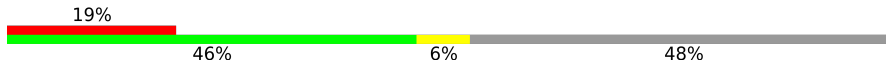


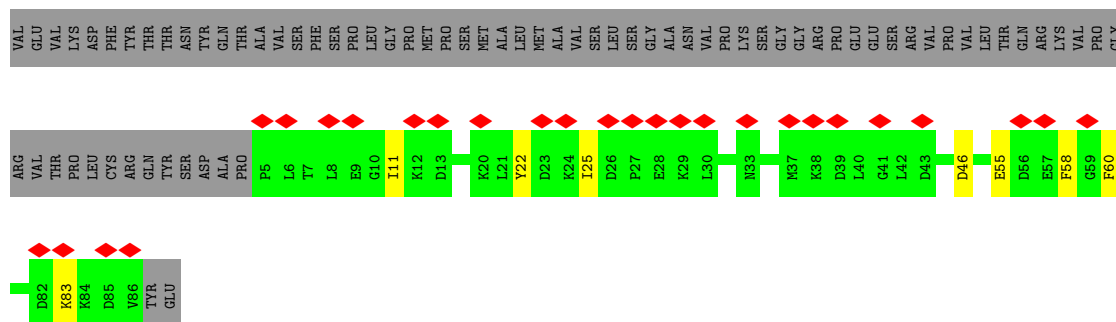
- Molecule 11: Acyl carrier protein

Chain X:  41% 14% 45%



- Molecule 11: Acyl carrier protein

Chain j:  19% 46% 6% 48%

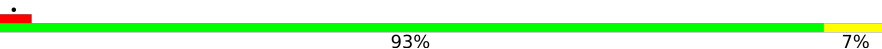


- Molecule 12: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain Y:  89% 11%

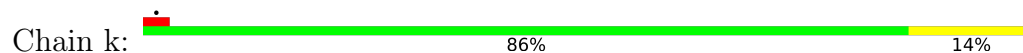


- Molecule 13: Complex I-PDSW

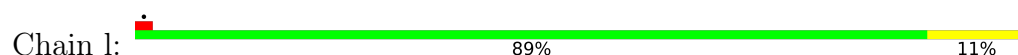
Chain Z:  93% 7%



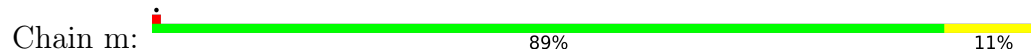
- Molecule 14: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial



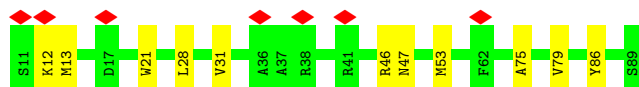
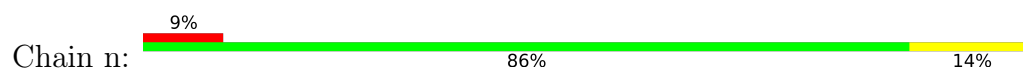
- Molecule 15: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5



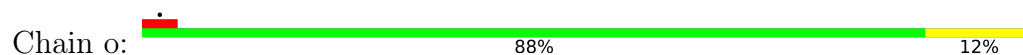
- Molecule 16: Complex I-B9



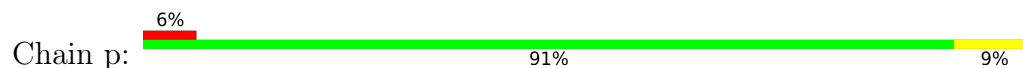
- Molecule 17: Complex I-B12



- Molecule 18: NADH dehydrogenase [ubiquinone] 1 subunit C2

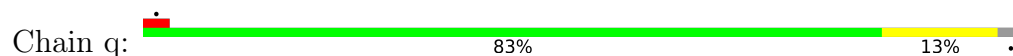


- Molecule 19: NADH:ubiquinone oxidoreductase subunit B4

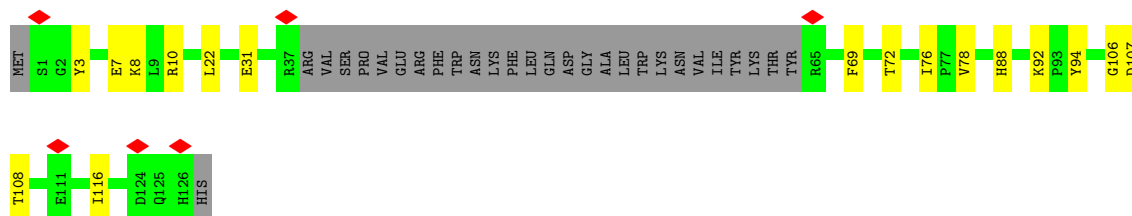




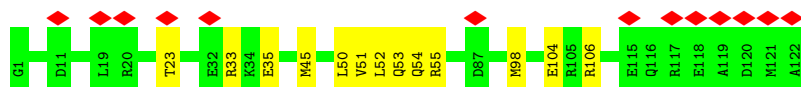
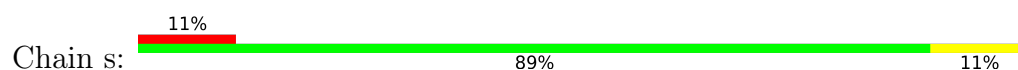
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



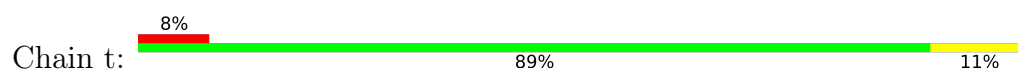
- Molecule 21: Mitochondrial complex I, B17 subunit



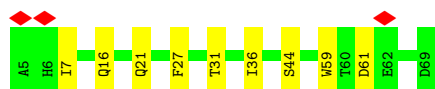
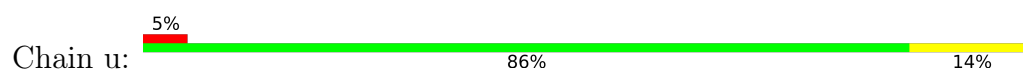
- Molecule 22: Complex I-B18



- Molecule 23: Complex I-B22



- Molecule 24: Complex I-AGGG

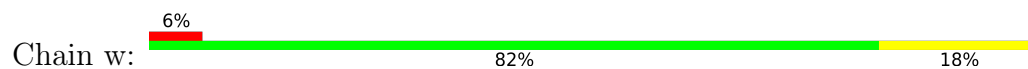


- Molecule 25: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial





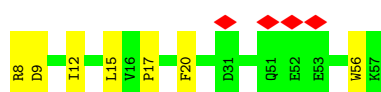
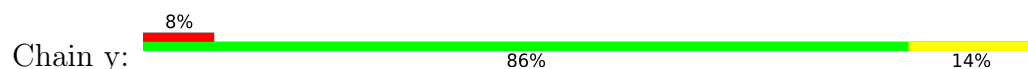
• Molecule 26: Complex I-ESSS



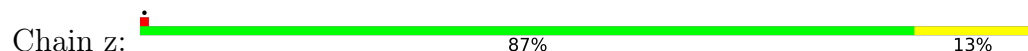
• Molecule 27: Complex I-KFYI



• Molecule 28: Complex I-MNLL



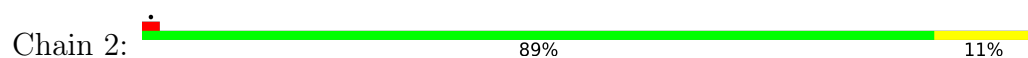
• Molecule 29: Complex I-MWFE



• Molecule 30: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

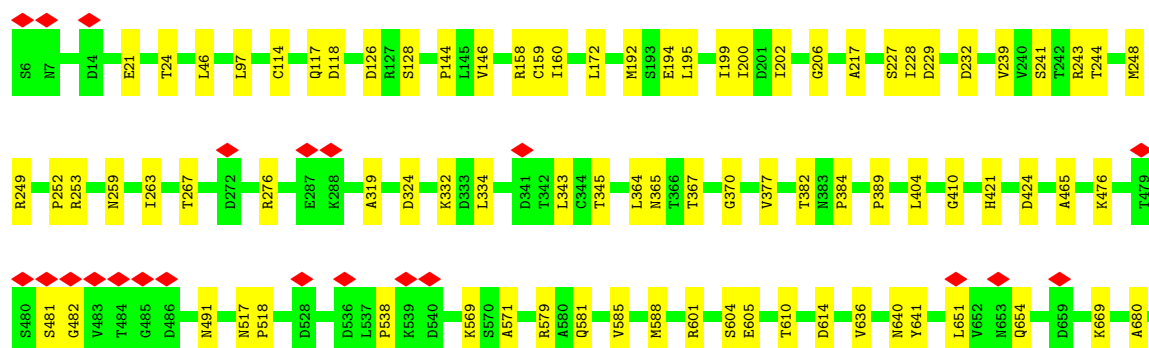
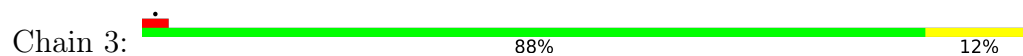


• Molecule 31: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

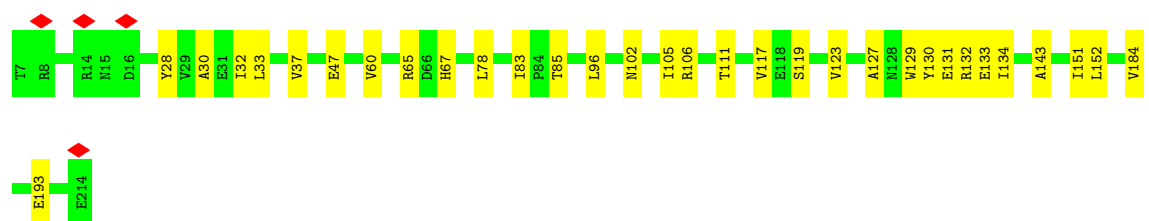
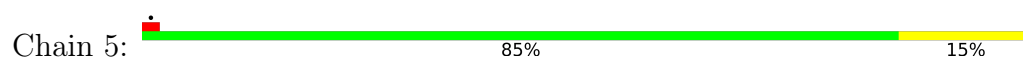




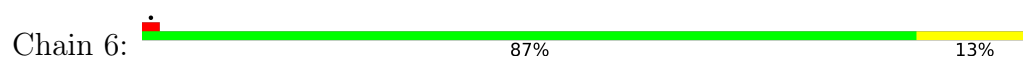
- Molecule 32: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial



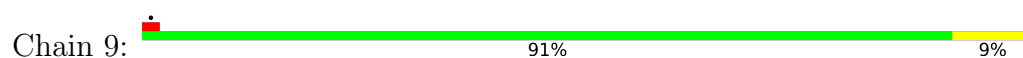
- Molecule 33: Complex I-30kD



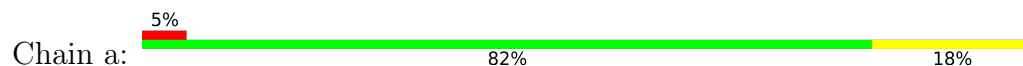
- Molecule 34: Complex I-20kD

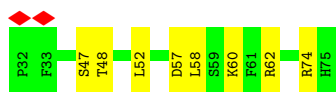


- Molecule 35: Complex I-23kD

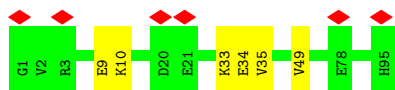


- Molecule 36: Complex I-9kD

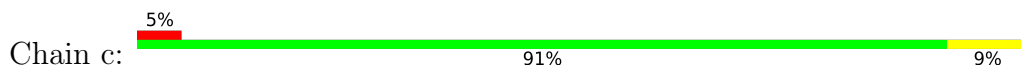




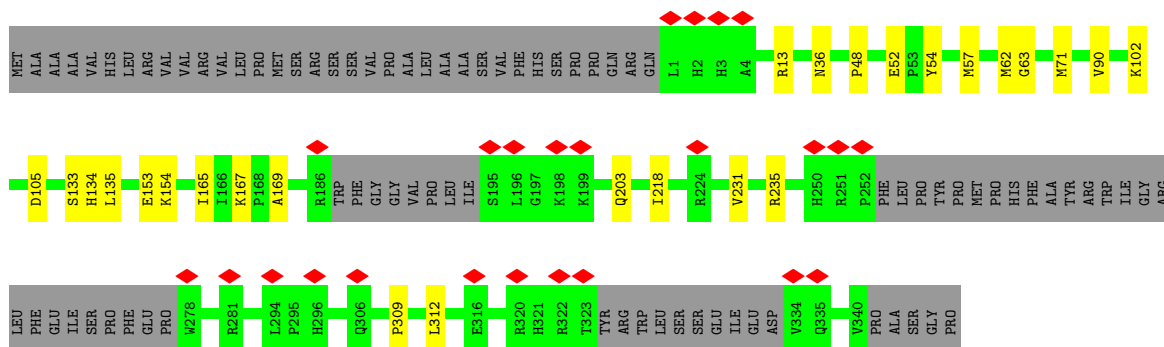
- Molecule 37: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



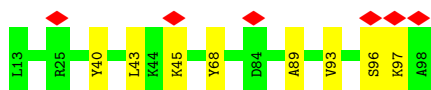
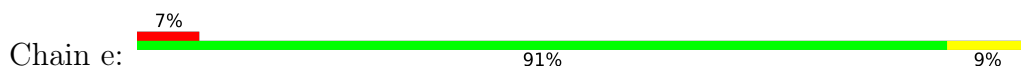
- Molecule 38: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



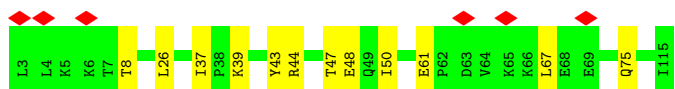
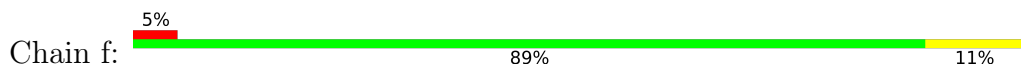
- Molecule 39: NADH:ubiquinone oxidoreductase subunit A9



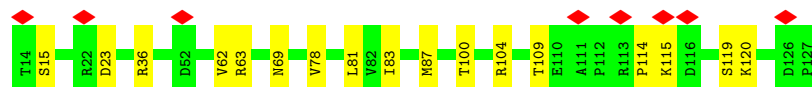
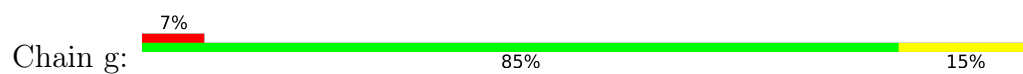
- Molecule 40: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



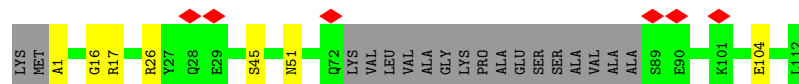
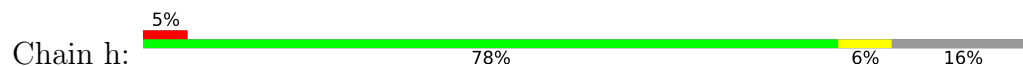
- Molecule 41: Complex I subunit B13



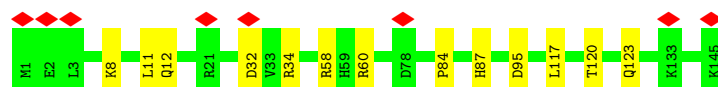
- Molecule 42: Complex I-B14



- Molecule 43: Mitochondrial complex I, B14.5a subunit



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97548	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	90	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	120000	Depositor
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.455	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.025	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	173.24, 201.3, 287.92	wwPDB
Map dimensions	236, 165, 142	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.22, 1.22, 1.22	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FME, ZMP, ZN, NAI, K, 2MR, FMN, SF4, SEP, FES, NDP, AYA, MYR

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	4	0.14	0/3463	0.31	0/4687
2	A	0.20	0/902	0.47	0/1234
3	H	0.25	1/2572 (0.0%)	0.47	0/3517
4	J	0.20	0/1324	0.46	0/1790
5	K	0.22	0/749	0.44	0/1014
6	L	0.20	0/4924	0.45	0/6698
7	M	0.22	0/3731	0.46	0/5085
8	N	0.22	0/2787	0.44	0/3795
9	V	0.14	0/1041	0.30	0/1412
10	W	0.17	0/1188	0.35	0/1607
11	X	0.15	0/713	0.44	0/963
11	j	0.17	0/670	0.45	0/902
12	Y	0.16	0/1440	0.34	0/1942
13	Z	0.16	0/1475	0.34	0/1989
14	k	0.14	0/2646	0.32	0/3579
15	l	0.16	0/896	0.45	2/1200 (0.2%)
16	m	0.16	0/647	0.40	0/890
17	n	0.16	0/653	0.34	0/882
18	o	0.17	0/1035	0.33	0/1398
19	p	0.16	0/1085	0.32	0/1467
20	q	0.19	0/1171	0.41	0/1579
21	r	0.19	0/874	0.45	0/1188
22	s	0.17	0/1072	0.42	0/1436
23	t	0.15	0/1573	0.37	0/2130
24	u	0.15	0/590	0.35	0/810
25	v	0.14	0/1361	0.34	0/1861
26	w	0.18	0/872	0.39	0/1185
27	x	0.15	0/425	0.36	0/576
28	y	0.23	0/449	0.38	0/605
29	z	0.19	0/591	0.39	0/795
30	1	0.16	0/3386	0.34	0/4575
31	2	0.16	0/1695	0.39	0/2306

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	3	0.15	0/5362	0.35	0/7266
33	5	0.16	0/1776	0.38	0/2417
34	6	0.18	0/1278	0.40	0/1728
35	9	0.17	0/1445	0.37	0/1956
36	a	0.11	0/383	0.27	0/518
37	b	0.12	0/749	0.28	0/1009
38	c	0.16	0/1047	0.36	0/1415
39	d	0.14	0/2424	0.32	0/3276
40	e	0.15	0/702	0.38	0/945
41	f	0.18	0/937	0.39	0/1271
42	g	0.19	0/993	0.41	0/1336
43	h	0.14	0/779	0.33	0/1053
44	i	0.13	0/1250	0.31	0/1698
All	All	0.17	1/67125 (0.0%)	0.39	2/90985 (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	4	0	1
32	3	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	87	ILE	C-N	5.68	1.38	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	1	103	LEU	CA-C-N	5.43	129.00	120.97
15	1	103	LEU	C-N-CA	5.43	129.00	120.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	3	259	ASN	Peptide

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Mol	Chain	Res	Type	Group
1	4	275	TYR	Peptide

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	4	3390	0	3334	41	0
2	A	880	0	920	13	0
3	H	2498	0	2609	33	0
4	J	1294	0	1317	26	0
5	K	749	0	793	10	0
6	L	4806	0	4945	52	0
7	M	3647	0	3849	42	0
8	N	2723	0	2930	34	0
9	V	1028	0	1036	5	0
10	W	1155	0	1177	13	0
11	X	701	0	692	17	0
11	j	660	0	662	6	0
12	Y	1403	0	1392	16	0
13	Z	1441	0	1419	11	0
14	k	2596	0	2559	26	0
15	l	874	0	869	9	0
16	m	626	0	635	7	0
17	n	634	0	616	7	0
18	o	1004	0	995	12	0
19	p	1059	0	1062	11	0
20	q	1142	0	1137	19	0
21	r	846	0	864	13	0
22	s	1047	0	1015	12	0
23	t	1520	0	1477	15	0
24	u	563	0	509	7	0
25	v	1307	0	1207	16	0
26	w	846	0	792	15	0
27	x	412	0	411	2	0
28	y	436	0	437	4	0
29	z	576	0	570	7	0
30	1	3312	0	3266	29	0
31	2	1655	0	1668	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	3	5275	0	5300	53	0
33	5	1726	0	1676	21	0
34	6	1247	0	1256	13	0
35	9	1414	0	1370	13	0
36	a	371	0	344	6	0
37	b	737	0	710	3	0
38	c	1024	0	1023	11	0
39	d	2372	0	2407	15	0
40	e	691	0	706	5	0
41	f	917	0	958	7	0
42	g	969	0	980	13	0
43	h	769	0	780	6	0
44	i	1209	0	1182	7	0
45	X	31	0	34	1	0
45	j	34	0	40	3	0
46	s	15	0	27	0	0
47	1	8	0	0	0	0
47	3	16	0	0	1	0
47	6	8	0	0	0	0
47	9	16	0	0	0	0
48	1	31	0	19	0	0
49	1	44	0	27	1	0
50	2	4	0	0	1	0
50	3	4	0	0	0	0
51	3	1	0	0	0	0
52	b	1	0	0	0	0
53	d	48	0	26	0	0
All	All	65812	0	66029	585	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 4.

All (585) 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)
10:W:124:GLN:HB2	18:o:4:GLY:HA3	1.76	0.67
11:X:20:LYS:HB3	11:X:27:PRO:HB3	1.78	0.66
1:4:328:ALA:HB3	32:3:126:ASP:HB2	1.78	0.64
3:H:141:SER:HB2	3:H:289:LEU:HD22	1.79	0.64
34:6:57:VAL:HA	34:6:60:MET:HE2	1.79	0.64
30:1:21:ILE:HG21	30:1:230:VAL:HG22	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:w:25:ARG:HE	26:w:26:TRP:H	1.47	0.63
6:L:221:THR:HG23	6:L:226:GLN:HB2	1.82	0.62
30:1:69:GLY:O	49:1:503:NAI:N7N	2.31	0.62
20:q:26:ARG:O	20:q:26:ARG:HG3	2.00	0.62
13:Z:98:ASP:HB3	26:w:108:MET:HE1	1.81	0.61
1:4:269:LEU:HB2	1:4:368:GLU:HB2	1.81	0.61
39:d:36:ASN:HB2	39:d:62:MET:HE2	1.81	0.61
14:k:173:ASP:OD1	14:k:207:LYS:NZ	2.34	0.60
7:M:130:LEU:HD22	7:M:150:LEU:HD13	1.83	0.60
11:X:21:LEU:HD23	17:n:47:ASN:HA	1.83	0.60
32:3:651:LEU:HD11	40:e:45:LYS:HD3	1.84	0.60
1:4:430:ARG:NH2	33:5:133:GLU:OE2	2.35	0.60
3:H:312:SER:HB3	20:q:54:ARG:HH21	1.67	0.60
33:5:32:ILE:HG22	33:5:33:LEU:HG	1.83	0.59
7:M:232:ALA:O	7:M:237:LYS:NZ	2.36	0.59
41:f:61:GLU:HG2	41:f:67:LEU:HB2	1.85	0.59
39:d:52:GLU:HG3	39:d:54:TYR:H	1.68	0.59
10:W:140:THR:O	10:W:143:ASN:ND2	2.36	0.59
12:Y:89:ASP:OD2	29:z:34:ARG:NH1	2.36	0.59
2:A:73:LEU:HD12	3:H:151:LEU:HD12	1.85	0.58
7:M:295:ALA:HA	7:M:298:ILE:HD12	1.85	0.58
32:3:243:ARG:HD2	32:3:244:THR:HG23	1.86	0.58
10:W:111:ARG:NH1	18:o:1:MET:SD	2.77	0.58
42:g:36:ARG:NH2	11:j:55:GLU:OE2	2.37	0.58
23:t:142:GLU:OE2	23:t:157:ARG:NH2	2.36	0.58
30:1:111:ILE:HD12	30:1:138:ILE:HD11	1.86	0.58
12:Y:165:ARG:NH2	18:o:87:ASP:OD1	2.37	0.57
7:M:243:MET:O	7:M:247:THR:OG1	2.19	0.57
14:k:52:PRO:O	14:k:107:GLN:NE2	2.37	0.57
2:A:68:GLU:HG2	4:J:161:LEU:HD13	1.86	0.57
5:K:44:ALA:HB1	5:K:59:MET:HE1	1.87	0.57
7:M:36:LEU:HB2	26:w:69:VAL:HG22	1.86	0.57
22:s:35:GLU:HA	25:v:156:TYR:HA	1.85	0.57
8:N:337:LEU:O	8:N:340:THR:OG1	2.22	0.57
15:l:50:ARG:O	15:l:54:GLU:HB2	2.04	0.56
32:3:194:GLU:HG2	32:3:195:LEU:HG	1.88	0.56
42:g:78:VAL:HG23	45:j:101:ZMP:HN1	1.70	0.56
14:k:53:GLU:OE2	14:k:126:ARG:NH1	2.37	0.56
26:w:25:ARG:NE	26:w:26:TRP:H	2.02	0.56
6:L:356:ILE:HG12	6:L:429:PHE:HB3	1.88	0.56
12:Y:6:LEU:HB3	20:q:87:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:7:THR:HG23	11:X:10:GLY:H	1.69	0.56
29:z:34:ARG:NH2	29:z:61:TYR:O	2.39	0.56
13:Z:159:LYS:NZ	18:o:112:VAL:O	2.39	0.55
14:k:235:VAL:HA	14:k:238:ILE:HG12	1.87	0.55
31:2:37:ASN:OD1	36:a:62:ARG:NH1	2.39	0.55
32:3:518:PRO:HB2	32:3:538:PRO:HD3	1.88	0.55
10:W:88:GLU:OE1	28:y:56:TRP:NE1	2.36	0.55
11:X:23:ASP:OD1	17:n:46:ARG:NH1	2.39	0.55
31:2:150:ASN:OD1	31:2:190:ARG:NH2	2.38	0.55
6:L:346:ILE:HG12	6:L:366:MET:HE1	1.88	0.55
16:m:27:LEU:O	16:m:31:LEU:HB2	2.07	0.55
1:4:33:TRP:HD1	14:k:158:VAL:HG11	1.71	0.55
1:4:335:ARG:NH2	35:9:129:ASP:OD1	2.38	0.55
14:k:88:SER:OG	14:k:90:ASP:OD1	2.24	0.55
32:3:118:ASP:OD2	38:c:46:GLN:NE2	2.40	0.55
32:3:252:PRO:HG3	32:3:263:ILE:HG12	1.90	0.55
2:A:73:LEU:HD23	4:J:55:MET:HE1	1.88	0.54
12:Y:121:LEU:HD13	20:q:61:ILE:HD11	1.88	0.54
21:r:31:GLU:HG2	23:t:114:TYR:HA	1.89	0.54
34:6:27:GLU:OE2	34:6:178:ARG:NH2	2.40	0.54
1:4:145:THR:HG1	1:4:181:TYR:HH	1.53	0.54
39:d:90:VAL:HG21	39:d:218:ILE:HD12	1.89	0.54
4:J:22:SER:OG	4:J:92:THR:OG1	2.26	0.54
1:4:169:TRP:HE1	3:H:32:GLN:HA	1.72	0.54
3:H:24:GLU:OE2	3:H:274:ARG:NH1	2.39	0.54
11:X:31:SER:H	11:X:34:SER:HG	1.53	0.54
31:2:153:MET:HG3	31:2:162:GLU:HG2	1.88	0.54
34:6:115:SER:OG	34:6:136:CYS:SG	2.66	0.54
6:L:542:LEU:HB2	25:v:83:MET:HE3	1.89	0.54
12:Y:48:GLU:OE1	12:Y:134:ARG:NH2	2.41	0.54
18:o:5:ARG:NH1	18:o:89:ASP:OD1	2.41	0.54
34:6:52:LEU:HB2	34:6:90:GLY:HA3	1.88	0.54
39:d:203:GLN:HG2	39:d:235:ARG:HG2	1.89	0.54
1:4:354:GLU:OE2	1:4:357:GLN:NE2	2.39	0.53
41:f:8:THR:O	41:f:75:GLN:NE2	2.41	0.53
35:9:143:THR:HB	35:9:146:GLU:HG3	1.90	0.53
1:4:3:GLN:NE2	7:M:135:ARG:O	2.36	0.53
11:X:26:ASP:OD1	11:X:26:ASP:N	2.38	0.53
32:3:217:ALA:HB2	32:3:248:MET:HE2	1.90	0.53
32:3:239:VAL:HG23	32:3:253:ARG:HG3	1.90	0.53
31:2:114:ASP:OD1	31:2:114:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:66:MET:HE1	1:4:414:VAL:HG21	1.91	0.53
7:M:256:PHE:O	7:M:259:TYR:HB2	2.08	0.53
32:3:199:ILE:HA	32:3:202:ILE:HG12	1.89	0.53
20:q:88:GLU:OE1	20:q:127:ARG:NH2	2.42	0.53
21:r:88:HIS:O	21:r:92:LYS:NZ	2.40	0.53
33:5:193:GLU:OE2	38:c:64:ARG:NH1	2.41	0.53
34:6:109:GLU:OE2	34:6:109:GLU:N	2.41	0.53
3:H:85:MET:HE3	3:H:108:MET:HB2	1.91	0.53
14:k:146:LYS:NZ	14:k:150:ASP:OD1	2.42	0.53
6:L:286:LEU:HD22	6:L:411:MET:HB3	1.91	0.53
32:3:382:THR:HG23	32:3:384:PRO:HD3	1.89	0.53
43:h:45:SER:O	43:h:51:ASN:ND2	2.40	0.53
7:M:328:CYS:HB3	7:M:437:MET:HE1	1.91	0.53
1:4:422:ASP:OD1	1:4:422:ASP:N	2.39	0.52
5:K:73:LEU:HD21	8:N:41:ILE:HG13	1.91	0.52
41:f:37:ILE:O	41:f:44:ARG:NH1	2.38	0.52
36:a:57:ASP:O	36:a:60:LYS:NZ	2.42	0.52
3:H:293:PHE:O	3:H:297:THR:OG1	2.24	0.52
7:M:131:ILE:O	7:M:135:ARG:HB2	2.10	0.52
22:s:106:ARG:NH1	24:u:61:ASP:OD1	2.42	0.52
30:1:139:ARG:NH2	31:2:144:CYS:O	2.35	0.52
7:M:158:LEU:HD13	8:N:283:ALA:HB1	1.90	0.52
14:k:311:ASP:OD1	14:k:311:ASP:N	2.43	0.52
37:b:9:GLU:OE2	37:b:33:LYS:NZ	2.40	0.52
1:4:352:TYR:HD1	35:9:86:VAL:HG21	1.73	0.52
22:s:50:LEU:O	22:s:55:ARG:NH2	2.33	0.52
6:L:337:ALA:O	6:L:341:MET:HG3	2.10	0.52
19:p:39:ARG:NH2	23:t:3:LEU:O	2.42	0.52
7:M:60:SER:HB3	7:M:457:PRO:HA	1.92	0.52
26:w:50:ASP:HB3	26:w:53:VAL:HB	1.90	0.52
30:1:260:GLY:O	31:2:111:ARG:NH1	2.42	0.52
8:N:25:HIS:HB3	8:N:28:LEU:HD23	1.93	0.51
28:y:17:PRO:O	28:y:20:PHE:HB3	2.10	0.51
30:1:270:GLU:HG3	30:1:274:VAL:HG21	1.92	0.51
32:3:367:THR:OG1	32:3:370:GLY:N	2.43	0.51
32:3:424:ASP:OD1	32:3:424:ASP:N	2.42	0.51
33:5:151:ILE:HG23	33:5:152:LEU:HG	1.91	0.51
3:H:123:SER:HB2	3:H:214:GLU:HG3	1.90	0.51
31:2:150:ASN:ND2	31:2:162:GLU:OE1	2.43	0.51
32:3:334:LEU:HD13	32:3:604:SER:HB3	1.92	0.51
1:4:238:ARG:NH1	3:H:279:ARG:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:59:MET:HE2	8:N:84:TRP:HH2	1.76	0.51
7:M:47:ASP:OD1	7:M:47:ASP:N	2.39	0.51
7:M:126:LEU:HD21	7:M:153:THR:HG21	1.91	0.51
30:1:228:VAL:O	30:1:231:SER:OG	2.27	0.51
32:3:579:ARG:HB2	32:3:636:VAL:HG22	1.90	0.51
22:s:23:THR:OG1	22:s:104:GLU:OE2	2.26	0.51
23:t:9:LEU:O	23:t:14:LYS:NZ	2.42	0.51
30:1:318:ASP:OD1	30:1:318:ASP:N	2.44	0.51
44:i:60:ARG:HH22	44:i:95:ASP:HA	1.76	0.51
22:s:45:MET:HG3	22:s:50:LEU:HD12	1.93	0.51
32:3:158:ARG:HB3	32:3:202:ILE:HD12	1.92	0.51
38:c:42:ARG:NH1	38:c:46:GLN:O	2.44	0.51
6:L:383:MET:HE2	24:u:36:ILE:HD13	1.92	0.51
7:M:105:PHE:O	7:M:109:THR:OG1	2.22	0.51
1:4:71:GLU:OE2	3:H:134:ARG:NH1	2.41	0.51
1:4:88:GLU:OE2	1:4:430:ARG:NH2	2.44	0.51
25:v:137:ASN:O	25:v:142:ARG:NH1	2.44	0.51
33:5:96:LEU:HB2	33:5:105:ILE:HG22	1.93	0.51
10:W:109:GLU:OE2	10:W:112:ARG:NH2	2.42	0.50
44:i:32:ASP:OD2	44:i:34:ARG:NH1	2.36	0.50
19:p:47:GLN:HG3	23:t:165:LEU:HD13	1.94	0.50
6:L:100:ILE:HG21	6:L:246:LEU:HB2	1.93	0.50
18:o:16:ASP:OD1	27:x:45:ARG:NH2	2.40	0.50
30:1:154:ARG:HA	36:a:58:LEU:HD21	1.94	0.50
33:5:127:ALA:HA	33:5:130:TYR:HB2	1.93	0.50
42:g:114:PRO:HB3	42:g:119:SER:HB2	1.93	0.50
22:s:52:LEU:HD11	25:v:141:GLU:HB3	1.94	0.50
30:1:213:VAL:HG13	30:1:217:GLY:HA2	1.93	0.50
32:3:160:ILE:HD12	32:3:160:ILE:H	1.77	0.50
8:N:320:THR:HB	14:k:1:LEU:HD21	1.94	0.49
18:o:52:PRO:HB2	18:o:55:SER:HB2	1.94	0.49
32:3:605:GLU:HA	32:3:610:THR:HG22	1.93	0.49
36:a:47:SER:OG	36:a:48:THR:N	2.45	0.49
3:H:70:MET:HE1	4:J:31:LEU:HD22	1.94	0.49
26:w:97:VAL:HG13	26:w:107:LEU:HD11	1.93	0.49
4:J:133:SER:OG	4:J:136:PHE:O	2.28	0.49
9:V:140:VAL:HG12	10:W:111:ARG:HH21	1.77	0.49
23:t:126:LYS:NZ	23:t:130:GLU:OE2	2.45	0.49
7:M:207:MET:HE1	7:M:294:MET:HE3	1.94	0.49
30:1:185:ILE:HG12	30:1:359:CYS:HB3	1.93	0.49
12:Y:129:LYS:NZ	16:m:65:VAL:O	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:o:52:PRO:HG2	18:o:56:ALA:HB2	1.94	0.49
32:3:640:ASN:OD1	32:3:641:TYR:N	2.39	0.49
35:9:1:THR:N	43:h:104:GLU:O	2.42	0.49
21:r:106:GLY:H	21:r:116:ILE:HG23	1.77	0.49
1:4:74:ARG:O	1:4:407:LYS:NZ	2.45	0.49
7:M:78:MET:HE1	7:M:439:LEU:HD12	1.95	0.49
30:1:291:TRP:O	30:1:309:LYS:NZ	2.43	0.49
1:4:377:TYR:HB3	1:4:390:LYS:HB3	1.95	0.48
26:w:114:ASP:HB3	26:w:117:LYS:HG2	1.93	0.48
32:3:324:ASP:HB3	32:3:571:ALA:HB1	1.94	0.48
2:A:33:LYS:HE2	34:6:105:ASP:HB3	1.94	0.48
18:o:109:TYR:HA	18:o:112:VAL:HG22	1.95	0.48
32:3:276:ARG:NH1	32:3:680:ALA:O	2.46	0.48
42:g:23:ASP:OD1	42:g:23:ASP:N	2.46	0.48
1:4:105:ARG:NH2	34:6:149:CYS:SG	2.83	0.48
6:L:10:VAL:HG21	21:r:78:VAL:HG22	1.94	0.48
11:X:31:SER:OG	11:X:32:VAL:N	2.46	0.48
39:d:48:PRO:HA	39:d:71:MET:O	2.13	0.48
12:Y:63:ASN:OD1	20:q:80:ARG:NH2	2.46	0.48
4:J:124:ASP:OD1	5:K:2:SER:OG	2.30	0.48
11:X:69:LYS:NZ	21:r:7:GLU:OE1	2.46	0.48
32:3:585:VAL:HG11	32:3:588:MET:HE2	1.95	0.48
41:f:44:ARG:O	41:f:48:GLU:HB2	2.14	0.48
42:g:69:ASN:HD21	42:g:81:LEU:HD22	1.79	0.48
7:M:20:ASN:OD1	7:M:20:ASN:N	2.46	0.48
7:M:403:THR:HA	7:M:406:TYR:CE2	2.49	0.48
12:Y:66:ALA:O	12:Y:69:PHE:HB3	2.14	0.48
3:H:62:ARG:HH22	3:H:68:ILE:HD11	1.79	0.48
32:3:228:ILE:HG13	32:3:581:GLN:HB3	1.96	0.48
8:N:218:LEU:HD13	8:N:244:VAL:HG12	1.96	0.48
14:k:310:GLU:HG2	14:k:317:ILE:HD12	1.94	0.48
19:p:66:ARG:NH2	25:v:8:MET:SD	2.86	0.48
44:i:8:LYS:O	44:i:12:GLN:HG2	2.14	0.48
7:M:54:LEU:HD23	10:W:93:ILE:HG12	1.96	0.47
7:M:221:VAL:HA	7:M:283:LYS:HD3	1.96	0.47
33:5:33:LEU:HD13	33:5:60:VAL:HG22	1.95	0.47
12:Y:124:LEU:HD13	20:q:69:ALA:HB2	1.96	0.47
20:q:35:PHE:O	20:q:39:ILE:HG12	2.14	0.47
30:1:87:ASP:OD1	30:1:87:ASP:N	2.42	0.47
14:k:35:LYS:O	14:k:38:LEU:HB3	2.13	0.47
17:n:21:TRP:HA	17:n:53:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:194:GLU:HG3	32:3:389:PRO:HB3	1.95	0.47
33:5:111:THR:HG21	33:5:117:VAL:HG22	1.96	0.47
39:d:169:ALA:HB2	39:d:231:VAL:HG12	1.96	0.47
25:v:145:ASP:N	25:v:145:ASP:OD1	2.40	0.47
32:3:241:SER:HB2	32:3:249:ARG:HG2	1.95	0.47
38:c:27:GLU:N	38:c:27:GLU:OE2	2.46	0.47
20:q:25:PRO:HG3	43:h:17:ARG:HH12	1.77	0.47
3:H:216:ALA:HB3	3:H:219:PRO:HD2	1.97	0.47
4:J:103:MET:HE1	4:J:115:ILE:HG13	1.95	0.47
19:p:47:GLN:O	19:p:51:ASN:ND2	2.45	0.47
30:1:314:THR:O	30:1:314:THR:OG1	2.33	0.47
32:3:144:PRO:HD2	32:3:192:MET:HE3	1.96	0.47
39:d:133:SER:OG	39:d:134:HIS:N	2.47	0.47
1:4:183:ARG:NH1	1:4:210:ASP:OD2	2.41	0.47
30:1:243:ALA:HA	30:1:251:SER:HB3	1.96	0.47
32:3:588:MET:HG3	38:c:63:GLU:HA	1.96	0.47
34:6:162:GLN:OE1	35:9:140:SER:OG	2.33	0.47
6:L:129:LEU:HA	6:L:132:VAL:HG22	1.97	0.47
8:N:139:MET:HE3	8:N:190:MET:HE2	1.95	0.47
11:j:11:ILE:HG22	11:j:77:VAL:HG23	1.96	0.47
29:z:49:GLU:HB3	29:z:53:ARG:HH21	1.80	0.47
32:3:227:SER:O	32:3:253:ARG:NH2	2.45	0.47
33:5:47:GLU:OE1	33:5:106:ARG:NH2	2.48	0.47
7:M:244:MET:HE2	7:M:301:ILE:HD11	1.96	0.47
13:Z:23:THR:OG1	13:Z:24:SER:N	2.47	0.47
39:d:102:LYS:HB3	39:d:102:LYS:HE3	1.72	0.47
11:j:22:TYR:HD2	11:j:25:ILE:HG22	1.80	0.47
15:l:72:MET:HG2	20:q:119:MET:HE1	1.97	0.46
11:X:47:GLN:NE2	11:X:70:LEU:O	2.48	0.46
12:Y:82:THR:HA	12:Y:85:TRP:CD1	2.49	0.46
1:4:413:ASP:OD1	3:H:281:ARG:NH1	2.49	0.46
2:A:64:LEU:HD13	4:J:165:VAL:HG22	1.97	0.46
14:k:104:ARG:NE	14:k:131:ASP:OD1	2.48	0.46
31:2:74:GLN:O	36:a:74:ARG:NH1	2.48	0.46
1:4:155:THR:HB	1:4:167:PHE:HA	1.96	0.46
4:J:99:MET:O	4:J:103:MET:HG2	2.14	0.46
6:L:26:THR:OG1	10:W:26:ARG:NH2	2.48	0.46
19:p:47:GLN:HA	19:p:50:TYR:HB3	1.98	0.46
4:J:167:VAL:HG13	8:N:42:PRO:HG3	1.97	0.46
6:L:526:LEU:HD23	6:L:530:PRO:HG2	1.98	0.46
31:2:134:ASP:N	31:2:134:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:V:80:ARG:HB3	9:V:82:LYS:HZ2	1.80	0.46
20:q:27:ARG:NH1	43:h:16:GLY:HA2	2.31	0.46
35:9:95:GLU:HB2	35:9:108:ARG:HB3	1.98	0.46
3:H:24:GLU:O	3:H:28:LEU:HB2	2.16	0.46
6:L:97:THR:HG21	6:L:125:LEU:HD22	1.98	0.46
14:k:31:ILE:HD11	14:k:183:ILE:HD11	1.97	0.46
16:m:39:LYS:O	16:m:43:MET:HG3	2.16	0.46
35:9:146:GLU:OE2	44:i:123:GLN:NE2	2.48	0.46
1:4:117:ALA:HB2	1:4:367:ILE:HG12	1.97	0.46
1:4:343:GLU:O	1:4:347:HIS:ND1	2.49	0.46
6:L:13:ILE:HA	6:L:16:THR:HG22	1.97	0.46
6:L:88:MET:HE3	6:L:472:ILE:HG22	1.98	0.46
8:N:36:ASN:OD1	8:N:134:GLN:NE2	2.49	0.46
31:2:105:THR:OG1	50:2:300:FES:S2	2.70	0.46
32:3:114:CYS:HB3	32:3:117:GLN:HB2	1.98	0.46
32:3:332:LYS:HG3	32:3:343:LEU:HD13	1.97	0.46
6:L:401:THR:HG22	6:L:486:LEU:HD23	1.98	0.46
23:t:53:GLU:OE1	23:t:58:LYS:NZ	2.47	0.46
23:t:133:GLU:HA	23:t:136:VAL:HG12	1.98	0.46
25:v:54:SER:HA	25:v:84:TYR:HB3	1.98	0.46
32:3:232:ASP:OD1	32:3:232:ASP:N	2.49	0.46
7:M:369:LEU:HD12	7:M:370:PRO:HD2	1.97	0.46
15:l:91:TYR:OH	20:q:92:GLU:OE1	2.32	0.46
11:j:60:PHE:HE2	11:j:83:LYS:HD3	1.81	0.46
6:L:108:MET:HE3	6:L:108:MET:HB3	1.84	0.45
14:k:28:ASP:OD1	14:k:206:TYR:OH	2.29	0.45
14:k:111:ALA:HB1	14:k:122:VAL:HG11	1.98	0.45
25:v:82:ASP:N	25:v:82:ASP:OD1	2.49	0.45
2:A:88:LEU:HD13	3:H:309:ILE:HG13	1.98	0.45
8:N:14:MET:HE2	8:N:14:MET:HB3	1.80	0.45
8:N:289:ASN:HA	8:N:292:PHE:CE2	2.51	0.45
12:Y:48:GLU:OE1	16:m:57:ARG:NH2	2.44	0.45
40:e:68:TYR:HH	40:e:96:SER:HG	1.60	0.45
6:L:313:MET:HG2	6:L:328:HIS:HD2	1.81	0.45
45:X:101:ZMP:H15	45:X:101:ZMP:H17	1.57	0.45
24:u:7:ILE:HG23	24:u:16:GLN:HB3	1.99	0.45
26:w:24:LEU:H	26:w:24:LEU:HD23	1.81	0.45
32:3:159:CYS:HB3	32:3:172:LEU:HD13	1.98	0.45
13:Z:72:ASP:OD1	13:Z:72:ASP:N	2.49	0.45
26:w:85:MET:O	26:w:88:TRP:HB3	2.16	0.45
32:3:410:GLY:O	32:3:421:HIS:NE2	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:3:476:LYS:HB2	32:3:476:LYS:HE3	1.78	0.45
42:g:100:THR:O	42:g:104:ARG:HG2	2.17	0.45
7:M:209:LEU:HD12	7:M:298:ILE:HD13	1.99	0.45
8:N:243:LEU:HD22	8:N:330:THR:HG21	1.98	0.45
1:4:143:GLU:OE2	1:4:278:TYR:OH	2.24	0.45
23:t:9:LEU:HD23	23:t:14:LYS:HG2	1.99	0.45
40:e:40:TYR:O	40:e:43:LEU:HB3	2.17	0.45
1:4:179:GLU:OE1	43:h:26:ARG:NH1	2.45	0.45
1:4:429:ASP:OD1	1:4:429:ASP:N	2.49	0.45
7:M:42:LEU:HD13	26:w:80:LEU:HD11	1.99	0.45
34:6:127:HIS:O	34:6:134:ARG:NH1	2.49	0.45
3:H:179:TRP:HE1	20:q:42:LEU:HG	1.82	0.45
6:L:227:PHE:N	6:L:284:THR:OG1	2.49	0.45
6:L:336:LYS:HA	6:L:336:LYS:HD3	1.77	0.45
8:N:249:LEU:HD22	8:N:254:LEU:HD12	1.99	0.45
17:n:12:LYS:NZ	17:n:13:MET:O	2.50	0.45
30:1:294:LEU:HD11	30:1:297:VAL:HG23	1.99	0.45
1:4:273:GLN:NE2	33:5:102:ASN:OD1	2.50	0.45
4:J:24:PRO:HB3	4:J:89:VAL:HG11	1.99	0.45
30:1:372:MET:HA	30:1:375:VAL:HG12	1.98	0.45
6:L:249:SER:HB2	6:L:336:LYS:HG3	1.98	0.44
11:X:17:TYR:OH	17:n:21:TRP:NE1	2.43	0.44
14:k:131:ASP:OD2	14:k:152:TYR:OH	2.33	0.44
14:k:174:VAL:HG22	14:k:225:ALA:HB2	1.99	0.44
33:5:119:SER:OG	33:5:131:GLU:OE2	2.34	0.44
1:4:341:SER:HB2	32:3:128:SER:HB3	1.98	0.44
13:Z:161:ARG:NH2	26:w:111:ASN:OD1	2.36	0.44
19:p:70:ALA:HB2	25:v:10:PRO:HG2	1.99	0.44
31:2:145:LEU:HB2	31:2:153:MET:HE1	1.99	0.44
33:5:83:ILE:HG22	33:5:85:THR:HG22	1.98	0.44
38:c:60:ASP:N	38:c:60:ASP:OD1	2.48	0.44
1:4:148:LEU:HD21	1:4:177:MET:HB2	1.99	0.44
7:M:373:ILE:HD11	7:M:444:LEU:HD12	1.99	0.44
8:N:98:MET:HE3	8:N:98:MET:HB2	1.86	0.44
14:k:253:ASP:OD1	14:k:253:ASP:N	2.51	0.44
17:n:28:LEU:HA	17:n:31:VAL:HG12	1.99	0.44
32:3:481:SER:OG	32:3:482:GLY:N	2.50	0.44
1:4:158:ALA:HB1	1:4:163:ALA:HB3	1.98	0.44
6:L:8:THR:HB	6:L:82:MET:HE1	1.99	0.44
22:s:98:MET:HG3	24:u:59:TRP:HH2	1.82	0.44
32:3:21:GLU:O	32:3:24:THR:OG1	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:88:GLU:HA	21:r:22:LEU:HB3	1.98	0.44
12:Y:76:HIS:HB3	12:Y:113:LYS:HE3	1.98	0.44
30:1:273:SER:O	30:1:273:SER:OG	2.31	0.44
33:5:184:VAL:HG21	42:g:109:THR:HG21	1.99	0.44
8:N:130:LEU:HD23	8:N:134:GLN:HG3	2.00	0.44
6:L:566:ILE:O	6:L:570:GLN:HG2	2.17	0.44
30:1:142:PHE:HB3	30:1:145:GLU:HB2	2.00	0.44
1:4:261:ARG:NH1	1:4:268:ASP:OD1	2.51	0.44
1:4:346:ILE:HG23	32:3:117:GLN:HG2	2.00	0.44
6:L:467:ILE:O	6:L:471:ASN:HB2	2.18	0.44
7:M:410:MET:HE2	7:M:410:MET:HB3	1.80	0.44
10:W:60:VAL:HA	10:W:61:PRO:HD3	1.88	0.44
40:e:96:SER:OG	40:e:97:LYS:N	2.51	0.44
2:A:13:LEU:HD22	3:H:10:ILE:HD12	1.99	0.44
6:L:543:THR:HG23	25:v:83:MET:HE1	1.99	0.44
8:N:258:SER:O	8:N:261:MET:HB3	2.16	0.44
11:X:83:LYS:HD2	11:X:83:LYS:HA	1.63	0.44
33:5:32:ILE:HG23	41:f:43:TYR:HB2	2.00	0.44
4:J:95:THR:O	4:J:99:MET:HG2	2.18	0.43
13:Z:144:ASP:OD2	19:p:122:ARG:NH2	2.39	0.43
45:j:101:ZMP:O2	45:j:101:ZMP:N2	2.50	0.43
3:H:106:LEU:HD21	3:H:147:ALA:HA	2.00	0.43
8:N:215:MET:HE3	8:N:215:MET:HB3	1.87	0.43
12:Y:39:ASN:HB3	20:q:72:PRO:HG2	2.00	0.43
22:s:51:VAL:HB	22:s:54:GLN:HB2	2.00	0.43
29:z:12:MET:HE2	29:z:12:MET:HB3	1.77	0.43
33:5:129:TRP:O	33:5:132:ARG:HB3	2.18	0.43
42:g:62:VAL:HG22	45:j:101:ZMP:H3A	1.99	0.43
7:M:31:SER:HB2	7:M:74:PRO:HG3	2.00	0.43
7:M:173:SER:HB2	10:W:101:ALA:HB2	2.01	0.43
10:W:8:LEU:HD21	11:X:88:GLU:HG3	2.01	0.43
30:1:292:ASP:O	30:1:339:ARG:NH1	2.51	0.43
32:3:46:LEU:O	38:c:116:LYS:NZ	2.42	0.43
39:d:105:ASP:OD1	39:d:105:ASP:N	2.40	0.43
1:4:189:MET:HE1	34:6:54:CYS:HB3	2.01	0.43
2:A:21:ALA:HB1	3:H:218:GLY:HA3	1.99	0.43
4:J:125:TRP:HB2	20:q:136:THR:HG21	2.00	0.43
5:K:62:ILE:H	5:K:62:ILE:HG12	1.62	0.43
6:L:356:ILE:HA	6:L:359:MET:SD	2.58	0.43
6:L:381:THR:HG22	6:L:420:ALA:HA	2.00	0.43
6:L:415:ALA:O	6:L:419:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:u:44:SER:O	24:u:44:SER:OG	2.32	0.43
11:X:55:GLU:HG2	11:X:62:ILE:H	1.84	0.43
25:v:55:GLN:NE2	25:v:69:LEU:O	2.45	0.43
7:M:371:PRO:O	7:M:448:SER:OG	2.36	0.43
42:g:83:ILE:O	42:g:87:MET:HG3	2.18	0.43
1:4:226:GLU:OE1	1:4:305:ARG:NH2	2.45	0.43
13:Z:140:ASP:O	13:Z:161:ARG:NH1	2.51	0.43
30:1:363:THR:HG21	32:3:97:LEU:HG	1.99	0.43
33:5:78:LEU:HB3	33:5:130:TYR:HB3	2.00	0.43
35:9:3:LYS:HB3	35:9:3:LYS:HE2	1.76	0.43
35:9:156:ASN:ND2	37:b:34:GLU:OE2	2.51	0.43
8:N:183:SER:O	8:N:187:MET:HG2	2.19	0.43
8:N:228:LEU:HD23	8:N:228:LEU:HA	1.90	0.43
12:Y:131:LYS:HA	12:Y:131:LYS:HD2	1.78	0.43
13:Z:100:GLU:OE2	26:w:86:GLN:NE2	2.51	0.43
29:z:37:ARG:HB3	29:z:48:MET:HE2	2.01	0.43
30:1:63:SER:HB2	30:1:242:PHE:HB3	2.01	0.43
31:2:168:ASP:HB3	31:2:187:ARG:HG2	2.01	0.43
42:g:114:PRO:HB2	42:g:120:LYS:HG2	2.00	0.43
44:i:117:LEU:O	44:i:120:THR:OG1	2.35	0.43
6:L:504:ILE:O	6:L:508:THR:HG23	2.19	0.43
29:z:59:ARG:HA	29:z:59:ARG:HD3	1.90	0.43
44:i:84:PRO:HA	44:i:87:HIS:HB3	2.01	0.43
6:L:102:GLU:OE1	6:L:456:ARG:NH2	2.42	0.43
6:L:309:GLN:O	6:L:313:MET:HG3	2.19	0.43
9:V:65:ILE:HD11	9:V:100:LEU:HB2	2.00	0.43
11:X:24:LYS:HE2	11:X:24:LYS:HB2	1.92	0.43
21:r:3:TYR:HB2	21:r:8:LYS:HG3	2.00	0.43
29:z:34:ARG:HE	29:z:34:ARG:HB2	1.53	0.43
32:3:669:LYS:HB3	32:3:669:LYS:HE3	1.77	0.43
4:J:107:VAL:HG11	5:K:3:LEU:HD11	2.00	0.42
6:L:103:PHE:HB2	6:L:341:MET:HE3	2.01	0.42
23:t:107:HIS:NE2	26:w:43:ASP:OD1	2.40	0.42
31:2:116:ILE:HD12	31:2:152:PRO:HB2	2.01	0.42
1:4:29:LYS:HD3	1:4:30:PRO:HD2	2.01	0.42
1:4:47:LEU:HD11	2:A:44:MET:HE2	2.01	0.42
6:L:299:LYS:HG2	6:L:340:PHE:HE1	1.83	0.42
23:t:157:ARG:HA	23:t:157:ARG:HD3	1.86	0.42
30:1:118:LEU:HD13	30:1:225:VAL:HG13	2.00	0.42
4:J:88:VAL:O	4:J:92:THR:HG23	2.18	0.42
30:1:389:ILE:HG23	30:1:419:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:27:MET:HE2	5:K:27:MET:HB2	1.86	0.42
6:L:581:LYS:H	6:L:581:LYS:HG2	1.62	0.42
15:l:78:ILE:HA	20:q:97:MET:HE2	2.01	0.42
25:v:138:LEU:HB3	25:v:141:GLU:HB2	2.02	0.42
32:3:227:SER:OG	32:3:228:ILE:N	2.51	0.42
39:d:309:PRO:HG2	39:d:312:LEU:HG	2.02	0.42
1:4:88:GLU:HA	1:4:91:ILE:HD12	2.02	0.42
39:d:154:LYS:HB3	39:d:154:LYS:HE2	1.72	0.42
2:A:87:MET:HE3	2:A:87:MET:HB3	1.90	0.42
6:L:100:ILE:O	6:L:104:SER:OG	2.29	0.42
8:N:20:VAL:HG13	8:N:29:ILE:HG23	2.02	0.42
8:N:170:LEU:HD13	8:N:288:LEU:HD23	2.02	0.42
14:k:128:ILE:HD12	14:k:160:VAL:HG23	2.02	0.42
20:q:25:PRO:HG3	43:h:17:ARG:NH1	2.34	0.42
22:s:33:ARG:HG2	25:v:156:TYR:HB3	2.00	0.42
22:s:45:MET:HE2	22:s:45:MET:HB3	1.89	0.42
30:1:292:ASP:HA	30:1:309:LYS:HZ1	1.83	0.42
33:5:131:GLU:O	33:5:134:ILE:HB	2.19	0.42
34:6:68:ASP:O	34:6:71:ARG:HG2	2.20	0.42
44:i:34:ARG:NH2	44:i:58:ARG:O	2.51	0.42
4:J:141:MET:HE3	4:J:141:MET:HB3	1.95	0.42
7:M:106:LEU:HD13	7:M:234:ILE:HG21	2.01	0.42
32:3:244:THR:HB	38:c:73:ALA:HB2	2.00	0.42
32:3:465:ALA:HB2	32:3:654:GLN:HB3	2.02	0.42
39:d:13:ARG:NH2	39:d:63:GLY:O	2.53	0.42
42:g:63:ARG:NH1	11:j:46:ASP:OD1	2.52	0.42
2:A:20:ILE:HD13	2:A:20:ILE:HA	1.87	0.42
6:L:141:PHE:HE2	7:M:375:LEU:HD21	1.85	0.42
6:L:554:ASP:OD2	7:M:288:TYR:OH	2.35	0.42
20:q:9:MET:HE3	20:q:9:MET:HB3	1.94	0.42
25:v:32:GLU:OE1	25:v:32:GLU:N	2.52	0.42
27:x:33:LYS:HE2	27:x:33:LYS:HB2	1.80	0.42
28:y:12:ILE:HG13	28:y:15:LEU:HD12	2.02	0.42
30:1:261:HIS:ND1	30:1:338:ASP:OD1	2.52	0.42
32:3:206:GLY:N	47:3:801:SF4:S2	2.80	0.42
3:H:318:THR:O	3:H:318:THR:OG1	2.33	0.42
10:W:95:GLN:HB2	13:Z:82:LEU:HD21	2.02	0.42
12:Y:100:ARG:HD3	12:Y:100:ARG:HA	1.88	0.42
13:Z:18:ALA:N	21:r:108:THR:O	2.50	0.42
3:H:103:LEU:HB3	4:J:54:LEU:HD13	2.02	0.41
6:L:102:GLU:HB3	6:L:453:SER:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:207:MET:HG3	7:M:298:ILE:HG12	2.02	0.41
10:W:93:ILE:O	10:W:97:GLU:HG2	2.20	0.41
14:k:32:CYS:SG	14:k:186:LYS:NZ	2.72	0.41
32:3:364:LEU:HD12	32:3:491:ASN:HB3	2.02	0.41
38:c:125:ASN:OD1	38:c:125:ASN:N	2.51	0.41
39:d:135:LEU:HA	39:d:167:LYS:HB3	2.02	0.41
42:g:115:LYS:HA	42:g:115:LYS:HD3	1.90	0.41
8:N:310:ASN:OD1	8:N:310:ASN:N	2.53	0.41
8:N:311:MET:HE2	8:N:311:MET:HB2	1.95	0.41
19:p:78:ASN:HB2	25:v:43:GLY:HA2	2.02	0.41
31:2:24:THR:OG1	31:2:27:ASN:ND2	2.52	0.41
32:3:229:ASP:OD2	32:3:267:THR:OG1	2.32	0.41
34:6:116:MET:HA	34:6:146:VAL:HB	2.01	0.41
38:c:10:LEU:HD23	42:g:15:SER:HB3	2.01	0.41
41:f:47:THR:HA	41:f:50:ILE:HG12	2.02	0.41
4:J:64:MET:HE1	5:K:37:MET:HE1	2.02	0.41
4:J:119:PHE:CG	5:K:6:MET:HB2	2.55	0.41
4:J:167:VAL:HG22	8:N:42:PRO:HG2	2.02	0.41
30:1:375:VAL:HG11	30:1:392:LEU:HD13	2.02	0.41
32:3:569:LYS:HG3	32:3:571:ALA:HB2	2.02	0.41
3:H:106:LEU:HD12	3:H:106:LEU:HA	1.87	0.41
4:J:94:ILE:HD13	4:J:94:ILE:HA	1.92	0.41
6:L:378:LEU:HD23	6:L:378:LEU:HA	1.89	0.41
7:M:25:ILE:HD11	26:w:53:VAL:HG13	2.02	0.41
7:M:142:ARG:HH21	8:N:303:THR:HG22	1.84	0.41
14:k:146:LYS:HD2	14:k:146:LYS:HA	1.79	0.41
31:2:53:LEU:HD12	36:a:52:LEU:HG	2.02	0.41
35:9:148:LEU:HD23	38:c:70:MET:HG3	2.03	0.41
1:4:88:GLU:H	1:4:88:GLU:HG2	1.74	0.41
6:L:217:ILE:HD11	6:L:277:MET:HE2	2.01	0.41
6:L:421:ILE:HG12	6:L:501:ALA:HB2	2.03	0.41
6:L:587:TYR:O	6:L:590:SER:OG	2.33	0.41
21:r:72:THR:HA	21:r:76:ILE:HD12	2.01	0.41
31:2:116:ILE:HD11	31:2:164:LEU:HB2	2.02	0.41
32:3:377:VAL:HG23	32:3:404:LEU:HD11	2.02	0.41
32:3:601:ARG:NH2	32:3:614:ASP:OD1	2.46	0.41
33:5:65:ARG:NH1	33:5:123:VAL:O	2.53	0.41
33:5:117:VAL:O	33:5:143:ALA:N	2.48	0.41
37:b:10:LYS:HD2	37:b:35:VAL:HG21	2.02	0.41
3:H:24:GLU:HA	3:H:271:LEU:HD13	2.02	0.41
4:J:17:PHE:HA	4:J:20:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:233:LEU:HD23	6:L:307:SER:HB3	2.02	0.41
8:N:241:THR:HA	8:N:244:VAL:HG22	2.03	0.41
8:N:284:ILE:HD13	8:N:284:ILE:HA	1.91	0.41
14:k:15:THR:OG1	14:k:253:ASP:OD2	2.38	0.41
14:k:214:MET:HG2	14:k:217:LYS:NZ	2.36	0.41
17:n:75:ALA:O	17:n:79:VAL:HG12	2.21	0.41
21:r:10:ARG:HB2	23:t:155:PRO:HB3	2.03	0.41
22:s:51:VAL:HG12	22:s:53:GLN:H	1.84	0.41
35:9:108:ARG:NH1	35:9:110:ASP:OD2	2.45	0.41
1:4:83:LEU:HD23	1:4:426:GLY:HA2	2.03	0.41
1:4:261:ARG:HG2	1:4:287:ILE:HD13	2.02	0.41
2:A:80:GLN:HG3	3:H:317:GLN:HG3	2.02	0.41
3:H:107:ALA:HB1	4:J:57:PHE:HB3	2.02	0.41
4:J:65:MET:HE3	4:J:65:MET:HB3	1.89	0.41
7:M:221:VAL:HG22	7:M:283:LYS:HB3	2.02	0.41
7:M:277:LEU:HD21	7:M:405:LEU:HB3	2.01	0.41
8:N:190:MET:HG2	8:N:204:ASN:HB3	2.01	0.41
12:Y:44:LEU:HB2	16:m:55:PRO:HG2	2.02	0.41
15:l:9:LEU:HD12	15:l:9:LEU:HA	1.94	0.41
15:l:16:TRP:CD1	15:l:16:TRP:H	2.38	0.41
18:o:120:ARG:NH1	19:p:112:GLU:OE2	2.49	0.41
8:N:77:ASN:O	8:N:81:SER:OG	2.33	0.41
9:V:87:LEU:HD12	9:V:90:LEU:HD23	2.02	0.41
18:o:11:LEU:HD23	18:o:11:LEU:HA	1.92	0.41
22:s:98:MET:HB3	25:v:128:VAL:HG12	2.01	0.41
35:9:114:THR:HG21	35:9:144:HIS:CD2	2.56	0.41
3:H:309:ILE:HG22	16:m:38:THR:HG23	2.03	0.41
6:L:39:THR:HA	21:r:69:PHE:HZ	1.85	0.41
6:L:40:ILE:HD12	6:L:101:MET:SD	2.61	0.41
6:L:292:ALA:HB2	6:L:304:PHE:HB3	2.02	0.41
7:M:296:LEU:HD23	7:M:315:LEU:HD21	2.02	0.41
7:M:336:ARG:NH2	7:M:428:PRO:O	2.54	0.41
14:k:192:MET:SD	14:k:192:MET:N	2.94	0.41
28:y:8:ARG:NH1	28:y:9:ASP:H	2.18	0.41
31:2:101:GLN:HG2	31:2:140:ILE:HD11	2.02	0.41
32:3:365:ASN:N	32:3:491:ASN:OD1	2.54	0.41
33:5:28:TYR:OH	33:5:67:HIS:NE2	2.44	0.41
33:5:30:ALA:HA	33:5:37:VAL:HG21	2.03	0.41
39:d:153:GLU:HG3	39:d:165:ILE:HG21	2.02	0.41
40:e:89:ALA:O	40:e:93:VAL:HG23	2.20	0.41
41:f:39:LYS:HE2	41:f:39:LYS:HB2	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:142:ILE:HG12	7:M:370:PRO:HB2	2.02	0.41
9:V:80:ARG:HA	9:V:80:ARG:HD2	1.82	0.41
18:o:90:MET:HE2	18:o:90:MET:HB3	1.89	0.41
21:r:107:ASP:OD1	21:r:107:ASP:N	2.40	0.41
23:t:136:VAL:O	23:t:140:GLN:HG3	2.21	0.41
32:3:319:ALA:HB3	32:3:345:THR:HG22	2.02	0.41
34:6:101:ARG:HA	34:6:101:ARG:HD2	1.94	0.41
3:H:67:SER:HG	4:J:28:TYR:HH	1.58	0.40
3:H:149:ILE:HG21	3:H:185:TRP:HB2	2.03	0.40
5:K:26:LEU:HD11	8:N:61:LEU:HD11	2.02	0.40
7:M:220:HIS:CE1	7:M:232:ALA:HB2	2.56	0.40
31:2:28:TYR:O	31:2:32:GLU:HG2	2.21	0.40
32:3:146:VAL:HG22	32:3:200:ILE:HD11	2.03	0.40
1:4:75:LYS:HE2	1:4:75:LYS:HB3	1.77	0.40
3:H:72:ILE:HD13	3:H:72:ILE:HA	1.93	0.40
6:L:420:ALA:O	6:L:424:THR:HG22	2.21	0.40
6:L:554:ASP:OD1	7:M:213:HIS:NE2	2.54	0.40
16:m:81:LYS:HE3	16:m:81:LYS:HB2	1.77	0.40
30:1:368:GLY:O	30:1:372:MET:HG3	2.22	0.40
11:j:11:ILE:HG23	11:j:58:PHE:HZ	1.86	0.40
6:L:67:HIS:NE2	6:L:70:THR:OG1	2.54	0.40
6:L:324:LEU:HD23	6:L:324:LEU:HA	1.90	0.40
8:N:41:ILE:HD13	8:N:41:ILE:HA	1.95	0.40
8:N:104:MET:HE3	8:N:104:MET:HB3	1.93	0.40
13:Z:10:PRO:O	21:r:94:TYR:OH	2.36	0.40
14:k:16:LYS:HA	14:k:16:LYS:HD3	1.96	0.40
19:p:46:TYR:O	19:p:50:TYR:HB3	2.21	0.40
2:A:54:LYS:HE2	2:A:54:LYS:HB2	1.83	0.40
3:H:18:ALA:O	3:H:21:THR:OG1	2.27	0.40
3:H:89:LEU:HA	3:H:90:PRO:HD3	1.99	0.40
6:L:445:GLU:OE2	24:u:21:GLN:NE2	2.54	0.40
11:X:35:HIS:HB3	11:X:38:LYS:HB3	2.02	0.40
11:X:65:ILE:HD12	11:X:65:ILE:HA	1.85	0.40
15:l:36:GLU:HB2	15:l:62:PHE:CZ	2.56	0.40
23:t:169:ILE:O	23:t:172:ARG:NH1	2.55	0.40
24:u:27:PHE:O	24:u:31:THR:OG1	2.32	0.40
26:w:25:ARG:HH21	26:w:26:TRP:HB3	1.86	0.40
30:1:138:ILE:HG21	30:1:146:ALA:HB2	2.02	0.40
3:H:311:LEU:HD23	3:H:311:LEU:HA	1.93	0.40
4:J:153:LEU:HD12	4:J:153:LEU:HA	1.96	0.40
8:N:24:THR:HG22	15:l:2:PHE:HZ	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:k:94:TYR:OH	14:k:151:HIS:ND1	2.40	0.40
15:l:104:ARG:HH22	20:q:80:ARG:HD2	1.87	0.40
19:p:44:ARG:HH12	23:t:143:THR:HG21	1.86	0.40
35:9:75:GLU:O	35:9:105:ARG:NH1	2.55	0.40
39:d:54:TYR:HA	39:d:57:MET:HG2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	4	414/463 (89%)	401 (97%)	13 (3%)	0	100	100
2	A	106/115 (92%)	102 (96%)	4 (4%)	0	100	100
3	H	310/318 (98%)	302 (97%)	8 (3%)	0	100	100
4	J	165/175 (94%)	155 (94%)	10 (6%)	0	100	100
5	K	96/98 (98%)	93 (97%)	3 (3%)	0	100	100
6	L	604/606 (100%)	577 (96%)	26 (4%)	1 (0%)	43	70
7	M	457/459 (100%)	450 (98%)	7 (2%)	0	100	100
8	N	345/347 (99%)	337 (98%)	8 (2%)	0	100	100
9	V	138/140 (99%)	136 (99%)	2 (1%)	0	100	100
10	W	137/139 (99%)	135 (98%)	2 (2%)	0	100	100
11	X	85/157 (54%)	81 (95%)	4 (5%)	0	100	100
11	j	80/157 (51%)	78 (98%)	2 (2%)	0	100	100
12	Y	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
13	Z	169/171 (99%)	168 (99%)	1 (1%)	0	100	100
14	k	317/320 (99%)	312 (98%)	5 (2%)	0	100	100
15	l	103/105 (98%)	98 (95%)	5 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	m	78/80 (98%)	73 (94%)	5 (6%)	0	100	100
17	n	77/79 (98%)	75 (97%)	2 (3%)	0	100	100
18	o	118/120 (98%)	115 (98%)	3 (2%)	0	100	100
19	p	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
20	q	137/144 (95%)	136 (99%)	1 (1%)	0	100	100
21	r	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
22	s	120/122 (98%)	116 (97%)	4 (3%)	0	100	100
23	t	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
24	u	63/65 (97%)	61 (97%)	2 (3%)	0	100	100
25	v	153/155 (99%)	151 (99%)	2 (1%)	0	100	100
26	w	99/101 (98%)	96 (97%)	3 (3%)	0	100	100
27	x	47/49 (96%)	47 (100%)	0	0	100	100
28	y	48/50 (96%)	47 (98%)	1 (2%)	0	100	100
29	z	68/70 (97%)	67 (98%)	1 (2%)	0	100	100
30	1	428/430 (100%)	418 (98%)	10 (2%)	0	100	100
31	2	211/213 (99%)	200 (95%)	11 (5%)	0	100	100
32	3	686/688 (100%)	663 (97%)	23 (3%)	0	100	100
33	5	206/208 (99%)	195 (95%)	11 (5%)	0	100	100
34	6	154/156 (99%)	149 (97%)	5 (3%)	0	100	100
35	9	174/176 (99%)	169 (97%)	5 (3%)	0	100	100
36	a	42/44 (96%)	42 (100%)	0	0	100	100
37	b	93/95 (98%)	91 (98%)	2 (2%)	0	100	100
38	c	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
39	d	289/380 (76%)	283 (98%)	6 (2%)	0	100	100
40	e	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
41	f	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
42	g	112/114 (98%)	107 (96%)	5 (4%)	0	100	100
43	h	92/114 (81%)	90 (98%)	2 (2%)	0	100	100
44	i	143/145 (99%)	142 (99%)	1 (1%)	0	100	100
All	All	8048/8497 (95%)	7819 (97%)	228 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	L	72	GLN

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	4	363/391 (93%)	362 (100%)	1 (0%)	86	86
2	A	99/103 (96%)	99 (100%)	0	100	100
3	H	274/278 (99%)	274 (100%)	0	100	100
4	J	138/144 (96%)	138 (100%)	0	100	100
5	K	86/86 (100%)	85 (99%)	1 (1%)	63	74
6	L	538/538 (100%)	534 (99%)	4 (1%)	76	79
7	M	411/411 (100%)	410 (100%)	1 (0%)	87	87
8	N	315/315 (100%)	313 (99%)	2 (1%)	78	81
9	V	101/101 (100%)	101 (100%)	0	100	100
10	W	122/122 (100%)	122 (100%)	0	100	100
11	X	80/141 (57%)	80 (100%)	0	100	100
11	j	76/141 (54%)	76 (100%)	0	100	100
12	Y	154/154 (100%)	154 (100%)	0	100	100
13	Z	155/155 (100%)	155 (100%)	0	100	100
14	k	283/283 (100%)	282 (100%)	1 (0%)	84	84
15	l	94/94 (100%)	94 (100%)	0	100	100
16	m	69/69 (100%)	69 (100%)	0	100	100
17	n	61/61 (100%)	60 (98%)	1 (2%)	55	70
18	o	107/107 (100%)	107 (100%)	0	100	100
19	p	114/114 (100%)	114 (100%)	0	100	100
20	q	119/122 (98%)	119 (100%)	0	100	100
21	r	95/122 (78%)	95 (100%)	0	100	100
22	s	110/110 (100%)	110 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
23	t	159/159 (100%)	159 (100%)	0	100	100
24	u	59/59 (100%)	59 (100%)	0	100	100
25	v	140/140 (100%)	140 (100%)	0	100	100
26	w	92/92 (100%)	91 (99%)	1 (1%)	65	75
27	x	44/44 (100%)	43 (98%)	1 (2%)	44	65
28	y	46/46 (100%)	46 (100%)	0	100	100
29	z	59/59 (100%)	58 (98%)	1 (2%)	53	69
30	1	344/344 (100%)	343 (100%)	1 (0%)	86	86
31	2	183/183 (100%)	183 (100%)	0	100	100
32	3	578/578 (100%)	577 (100%)	1 (0%)	87	87
33	5	189/189 (100%)	189 (100%)	0	100	100
34	6	132/132 (100%)	132 (100%)	0	100	100
35	9	151/151 (100%)	151 (100%)	0	100	100
36	a	43/43 (100%)	43 (100%)	0	100	100
37	b	79/79 (100%)	78 (99%)	1 (1%)	61	73
38	c	113/113 (100%)	113 (100%)	0	100	100
39	d	255/326 (78%)	255 (100%)	0	100	100
40	e	76/76 (100%)	76 (100%)	0	100	100
41	f	101/101 (100%)	100 (99%)	1 (1%)	68	75
42	g	107/107 (100%)	107 (100%)	0	100	100
43	h	84/96 (88%)	84 (100%)	0	100	100
44	i	131/131 (100%)	130 (99%)	1 (1%)	73	78
All	All	7129/7410 (96%)	7110 (100%)	19 (0%)	84	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	4	240	VAL
5	K	7	ASN
6	L	136	ASN
6	L	320	ASN
6	L	356	ILE
6	L	578	THR
7	M	247	THR

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Mol	Chain	Res	Type
8	N	37	MET
8	N	235	ASN
14	k	96	LEU
17	n	86	TYR
26	w	33	GLU
27	x	4	ILE
29	z	54	VAL
30	1	359	CYS
32	3	517	ASN
37	b	49	VAL
41	f	26	LEU
44	i	11	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	4	79	HIS
1	4	273	GLN
3	H	157	ASN
3	H	235	ASN
5	K	94	ASN
6	L	210	ASN
6	L	479	GLN
6	L	506	ASN
7	M	169	ASN
8	N	77	ASN
8	N	120	GLN
8	N	171	ASN
8	N	316	GLN
9	V	78	GLN
12	Y	72	GLN
13	Z	90	GLN
13	Z	114	GLN
13	Z	120	HIS
13	Z	123	ASN
14	k	141	GLN
14	k	188	ASN
14	k	200	GLN
14	k	288	GLN
15	l	100	GLN
18	o	12	GLN
18	o	117	HIS

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Mol	Chain	Res	Type
19	p	32	GLN
20	q	53	ASN
20	q	75	GLN
22	s	3	HIS
22	s	46	ASN
22	s	53	GLN
24	u	21	GLN
25	v	56	GLN
25	v	97	ASN
25	v	104	HIS
26	w	86	GLN
27	x	34	GLN
30	1	116	HIS
30	1	326	GLN
30	1	421	HIS
31	2	27	ASN
32	3	459	GLN
32	3	655	GLN
33	5	15	ASN
33	5	160	HIS
34	6	106	GLN
39	d	58	HIS
39	d	67	GLN
39	d	148	ASN
40	e	47	ASN
41	f	49	GLN
41	f	110	GLN
42	g	57	GLN
42	g	69	ASN
43	h	24	GLN
43	h	46	HIS
44	i	112	ASN
11	j	74	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
6	FME	L	1	6	8,9,10	0.97	0	8,9,11	0.86	0
7	FME	M	1	7	8,9,10	1.00	0	8,9,11	0.83	0
14	SEP	k	36	14	8,9,10	1.63	1 (12%)	7,12,14	1.38	1 (14%)
9	AYA	V	1	9	6,7,8	1.25	1 (16%)	6,8,10	1.58	2 (33%)
43	AYA	h	1	43	6,7,8	1.25	1 (16%)	6,8,10	1.12	1 (16%)
1	2MR	4	85	1	10,12,13	2.49	2 (20%)	5,13,15	1.03	0
5	FME	K	1	5	8,9,10	0.97	0	8,9,11	0.89	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	FME	L	1	6	-	4/7/9/11	-
7	FME	M	1	7	-	3/7/9/11	-
14	SEP	k	36	14	-	3/6/8/10	-
9	AYA	V	1	9	-	3/5/6/8	-
43	AYA	h	1	43	-	1/5/6/8	-
1	2MR	4	85	1	-	2/10/13/15	-
5	FME	K	1	5	-	3/7/9/11	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	4	85	2MR	CZ-NH2	5.32	1.44	1.33
1	4	85	2MR	CZ-NE	5.17	1.45	1.34
14	k	36	SEP	P-O1P	3.53	1.61	1.50
43	h	1	AYA	CA-N	-2.35	1.44	1.46
9	V	1	AYA	CA-N	-2.27	1.44	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	k	36	SEP	OG-CB-CA	2.99	111.05	108.14
9	V	1	AYA	CB-CA-N	2.91	112.96	109.68
43	h	1	AYA	CB-CA-N	2.55	112.55	109.68
9	V	1	AYA	CA-N-CT	2.14	124.26	121.50

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	K	1	FME	O1-CN-N-CA
5	K	1	FME	C-CA-CB-CG
6	L	1	FME	N-CA-CB-CG
7	M	1	FME	C-CA-CB-CG
9	V	1	AYA	O-C-CA-CB
14	k	36	SEP	CB-OG-P-O1P
14	k	36	SEP	CB-OG-P-O2P
14	k	36	SEP	CB-OG-P-O3P
43	h	1	AYA	O-C-CA-CB
9	V	1	AYA	OT-CT-N-CA
9	V	1	AYA	CM-CT-N-CA
6	L	1	FME	CA-CB-CG-SD
5	K	1	FME	N-CA-CB-CG
7	M	1	FME	N-CA-CB-CG
7	M	1	FME	CB-CG-SD-CE
1	4	85	2MR	C-CA-CB-CG
6	L	1	FME	CB-CG-SD-CE
1	4	85	2MR	CA-CB-CG-CD
6	L	1	FME	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	SF4	3	801	32	0,12,12	-	-	-		
47	SF4	9	202	35	0,12,12	-	-	-		
50	FES	2	300	31	0,4,4	-	-	-		
46	MYR	s	201	22	13,14,15	0.18	0	12,13,15	0.13	0
48	FMN	1	502	-	33,33,33	1.05	2 (6%)	48,50,50	1.24	7 (14%)
50	FES	3	803	32	0,4,4	-	-	-		
47	SF4	3	802	32	0,12,12	-	-	-		
47	SF4	9	201	35	0,12,12	-	-	-		
47	SF4	6	300	34	0,12,12	-	-	-		
49	NAI	1	503	-	47,48,48	0.41	1 (2%)	64,73,73	1.79	4 (6%)
45	ZMP	X	101	11	25,30,36	0.79	1 (4%)	29,37,45	0.93	1 (3%)
45	ZMP	j	101	11	28,33,36	0.64	1 (3%)	32,40,45	1.00	1 (3%)
53	NDP	d	401	-	51,52,52	0.32	0	71,80,80	0.35	0
47	SF4	1	501	30	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
47	SF4	3	801	32	-	-	0/6/5/5
47	SF4	9	202	35	-	-	0/6/5/5
50	FES	2	300	31	-	-	0/1/1/1
46	MYR	s	201	22	-	1/12/12/13	-
48	FMN	1	502	-	-	8/18/18/18	0/3/3/3
50	FES	3	803	32	-	-	0/1/1/1
47	SF4	3	802	32	-	-	0/6/5/5
47	SF4	9	201	35	-	-	0/6/5/5
49	NAI	1	503	-	-	8/29/72/72	0/5/5/5
47	SF4	6	300	34	-	-	0/6/5/5
45	ZMP	X	101	11	-	6/35/37/43	-
45	ZMP	j	101	11	-	3/38/40/43	-
53	NDP	d	401	-	-	10/34/77/77	0/5/5/5
47	SF4	1	501	30	-	-	0/6/5/5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	1	502	FMN	C4A-N5	3.31	1.37	1.30
45	X	101	ZMP	C9-C10	2.64	1.53	1.50
48	1	502	FMN	C10-N1	2.33	1.37	1.33
45	j	101	ZMP	C9-C10	2.27	1.53	1.50
49	1	503	NAI	PA-O5B	2.08	1.67	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	1	503	NAI	O5B-PA-O1A	-9.58	70.95	108.94
49	1	503	NAI	O2A-PA-O1A	-8.34	73.65	112.44
49	1	503	NAI	O3-PA-O1A	-5.62	93.81	110.70
48	1	502	FMN	C4-N3-C2	-3.37	119.66	125.64
45	j	101	ZMP	O1-C10-C9	-2.91	120.62	123.98
48	1	502	FMN	C4A-C10-N10	2.79	120.47	116.48
48	1	502	FMN	C4A-C4-N3	2.67	120.06	113.25
48	1	502	FMN	O4-C4-C4A	-2.61	119.65	126.53
49	1	503	NAI	O2A-PA-O5B	2.60	119.37	107.57
45	X	101	ZMP	O1-C10-C9	-2.26	121.37	123.98
48	1	502	FMN	C10-C4A-N5	-2.25	120.21	124.81
48	1	502	FMN	C5A-C9A-N10	2.17	119.93	117.97
48	1	502	FMN	C4A-C10-N1	-2.10	119.43	124.59

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	X	101	ZMP	C17-C16-N2-C15
45	j	101	ZMP	S1-C11-C12-N1
48	1	502	FMN	N10-C1'-C2'-O2'
48	1	502	FMN	N10-C1'-C2'-C3'
48	1	502	FMN	C5'-O5'-P-O2P
48	1	502	FMN	C5'-O5'-P-O3P
49	1	503	NAI	C5B-O5B-PA-O1A
49	1	503	NAI	C5B-O5B-PA-O3
49	1	503	NAI	C2D-C1D-N1N-C6N
53	d	401	NDP	C2N-C3N-C7N-N7N
45	X	101	ZMP	O3-C16-N2-C15
49	1	503	NAI	C2D-C1D-N1N-C2N
45	X	101	ZMP	O3-C16-C17-O4
48	1	502	FMN	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
46	s	201	MYR	C1-C2-C3-C4
48	1	502	FMN	O2'-C2'-C3'-C4'
45	X	101	ZMP	C16-C17-C18-C21
53	d	401	NDP	C2N-C3N-C7N-O7N
53	d	401	NDP	C5B-O5B-PA-O2A
53	d	401	NDP	C5B-O5B-PA-O3
49	1	503	NAI	O4D-C1D-N1N-C6N
53	d	401	NDP	O4D-C1D-N1N-C6N
49	1	503	NAI	C4D-C5D-O5D-PN
48	1	502	FMN	O2'-C2'-C3'-O3'
49	1	503	NAI	C2N-C3N-C7N-N7N
53	d	401	NDP	PA-O3-PN-O1N
45	X	101	ZMP	C3-C4-C5-C6
49	1	503	NAI	O4D-C1D-N1N-C2N
48	1	502	FMN	C1'-C2'-C3'-C4'
53	d	401	NDP	C2D-C1D-N1N-C6N
53	d	401	NDP	PA-O3-PN-O2N
53	d	401	NDP	O4B-C4B-C5B-O5B
45	j	101	ZMP	C13-C14-C15-N2
53	d	401	NDP	C2B-O2B-P2B-O1X
45	X	101	ZMP	N2-C16-C17-O4
45	j	101	ZMP	N2-C16-C17-O4

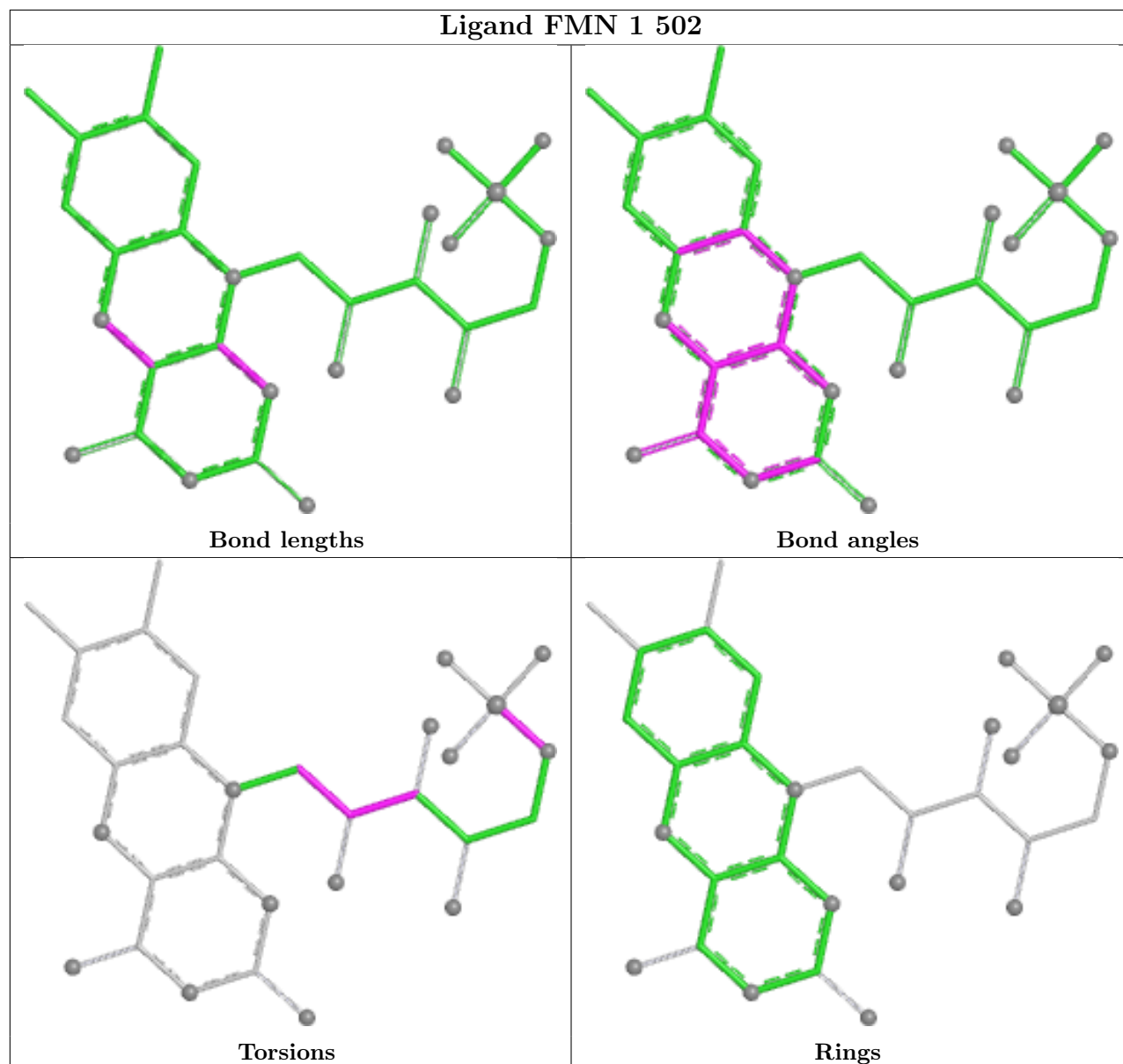
There are no ring outliers.

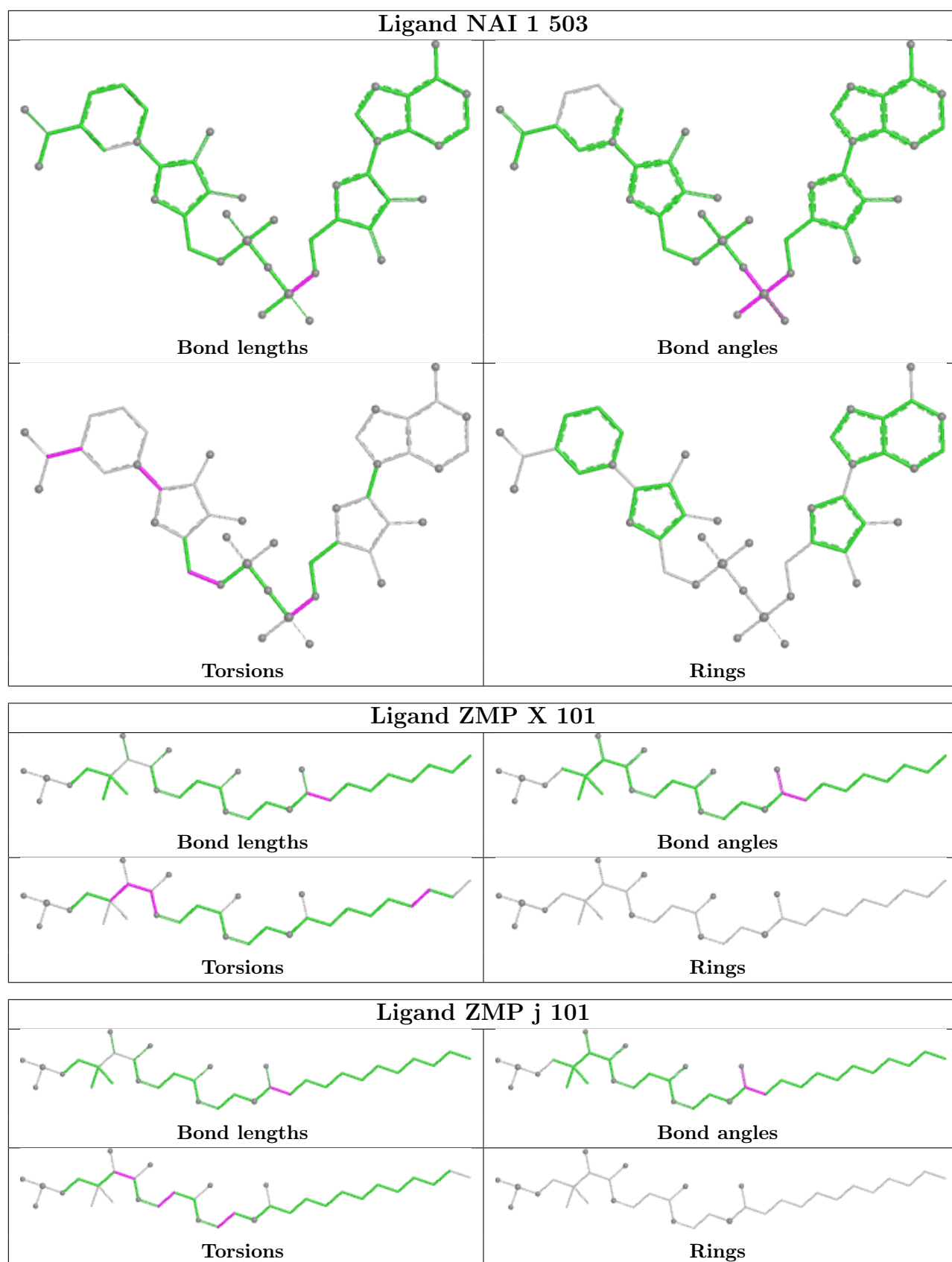
5 monomers are involved in 7 short contacts:

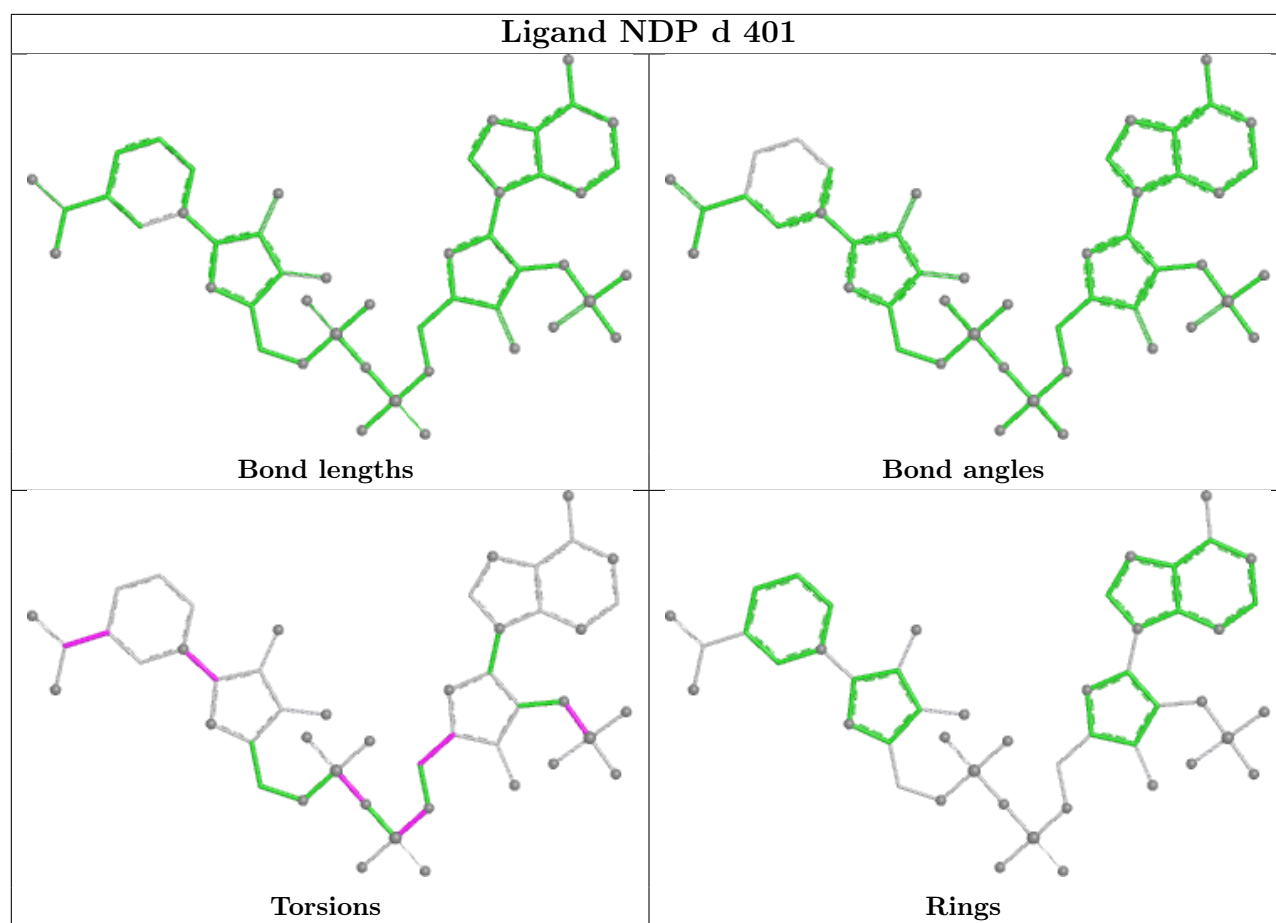
Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	3	801	SF4	1	0
50	2	300	FES	1	0
49	1	503	NAI	1	0
45	X	101	ZMP	1	0
45	j	101	ZMP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

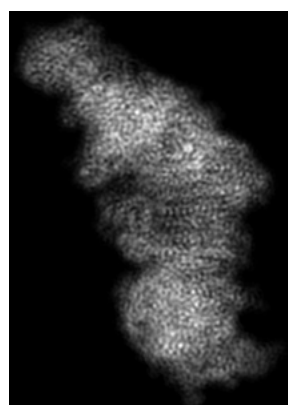
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14651. These allow visual inspection of the internal detail of the map and identification of artifacts.

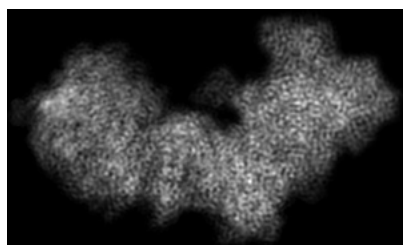
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

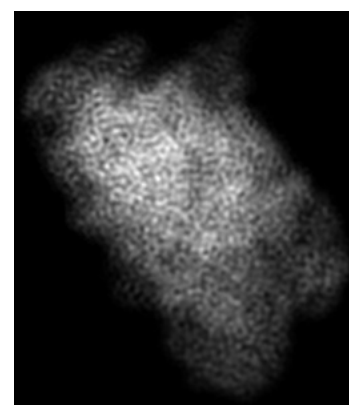
6.1.1 Primary map



X



Y



Z

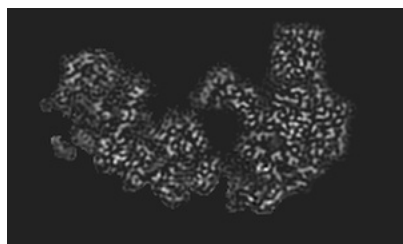
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 71



Y Index: 82



Z Index: 118

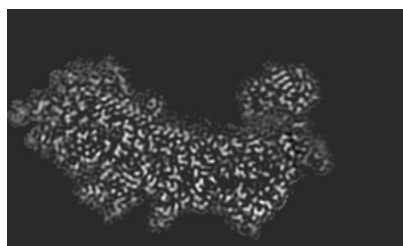
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

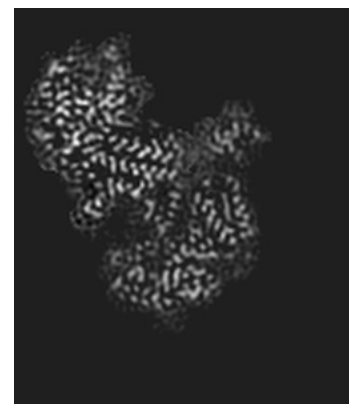
6.3.1 Primary map



X Index: 50



Y Index: 108

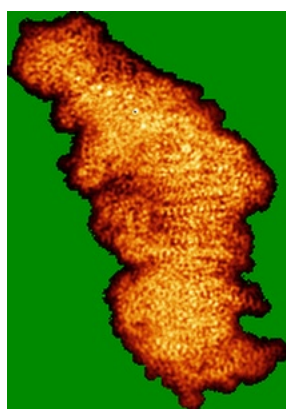


Z Index: 143

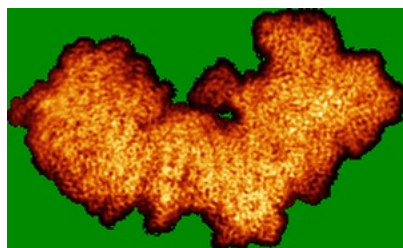
The images above show the largest variance slices of the map in three orthogonal directions.

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

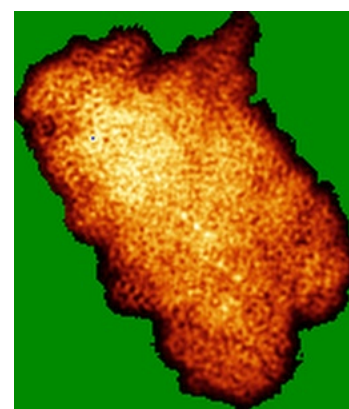
6.4.1 Primary map



X



Y

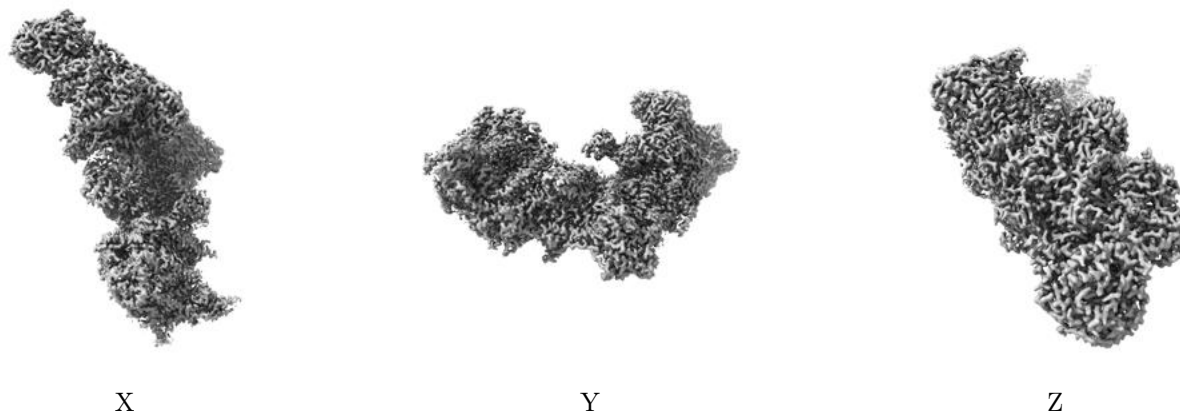


Z

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 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

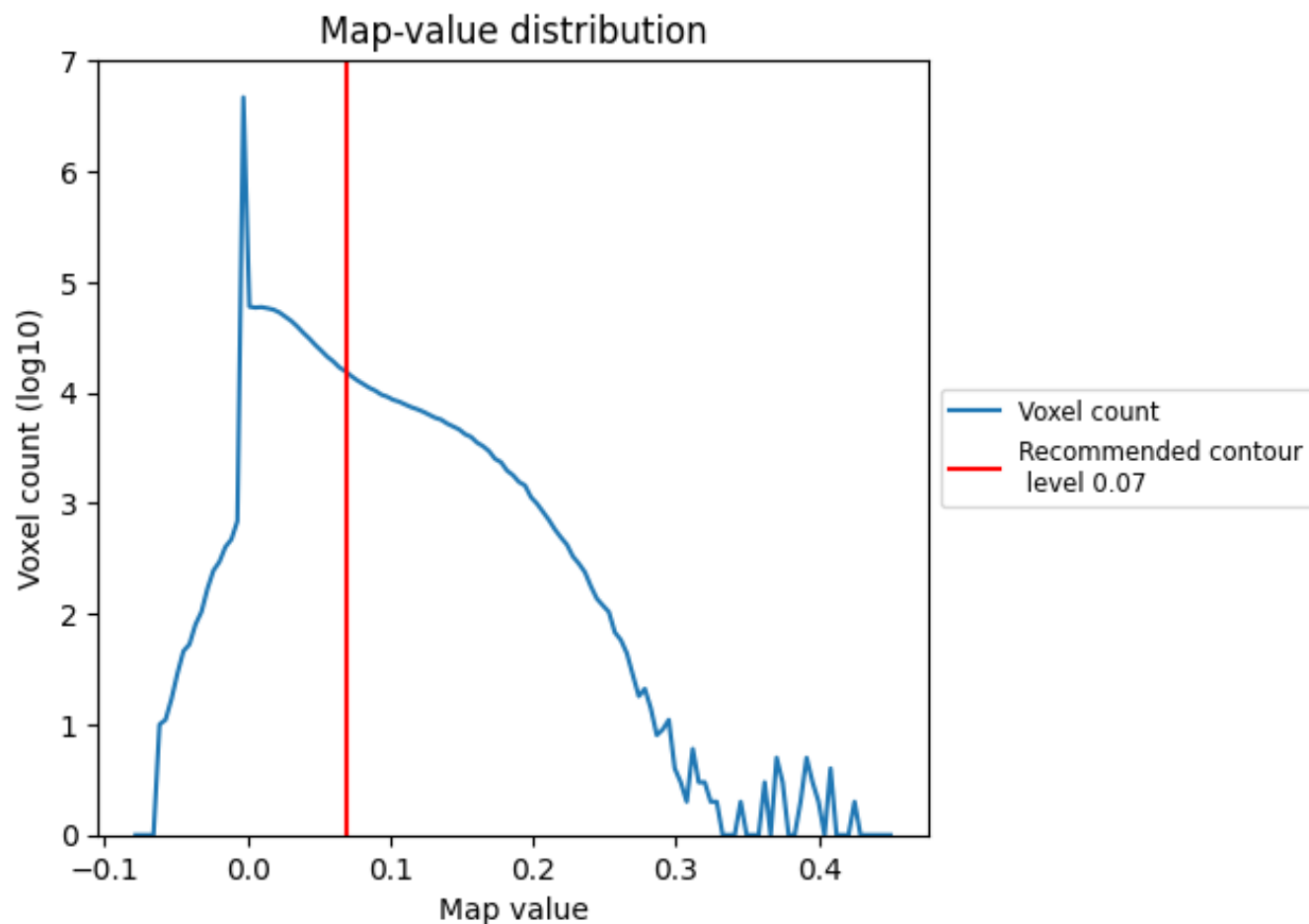
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

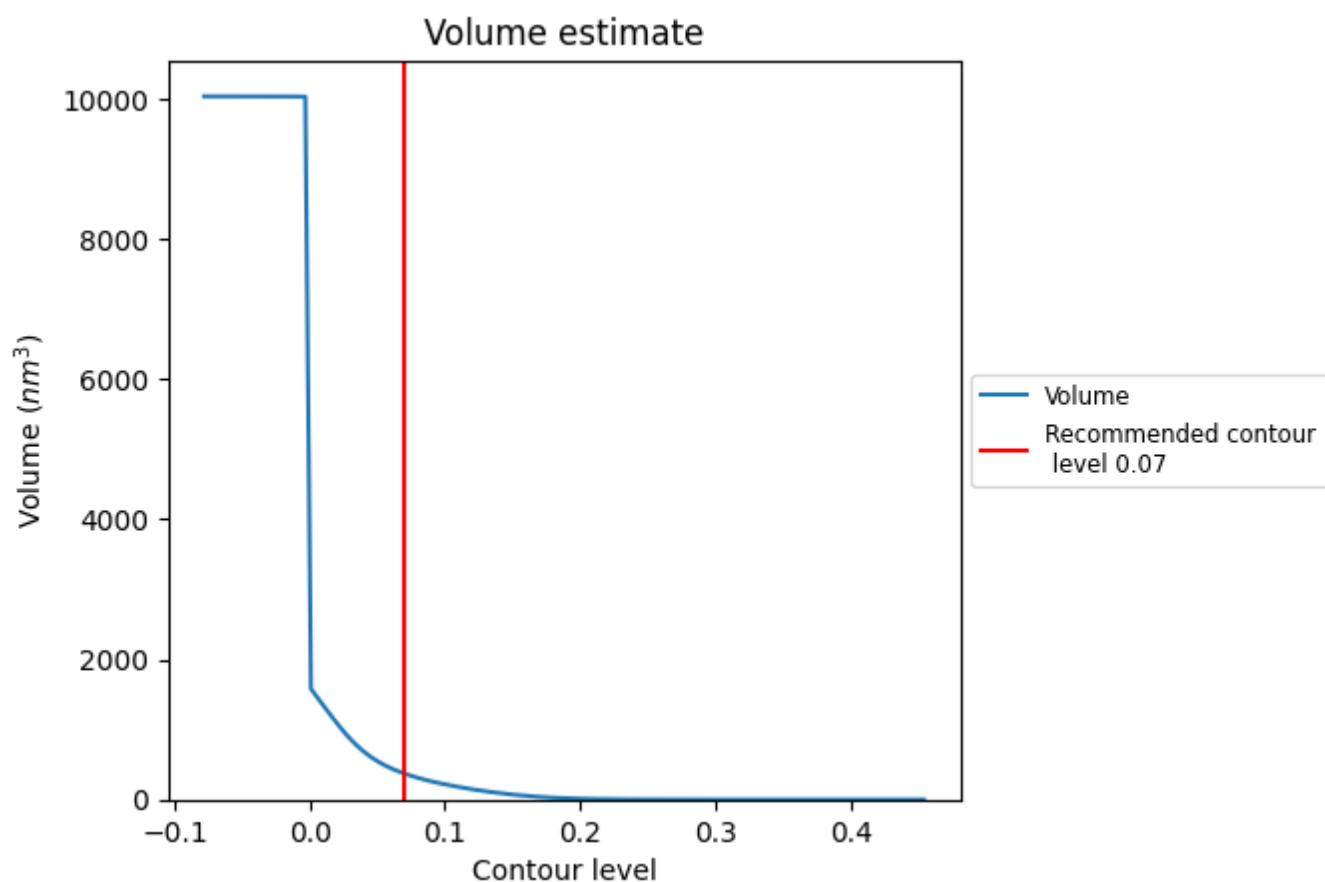
This section contains the results of statistical analysis of the map.

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 371 nm³; this corresponds to an approximate mass of 336 kDa.

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

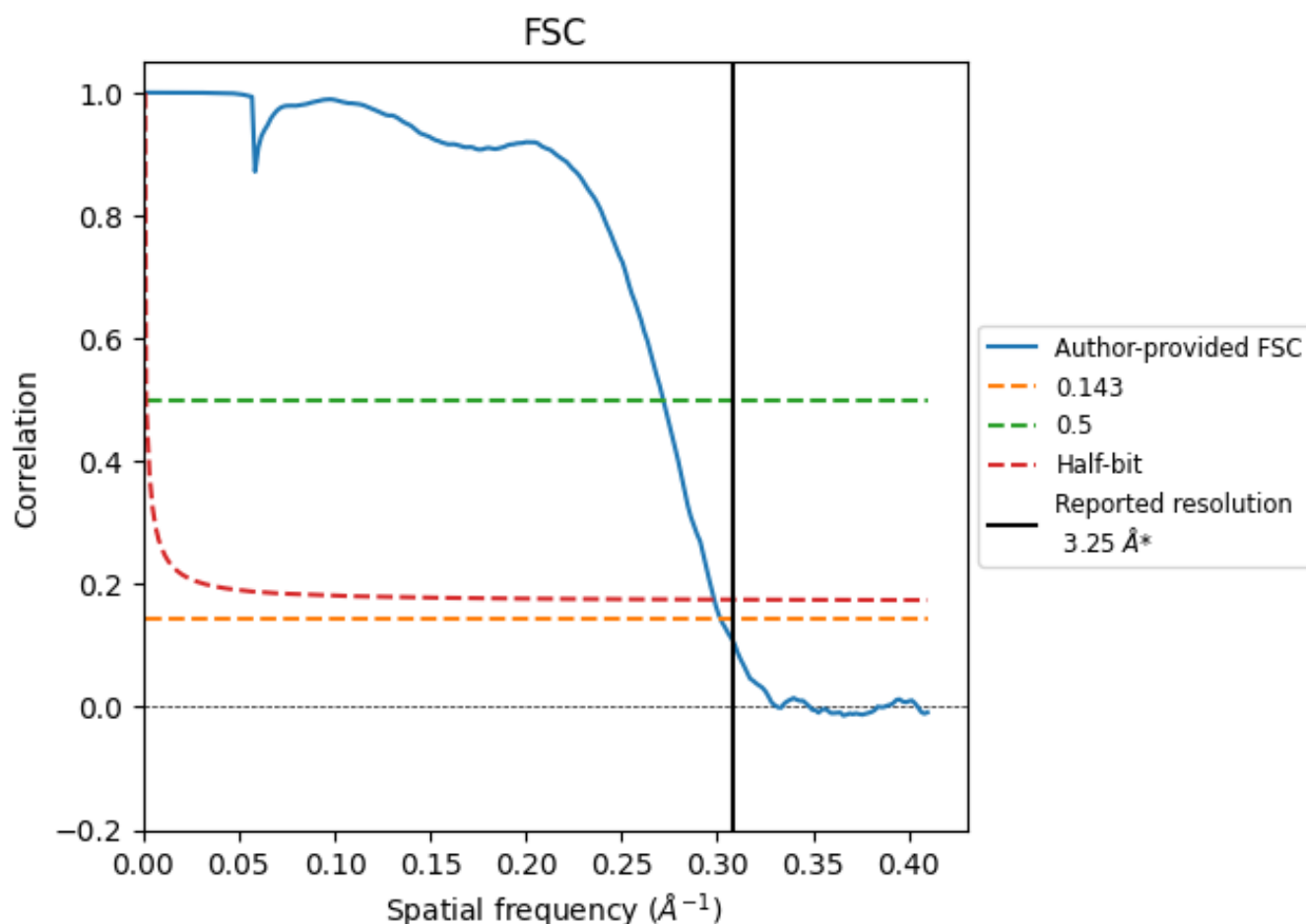
7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.308 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

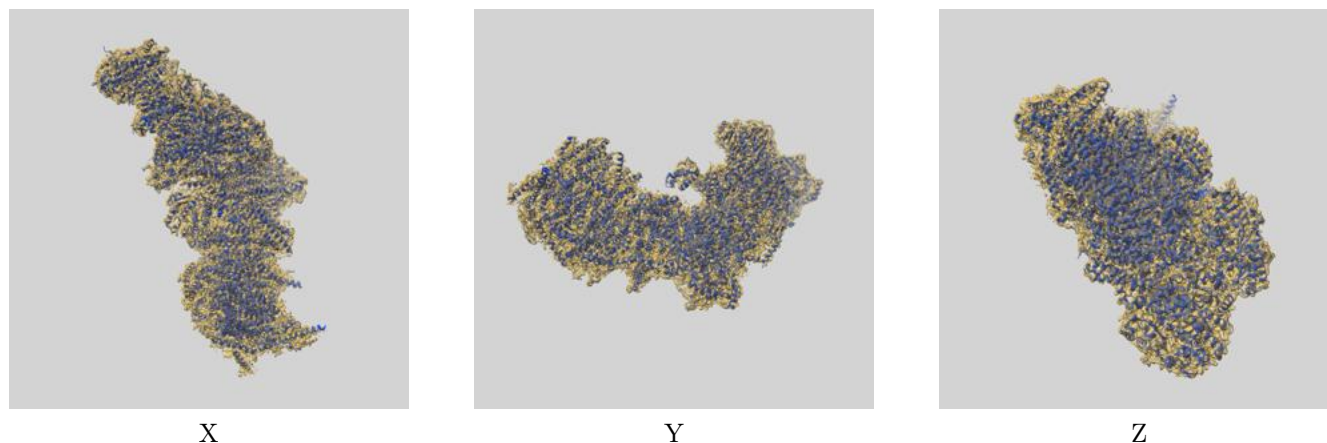
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.25	-	-
Author-provided FSC curve	3.31	3.68	3.35
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

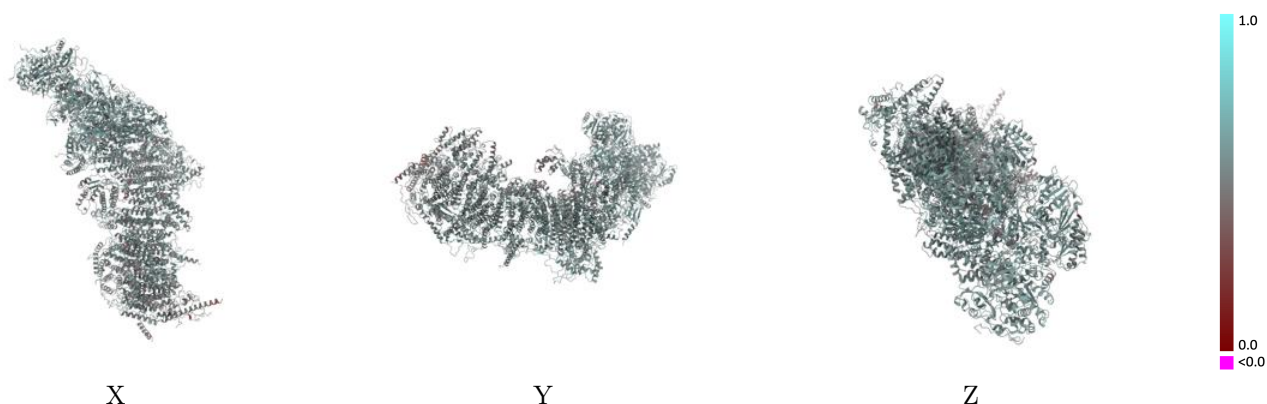
This section contains information regarding the fit between EMDB map EMD-14651 and PDB model 7ZDJ. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



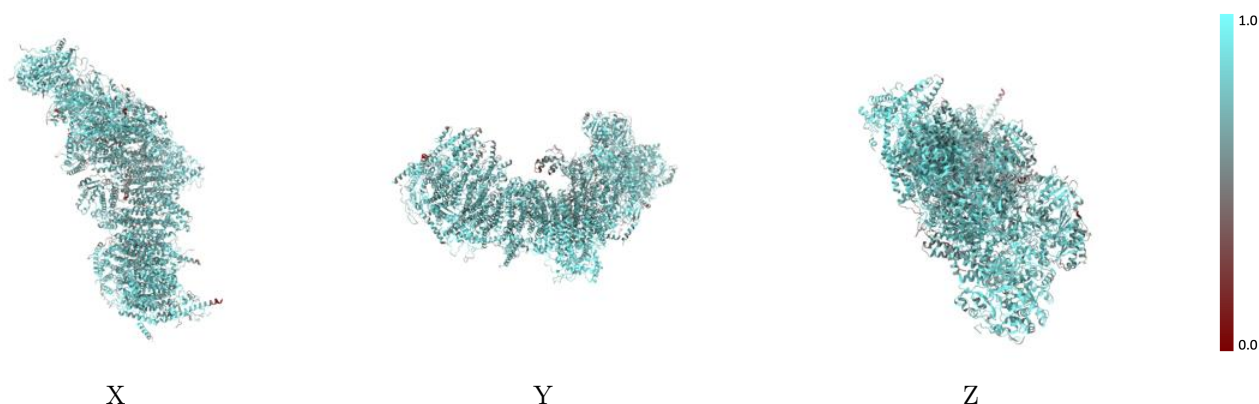
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



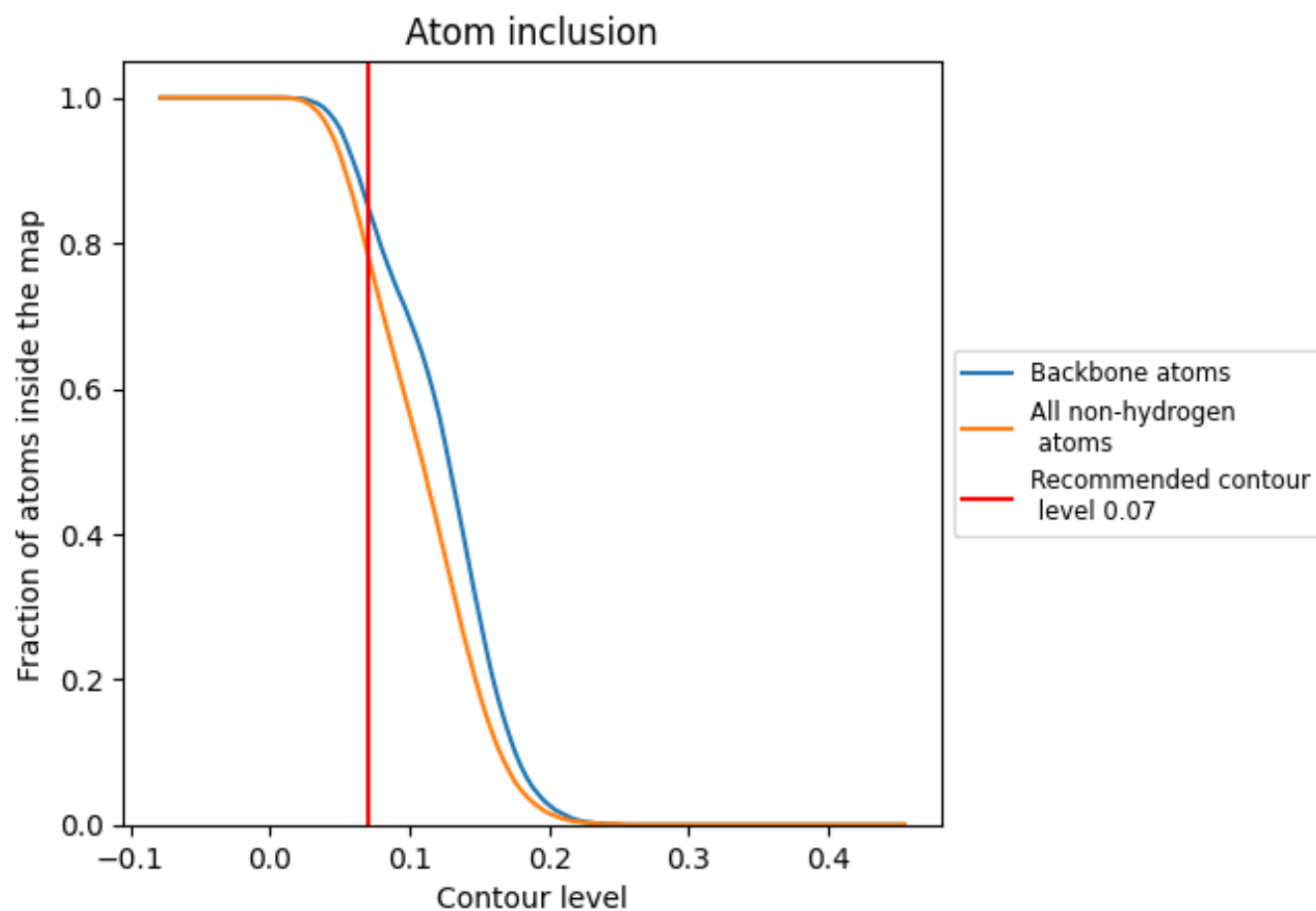
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 79% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7860	 0.5470
1	 0.8010	 0.5540
2	 0.7740	 0.5510
3	 0.7830	 0.5640
4	 0.7670	 0.5710
5	 0.8050	 0.5800
6	 0.8020	 0.5710
9	 0.8470	 0.5730
A	 0.7060	 0.5090
H	 0.8370	 0.5510
J	 0.7810	 0.5320
K	 0.8020	 0.5460
L	 0.8090	 0.5300
M	 0.8370	 0.5570
N	 0.8380	 0.5610
V	 0.7410	 0.5280
W	 0.8380	 0.5540
X	 0.7380	 0.4930
Y	 0.8540	 0.5550
Z	 0.8120	 0.5400
a	 0.7620	 0.5610
b	 0.7310	 0.5690
c	 0.7560	 0.5730
d	 0.7230	 0.5490
e	 0.7540	 0.5590
f	 0.7020	 0.5390
g	 0.7150	 0.5570
h	 0.7300	 0.5710
i	 0.7620	 0.5710
j	 0.5220	 0.4850
k	 0.7440	 0.5340
l	 0.8250	 0.5520
m	 0.8360	 0.5440
n	 0.7300	 0.4890
o	 0.8240	 0.5470



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Chain	Atom inclusion	Q-score
p	 0.7410	 0.5310
q	 0.8390	 0.5560
r	 0.7610	 0.5150
s	 0.7290	 0.4670
t	 0.7810	 0.5140
u	 0.7880	 0.4950
v	 0.7960	 0.5330
w	 0.7680	 0.5420
x	 0.7640	 0.5230
y	 0.7660	 0.5260
z	 0.8860	 0.5550