



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Dec 3, 2019 – 06:41 PM EST

PDB ID : 5LC5
EMDB ID: : EMD-4032
Title : Structure of mammalian respiratory Complex I, class2
Authors : Vinothkumar, K.R.; Zhu, J.; Hirst, J.
Deposited on : 2016-06-19
Resolution : 4.35 Å(reported)

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

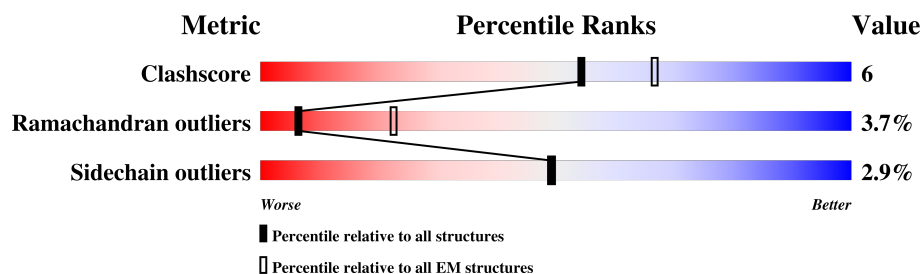
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.35 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.








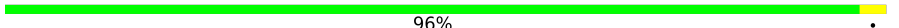
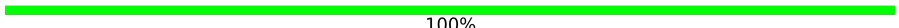

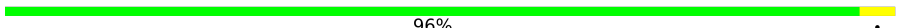
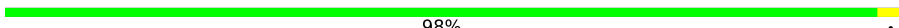
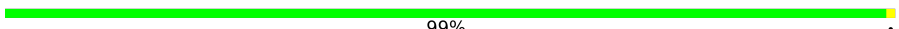
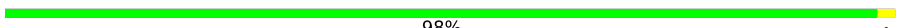






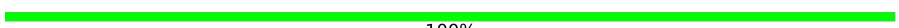

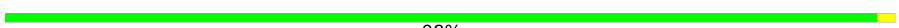




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	111	
2	B	147	
3	C	206	
4	D	426	
5	E	249	
6	F	464	
7	G	715	
8	H	313	
9	I	176	

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Mol	Chain	Length	Quality of chain
10	J	171	
11	K	95	
12	L	604	
13	M	457	
14	N	344	
15	O	314	
16	P	335	
17	Q	113	
18	R	89	
19	S	80	
20	T	75	
21	U	85	
22	V	116	
23	W	128	
24	X	169	
25	Y	138	
26	Z	138	
27	a	70	
28	b	80	
29	c	76	
30	d	114	
31	e	106	
32	f	57	
33	g	154	
34	h	186	

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Mol	Chain	Length	Quality of chain
35	i	121	 85% .. 12%
36	j	52	 100%
37	k	74	 100%
38	l	118	 100%
39	m	118	 95% . .
40	n	166	 98% .
41	o	58	 98% .
42	p	169	 98% .
43	q	138	 93% 7%
44	r	87	 100%
45	s	35	 100%

2 Entry composition

There are 50 unique types of molecules in this entry. The entry contains 51718 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	111	Total	C	N	O	S	0	0
			806	545	122	136	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	147	Total	C	N	O	S	0	0
			1159	740	203	202	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	206	Total	C	N	O	S	0	0
			1684	1091	285	305	3		

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	426	Total	C	N	O	S	0	0
			3301	2102	575	600	24		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	129	ARG	GLN	conflict	UNP P17694

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	186	Total	C	N	O	S	0	0
			959	583	186	186	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	425	Total	C	N	O	S	0	0
			2356	1432	463	455	6		

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial, NADH-ubiquinone oxidoreductase 75 kDa subunit, NDUF51.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	685	Total	C	N	O	S	0	0
			3614	2172	715	712	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	313	Total	C	N	O	S	0	0
			2389	1600	374	393	22		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	176	Total	C	N	O	S	0	0
			1366	857	238	261	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	171	Total	C	N	O	S	0	0
			1211	814	179	207	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	95	Total	C	N	O	S	0	0
			720	472	108	126	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	604	Total	C	N	O	S	0	0
			4538	3005	708	787	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	457	Total	C	N	O	S	0	0
			3536	2352	555	591	38		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	344	Total	C	N	O	S	0	0
			2592	1713	405	440	34		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	314	Total	C	N	O	S	0	0
			1854	1151	347	353	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
16	P	335	Total	C	N	O	0	0
			1675	1005	335	335		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
17	Q	113	Total	C	N	O	0	0
			565	339	113	113		

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

iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	89	Total	C	N	O	S	0	0
			501	304	99	95	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
19	S	80	Total	C	N	O	0	0
			405	245	80	80		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
20	T	75	Total	C	N	O	0	0
			378	228	75	75		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
21	U	85	Total	C	N	O	0	0
			432	262	85	85		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	106	Total	C	N	O	S	0	0
			685	430	126	128	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	111	Total	C	N	O	S	0	0
			817	516	154	144	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	164	Total	C	N	O	S	0	0
			1133	703	213	208	9		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	138	Total	C	N	O	S	0	0
			1011	644	173	188	6		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	138	Total	C	N	O	S	0	0
			921	573	172	170	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
27	a	64	Total	C	N	O	S	0	0
			480	312	86	77	5		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	b	80	Total	C	N	O	S	0	0
			519	336	89	93	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
29	c	46	Total	C	N	O	0	0
			320	211	56	53		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	d	114	Total	C	N	O	S	0	0
			790	504	146	137	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	e	89	Total	C	N	O	S	0	0
			616	382	121	108	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	f	54	Total	C	N	O	S	0	0
			350	223	62	64	1		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	g	97	Total	C	N	O	S	0	0
			677	438	120	117	2		

- Molecule 34 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	h	134	Total	C	N	O	0	0
			770	486	143	141		

- Molecule 35 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	i	106	Total	C	N	O	0	0
			616	376	126	114		

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUF2.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	j	52	Total	C	N	O	0	0
			260	156	52	52		

- Molecule 37 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUF3.

Mol	Chain	Residues	Atoms				AltConf	Trace
37	k	74	Total	C	N	O	0	0
			370	222	74	74		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUF8.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	l	118	Total	C	N	O	0	0
			590	354	118	118		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	m	118	Total	C	N	O	0	0
			887	566	165	156		

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	n	166	Total	C	N	O	S	0	0
			1088	677	212	196	3		

- Molecule 41 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit

7.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	o	58	Total	C	N	O	S	0	0
			296	176	58	58	4		

- Molecule 42 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUF10, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUF10.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	p	169	Total	C	N	O	S	0	0
			1039	633	198	202	6		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	q	138	Total	C	N	O	0	0
			696	420	138	138		

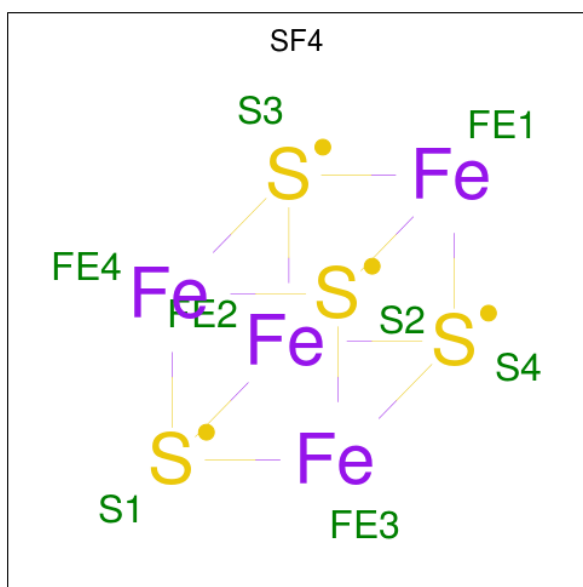
- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUF7.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	r	87	Total	C	N	O	0	0
			435	261	87	87		

- Molecule 45 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUF3.

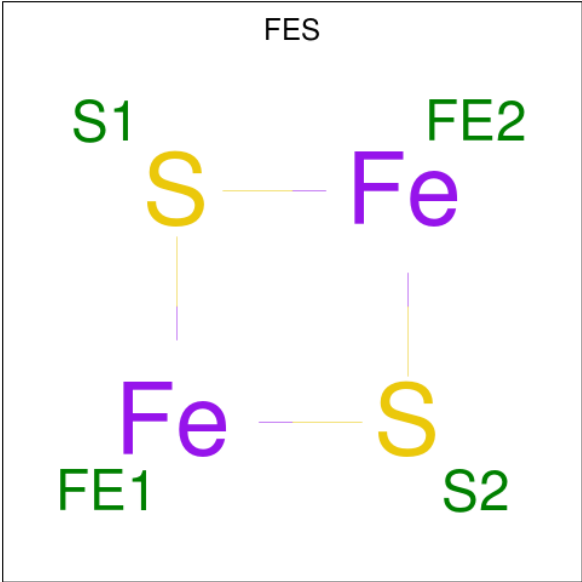
Mol	Chain	Residues	Atoms				AltConf	Trace
45	s	35	Total	C	N	O	0	0
			175	105	35	35		

- Molecule 46 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



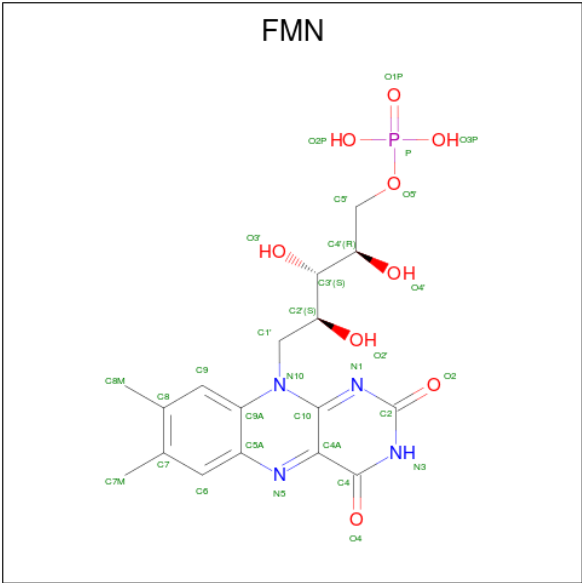
Mol	Chain	Residues	Atoms			AltConf
46	B	1	Total	Fe	S	0
			8	4	4	
46	F	1	Total	Fe	S	0
			8	4	4	
46	G	1	Total	Fe	S	0
			16	8	8	
46	G	1	Total	Fe	S	0
			16	8	8	
46	I	1	Total	Fe	S	0
			16	8	8	
46	I	1	Total	Fe	S	0
			16	8	8	

- Molecule 47 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

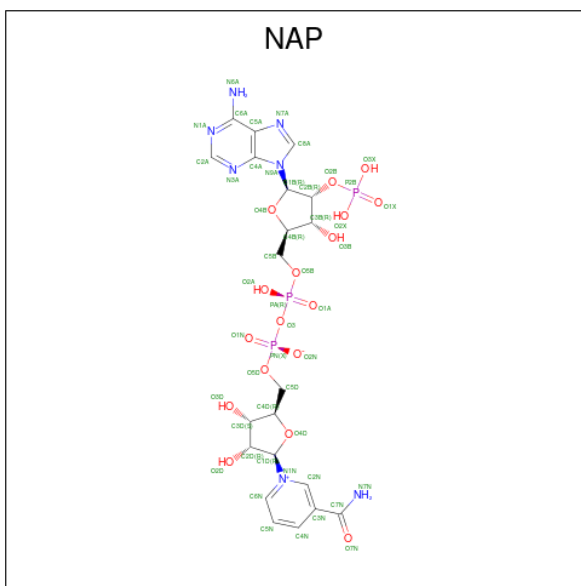
- Molecule 48 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



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

- Molecule 49 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE

(three-letter code: NAP) (formula: $\text{C}_{21}\text{H}_{28}\text{N}_7\text{O}_{17}\text{P}_3$).



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


- Molecule 50 is ZINC ION (three-letter code: ZN) (formula: Zn).

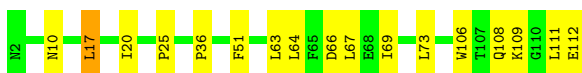
Mol	Chain	Residues	Atoms	AltConf
50	R	1	Total Zn 1 1	0

3 Residue-property plots


These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: NADH-ubiquinone oxidoreductase chain 3

Chain A: 




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

Chain B: 




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

Chain C: 



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

Chain D: 

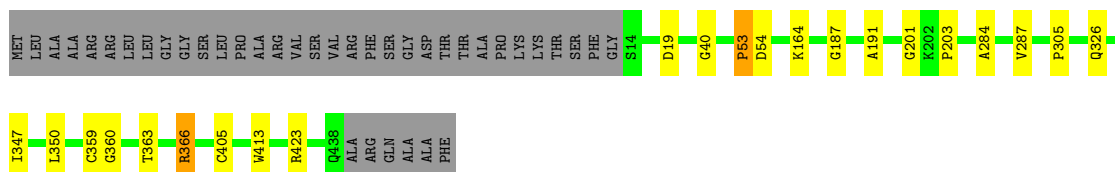


- Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E: 

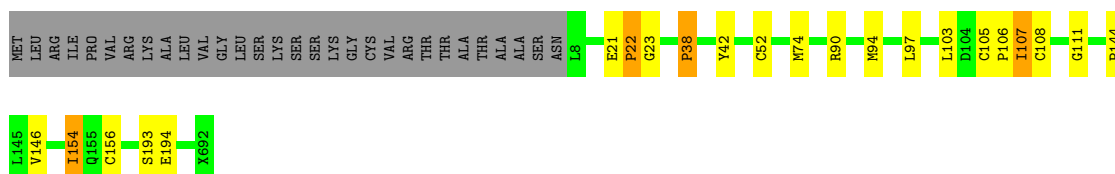
- Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F: 87% 0% 8%



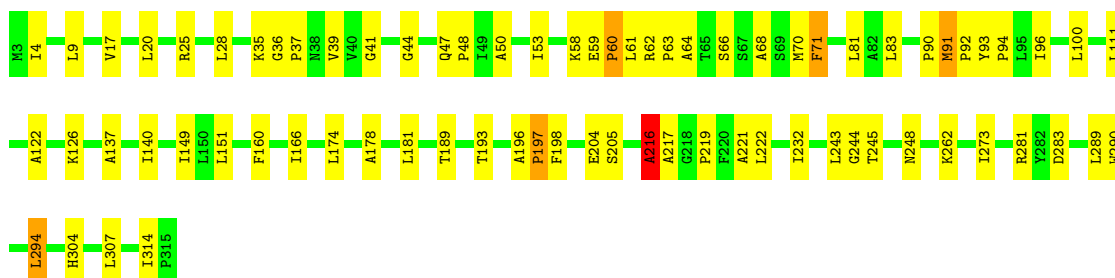
- Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial,NADH-ubiquinone oxidoreductase 75 kDa subunit, NDUFS1

Chain G:  93% . . .

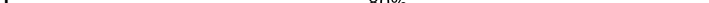


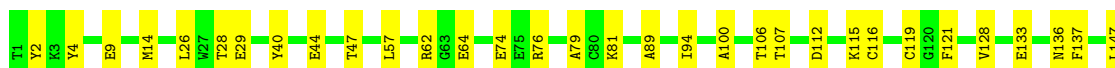
- Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H: 76% 22%



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

Chain I:  80% 20%





- Molecule 10: NADH-ubiquinone oxidoreductase chain 6

Chain J: 90% 9% .



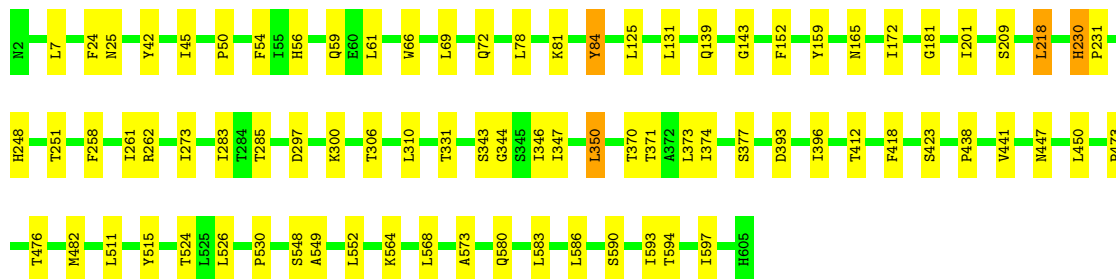
- Molecule 11: NADH-ubiquinone oxidoreductase chain 4L

Chain K: 82% 18% .



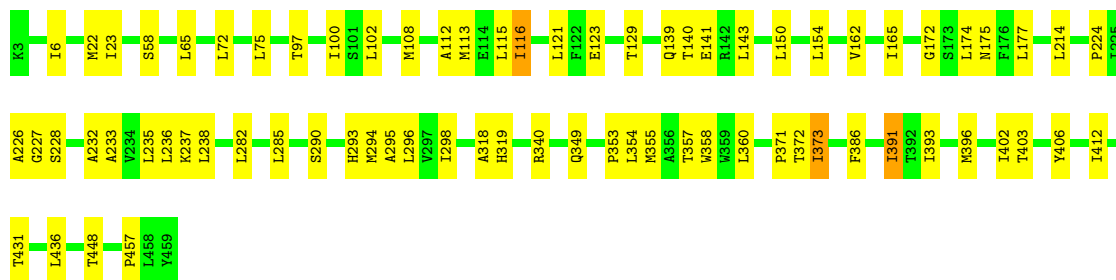
- Molecule 12: NADH-ubiquinone oxidoreductase chain 5

Chain L: 86% 13% .



- Molecule 13: NADH-ubiquinone oxidoreductase chain 4

Chain M: 84% 16% .



- Molecule 14: NADH-ubiquinone oxidoreductase chain 2

Chain N: 82% 17% .





- Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, NDUFA10, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial

Chain O: 96%



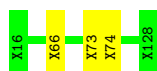
- Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P: 100%

There are no outlier residues recorded for this chain.

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

Chain Q: 97%



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

Chain R: 96%



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

Chain S: 98%

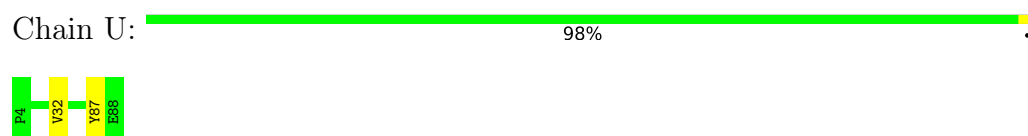


- Molecule 20: Acyl carrier protein, mitochondrial

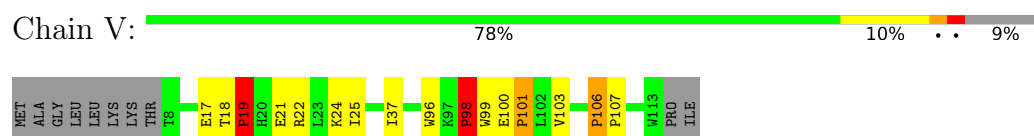
Chain T: 99%



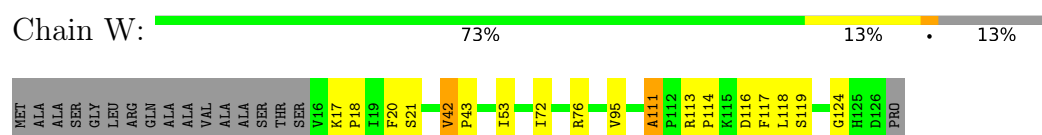
- Molecule 21: Acyl carrier protein, mitochondrial



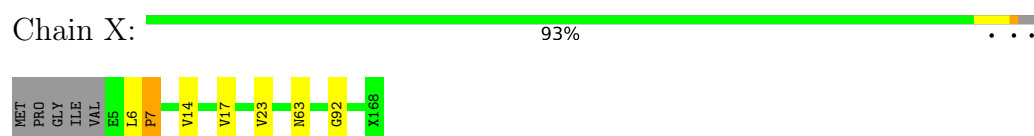
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5



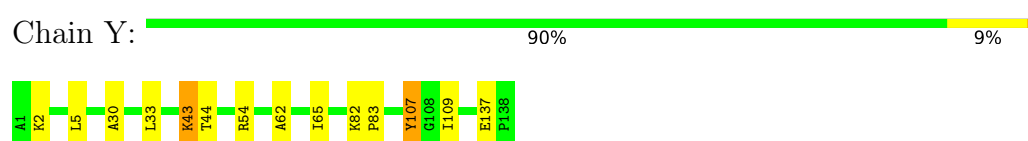
- Molecule 23: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



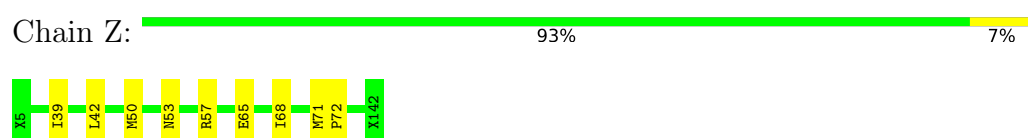
- Molecule 24: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8




- Molecule 25: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11



- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13, NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13



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

Chain a:  86% 6% 9%



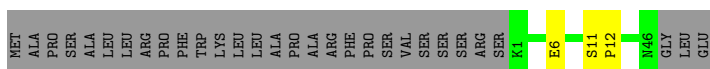
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3,NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3

Chain b:  100%

There are no outlier residues recorded for this chain.

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

Chain c:  57% . 39%




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

Chain d:  98% .




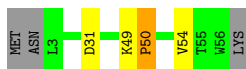
- Molecule 31: NADH dehydrogenase [ubiquinone] iron-sulfur protein 5

Chain e:  80% . 16%



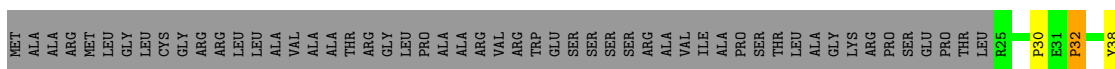
- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1

Chain f:  88% 5% . 5%



- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial

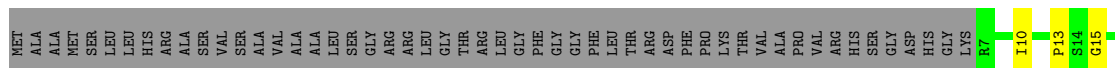
Chain g:  53% 8% . 37%





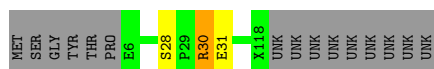
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial

Chain h: 70% 28%



- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6

Chain i: 85% 12%



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, NDUF2

Chain j: 100%

There are no outlier residues recorded for this chain.

- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3, NDUF3

Chain k: 100%

There are no outlier residues recorded for this chain.

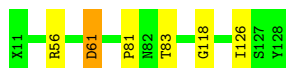
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, NDUF8

Chain l: 100%

There are no outlier residues recorded for this chain.

- Molecule 39: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4,NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

Chain m: 95%



- Molecule 40: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

Chain n:  98%



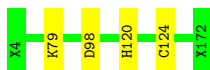
- Molecule 41: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

Chain o:  98%



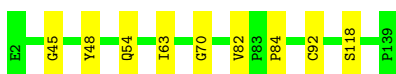
- Molecule 42: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10, NDUFB10

Chain p:  98%



- Molecule 43: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain q:  93% 7%



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7, NDUFA7

Chain r:  100%

There are no outlier residues recorded for this chain.

- Molecule 45: NADH dehydrogenase [ubiquinone] flavoprotein 3, NDUFV3

Chain s:  100%

There are no outlier residues recorded for this chain.

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	33301	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE; Ctf was estimated from the whole micrograph. Ctf was corrected per particle.	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	5500	Depositor
Magnification	105263	Depositor
Image detector	FEI FALCON II (4k x 4k)	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, ZN, SF4, NAP, FES

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 >2	RMSZ	# Z >2
1	A	0.43	0/825	0.63	0/1137
10	J	0.45	0/1239	0.55	0/1688
11	K	0.37	0/730	0.63	0/988
12	L	0.41	0/4653	0.57	0/6350
13	M	0.40	0/3624	0.60	0/4949
14	N	0.40	0/2656	0.61	0/3630
15	O	0.36	0/1449	0.53	0/2001
18	R	0.36	0/235	0.54	0/316
19	S	0.30	0/408	0.50	0/571
2	B	0.37	0/1187	0.61	0/1607
20	T	0.32	0/380	0.51	0/531
21	U	0.30	0/436	0.50	0/610
22	V	0.54	0/696	0.81	3/954 (0.3%)
23	W	0.49	0/831	0.69	2/1128 (0.2%)
24	X	0.43	0/877	0.63	1/1181 (0.1%)
25	Y	0.41	0/1031	0.56	0/1400
26	Z	0.37	0/585	0.54	0/781
27	a	0.45	0/494	0.57	0/669
28	b	0.42	0/352	0.54	0/481
29	c	0.46	0/330	0.62	0/455
3	C	0.43	0/1735	0.66	2/2365 (0.1%)
30	d	0.40	0/581	0.51	0/782
31	e	0.54	0/627	0.78	2/848 (0.2%)
32	f	0.49	0/356	0.69	1/488 (0.2%)
33	g	0.55	0/696	0.94	6/957 (0.6%)
34	h	0.54	0/301	0.68	0/409
35	i	0.55	0/224	2.89	2/300 (0.7%)
39	m	0.42	0/801	0.57	0/1085
4	D	0.43	0/3382	0.67	2/4587 (0.0%)
40	n	0.37	0/914	0.53	0/1247
41	o	0.32	0/296	0.51	0/412
42	p	0.36	0/535	0.53	0/718

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
43	q	0.36	0/704	0.57	0/984
5	E	0.62	0/975	1.04	12/1370 (0.9%)
6	F	0.38	0/2389	0.55	1/3299 (0.0%)
7	G	0.40	0/1213	0.65	2/1658 (0.1%)
8	H	0.41	0/2455	0.66	4/3359 (0.1%)
9	I	0.39	0/1395	0.62	0/1893
All	All	0.42	0/42597	0.66	40/58188 (0.1%)

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
2	B	0	1
35	i	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	i	30	ARG	O-C-N	-38.63	60.90	122.70
35	i	30	ARG	CA-C-N	28.54	179.99	117.20
5	E	166	PRO	CA-N-CD	-9.19	98.63	111.50
7	G	22	PRO	CA-N-CD	-9.17	98.66	111.50
6	F	53	PRO	CA-N-CD	-9.12	98.73	111.50

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	149	CYS	Peptide
35	i	30	ARG	Mainchain

5.2 Too-close contacts ⓘ

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

the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	806	0	789	8	0
2	B	1159	0	1166	13	0
3	C	1684	0	1610	63	0
4	D	3301	0	3185	76	0
5	E	959	0	509	81	0
6	F	2356	0	1535	9	0
7	G	3614	0	1337	16	0
8	H	2389	0	2462	57	0
9	I	1366	0	1286	9	0
10	J	1211	0	1165	8	0
11	K	720	0	761	18	0
12	L	4538	0	4480	33	0
13	M	3536	0	3652	35	0
14	N	2592	0	2631	44	0
15	O	1854	0	1139	3	0
16	P	1675	0	354	0	0
17	Q	565	0	122	2	0
18	R	501	0	246	3	0
19	S	405	0	197	1	0
20	T	378	0	176	0	0
21	U	432	0	207	0	0
22	V	685	0	563	27	0
23	W	817	0	743	25	0
24	X	1133	0	838	2	0
25	Y	1011	0	1018	5	0
26	Z	921	0	656	6	0
27	a	480	0	440	0	0
28	b	519	0	407	0	0
29	c	320	0	277	0	0
30	d	790	0	598	0	0
31	e	616	0	506	0	0
32	f	350	0	260	0	0
33	g	677	0	559	0	0
34	h	770	0	402	0	0
35	i	616	0	298	0	0
36	j	260	0	55	0	0
37	k	370	0	77	0	0
38	l	590	0	121	0	0
39	m	887	0	781	0	0
40	n	1088	0	768	0	0
41	o	296	0	134	0	0
42	p	1039	0	583	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	q	696	0	338	0	0
44	r	435	0	95	0	0
45	s	175	0	39	0	0
46	B	8	0	0	0	0
46	F	8	0	0	0	0
46	G	16	0	0	0	0
46	I	16	0	0	0	0
47	E	4	0	0	0	0
47	G	4	0	0	0	0
48	F	31	0	19	0	0
49	P	48	0	25	0	0
50	R	1	0	0	0	0
All	All	51718	0	39609	453	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 6.

The worst 5 of 453 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:31:PRO:HG3	14:N:174:GLN:NE2	1.12	1.45
3:C:39:GLN:NE2	22:V:107:PRO:HD3	1.32	1.44
4:D:31:PRO:CG	14:N:174:GLN:NE2	1.75	1.43
4:D:31:PRO:CG	14:N:174:GLN:HE22	1.26	1.41
5:E:46:ALA:O	5:E:49:PRO:CD	1.74	1.34

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	109/111 (98%)	89 (82%)	17 (16%)	3 (3%)	5	38
2	B	145/147 (99%)	125 (86%)	14 (10%)	6 (4%)	3	29
3	C	204/206 (99%)	174 (85%)	23 (11%)	7 (3%)	4	34
4	D	424/426 (100%)	367 (87%)	40 (9%)	17 (4%)	3	30
5	E	184/249 (74%)	158 (86%)	11 (6%)	15 (8%)	1	15
6	F	423/464 (91%)	374 (88%)	40 (10%)	9 (2%)	8	44
7	G	201/715 (28%)	168 (84%)	26 (13%)	7 (4%)	4	33
8	H	311/313 (99%)	277 (89%)	21 (7%)	13 (4%)	3	29
9	I	174/176 (99%)	144 (83%)	18 (10%)	12 (7%)	1	19
10	J	169/171 (99%)	147 (87%)	17 (10%)	5 (3%)	5	36
11	K	93/95 (98%)	88 (95%)	3 (3%)	2 (2%)	7	43
12	L	602/604 (100%)	537 (89%)	50 (8%)	15 (2%)	6	40
13	M	455/457 (100%)	413 (91%)	29 (6%)	13 (3%)	5	37
14	N	342/344 (99%)	305 (89%)	30 (9%)	7 (2%)	8	45
15	O	227/314 (72%)	201 (88%)	19 (8%)	7 (3%)	4	36
18	R	34/89 (38%)	28 (82%)	6 (18%)	0	100	100
19	S	78/80 (98%)	74 (95%)	4 (5%)	0	100	100
20	T	73/75 (97%)	68 (93%)	4 (6%)	1 (1%)	12	51
21	U	83/85 (98%)	74 (89%)	7 (8%)	2 (2%)	6	41
22	V	104/116 (90%)	88 (85%)	10 (10%)	6 (6%)	2	22
23	W	109/128 (85%)	90 (83%)	12 (11%)	7 (6%)	1	21
24	X	108/169 (64%)	96 (89%)	8 (7%)	4 (4%)	4	32
25	Y	136/138 (99%)	122 (90%)	8 (6%)	6 (4%)	3	28
26	Z	69/138 (50%)	65 (94%)	4 (6%)	0	100	100
27	a	62/70 (89%)	55 (89%)	4 (6%)	3 (5%)	2	26
28	b	44/80 (55%)	41 (93%)	3 (7%)	0	100	100
29	c	44/76 (58%)	39 (89%)	2 (4%)	3 (7%)	1	19
30	d	69/114 (60%)	65 (94%)	3 (4%)	1 (1%)	12	51
31	e	87/106 (82%)	76 (87%)	9 (10%)	2 (2%)	7	42
32	f	52/57 (91%)	44 (85%)	5 (10%)	3 (6%)	2	22
33	g	95/154 (62%)	64 (67%)	19 (20%)	12 (13%)	0	6
34	h	38/186 (20%)	35 (92%)	0	3 (8%)	1	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
35	i	25/121 (21%)	23 (92%)	0	2 (8%)	1	16
39	m	96/118 (81%)	83 (86%)	7 (7%)	6 (6%)	1	21
40	n	126/166 (76%)	113 (90%)	10 (8%)	3 (2%)	6	41
41	o	56/58 (97%)	55 (98%)	0	1 (2%)	9	47
42	p	67/169 (40%)	60 (90%)	4 (6%)	3 (4%)	3	27
43	q	136/138 (99%)	109 (80%)	18 (13%)	9 (7%)	1	20
All	All	5854/7423 (79%)	5134 (88%)	505 (9%)	215 (4%)	6	32

5 of 215 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	150	PRO
3	C	9	PRO
4	D	35	ASP
4	D	53	PRO
4	D	258	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	75/97 (77%)	68 (91%)	7 (9%)	10	36
2	B	124/124 (100%)	116 (94%)	8 (6%)	19	51
3	C	179/187 (96%)	171 (96%)	8 (4%)	30	61
4	D	338/368 (92%)	323 (96%)	15 (4%)	31	61
5	E	21/205 (10%)	21 (100%)	0	100	100
6	F	84/368 (23%)	81 (96%)	3 (4%)	38	66
7	G	64/196 (33%)	57 (89%)	7 (11%)	7	30
8	H	249/270 (92%)	239 (96%)	10 (4%)	34	63
9	I	138/151 (91%)	130 (94%)	8 (6%)	22	54
10	J	112/139 (81%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	K	83/83 (100%)	81 (98%)	2 (2%)	52	75
12	L	463/532 (87%)	451 (97%)	12 (3%)	49	73
13	M	384/411 (93%)	376 (98%)	8 (2%)	56	78
14	N	277/313 (88%)	271 (98%)	6 (2%)	55	77
15	O	84/205 (41%)	83 (99%)	1 (1%)	74	87
18	R	17/26 (65%)	16 (94%)	1 (6%)	21	54
19	S	4/72 (6%)	4 (100%)	0	100	100
20	T	3/69 (4%)	3 (100%)	0	100	100
21	U	5/79 (6%)	5 (100%)	0	100	100
22	V	47/102 (46%)	47 (100%)	0	100	100
23	W	71/114 (62%)	70 (99%)	1 (1%)	69	85
24	X	83/103 (81%)	83 (100%)	0	100	100
25	Y	99/99 (100%)	98 (99%)	1 (1%)	78	89
26	Z	59/59 (100%)	59 (100%)	0	100	100
27	a	41/59 (70%)	40 (98%)	1 (2%)	52	75
28	b	36/36 (100%)	36 (100%)	0	100	100
29	c	26/68 (38%)	26 (100%)	0	100	100
30	d	56/60 (93%)	55 (98%)	1 (2%)	62	82
31	e	45/96 (47%)	45 (100%)	0	100	100
32	f	22/54 (41%)	21 (96%)	1 (4%)	30	61
33	g	51/131 (39%)	50 (98%)	1 (2%)	58	79
34	h	28/73 (38%)	27 (96%)	1 (4%)	38	66
35	i	20/32 (62%)	20 (100%)	0	100	100
39	m	75/86 (87%)	74 (99%)	1 (1%)	71	86
40	n	65/117 (56%)	65 (100%)	0	100	100
41	o	5/56 (9%)	5 (100%)	0	100	100
42	p	50/62 (81%)	49 (98%)	1 (2%)	58	79
43	q	9/124 (7%)	9 (100%)	0	100	100
All	All	3592/5426 (66%)	3487 (97%)	105 (3%)	49	70

5 of 105 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	G	156	CYS
9	I	26	LEU
25	Y	107	TYR
8	H	4	ILE
8	H	174	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
12	L	580	GLN
13	M	319	HIS
30	d	59	HIS
13	M	192	ASN
13	M	279	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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
46	SF4	B	201	2	0,12,12	0.00	-	-		
47	FES	E	301	5	0,4,4	0.00	-	-		
48	FMN	F	501	-	31,33,33	2.52	6 (19%)	40,50,50	2.15	8 (20%)
46	SF4	F	502	6	0,12,12	0.00	-	-		
46	SF4	G	801	7	0,12,12	0.00	-	-		
46	SF4	G	802	7	0,12,12	0.00	-	-		
47	FES	G	803	7	0,4,4	0.00	-	-		
46	SF4	I	201	9	0,12,12	0.00	-	-		
46	SF4	I	202	9	0,12,12	0.00	-	-		
49	NAP	P	501	-	43,52,52	0.96	2 (4%)	53,80,80	1.22	5 (9%)

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	SF4	B	201	2	-	-	0/6/5/5
47	FES	E	301	5	-	-	0/1/1/1
48	FMN	F	501	-	-	10/18/18/18	0/3/3/3
46	SF4	F	502	6	-	-	0/6/5/5
46	SF4	G	801	7	-	-	0/6/5/5
46	SF4	G	802	7	-	-	0/6/5/5
47	FES	G	803	7	-	-	0/1/1/1
46	SF4	I	201	9	-	-	0/6/5/5
46	SF4	I	202	9	-	-	0/6/5/5
49	NAP	P	501	-	-	6/27/67/67	0/5/5/5

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	F	501	FMN	C4A-C10	10.48	1.49	1.38
48	F	501	FMN	C4-C4A	4.50	1.49	1.41
48	F	501	FMN	C9A-C5A	4.14	1.50	1.42
48	F	501	FMN	C8-C7	3.92	1.50	1.40
48	F	501	FMN	C9A-N10	3.67	1.43	1.38

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	F	501	FMN	C4-N3-C2	8.25	122.11	115.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	F	501	FMN	C4A-N5-C5A	4.51	121.40	116.77
48	F	501	FMN	C1'-N10-C9A	3.97	121.76	118.31
48	F	501	FMN	C4-C4A-C10	-3.92	117.05	119.95
49	P	501	NAP	PN-O3-PA	-3.66	120.93	132.57

There are no chirality outliers.

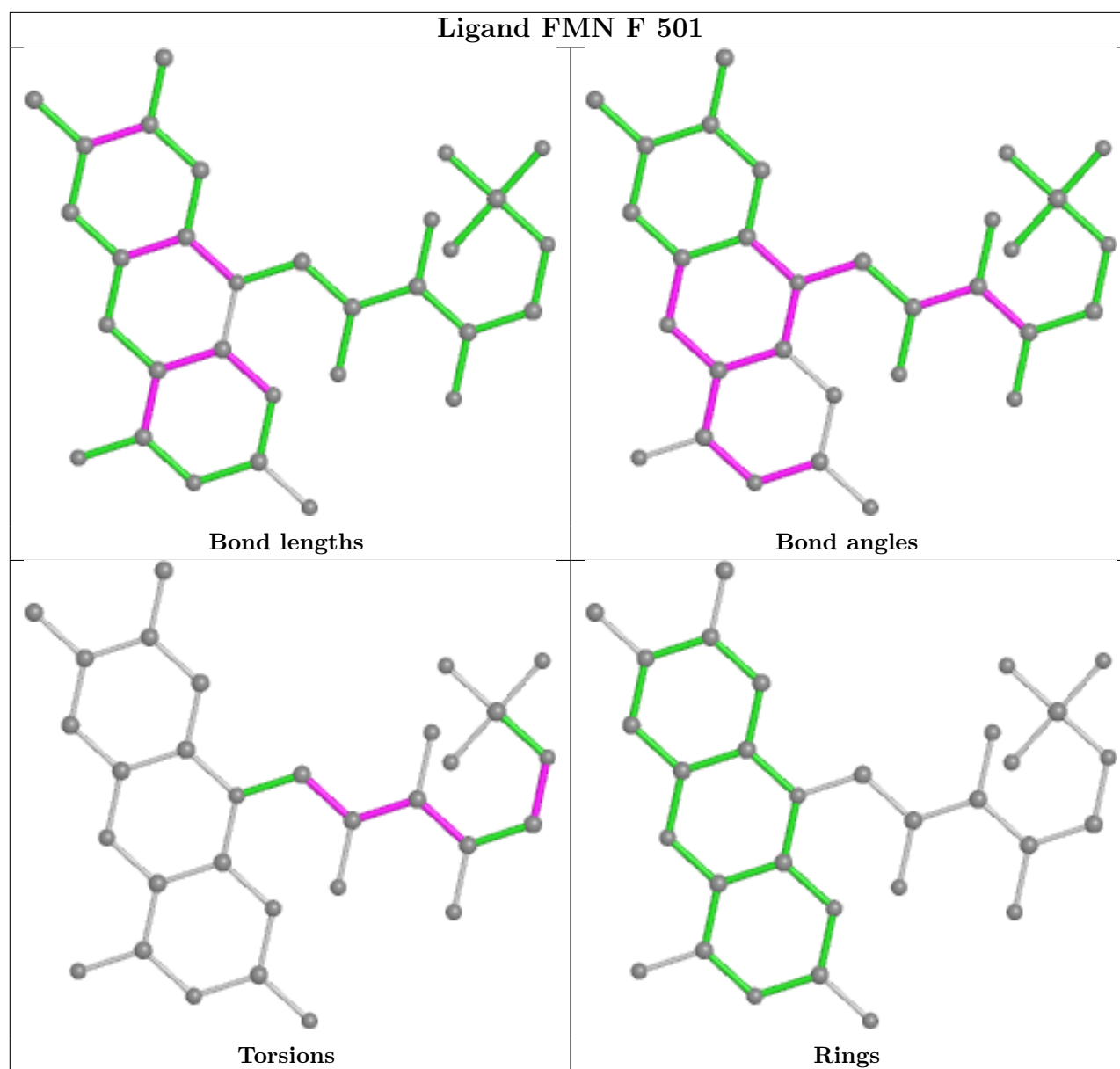
5 of 16 torsion outliers are listed below:

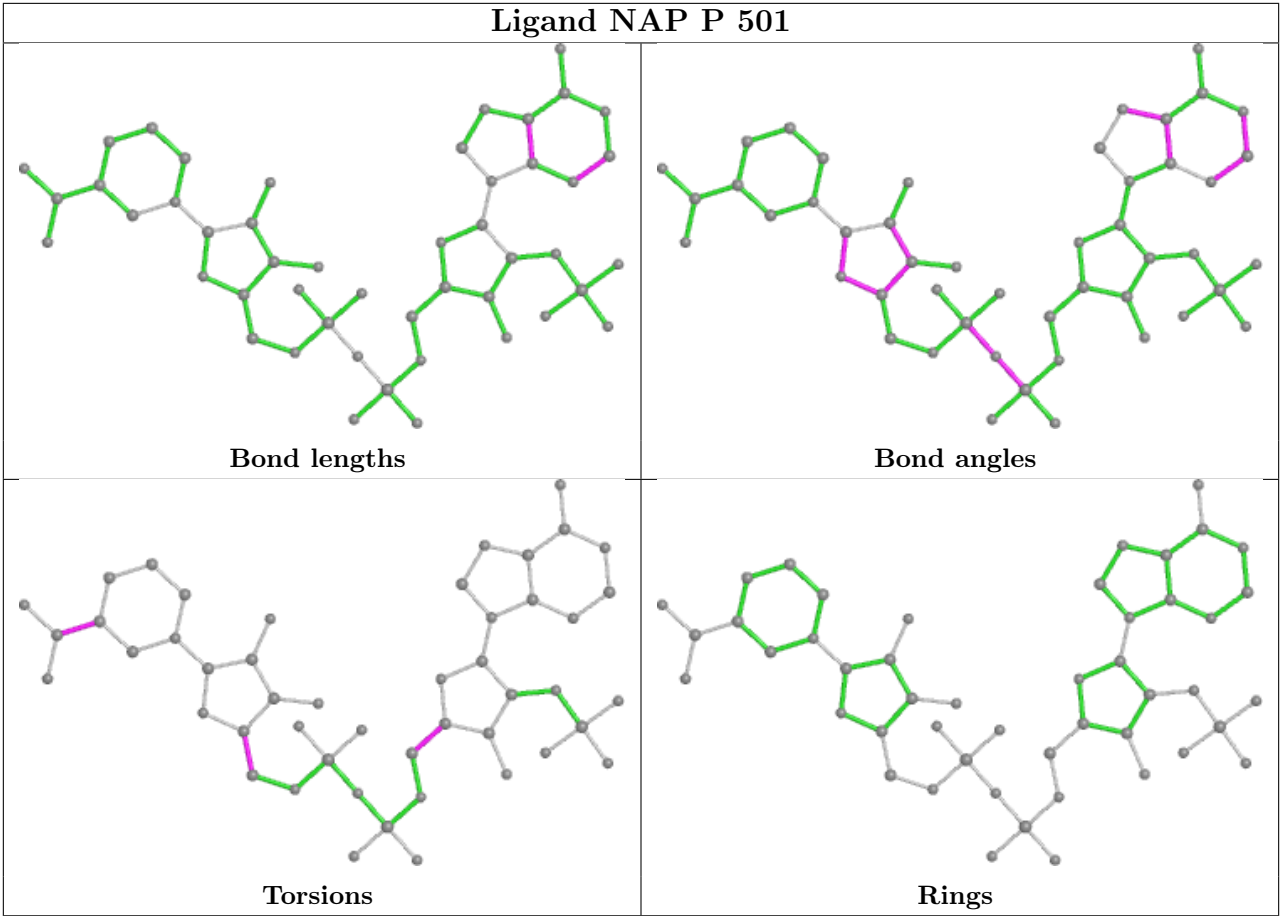
Mol	Chain	Res	Type	Atoms
48	F	501	FMN	N10-C1'-C2'-O2'
48	F	501	FMN	N10-C1'-C2'-C3'
48	F	501	FMN	C1'-C2'-C3'-O3'
49	P	501	NAP	C2N-C3N-C7N-O7N
49	P	501	NAP	C2N-C3N-C7N-N7N

There are no ring outliers.

No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
44	r	1
35	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	70:UNK	C	100:UNK	N	23.03
1	i	32:PRO	C	40:UNK	N	15.86