



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 06:02 AM JST

PDB ID : 7DGZ / pdb_00007dgz
EMDB ID : EMD-30676
Title : Activity optimized complex I (closed form)
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Deposited on : 2020-11-12
Resolution : 3.80 Å(reported)

This is a wwPDB EM Validation Summary 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.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

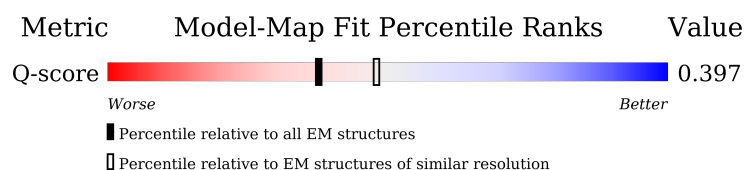
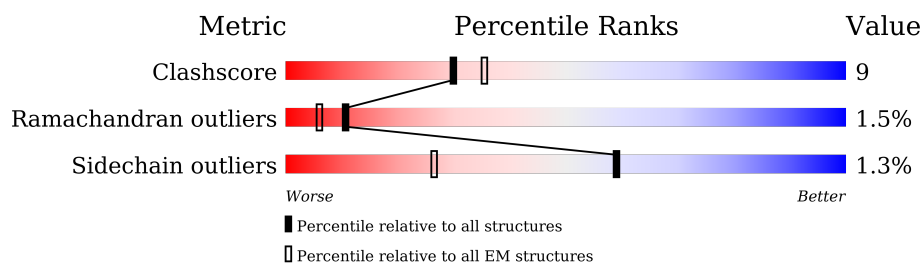
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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	10198 (3.30 - 4.30)

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	2	347	
2	3	115	
3	4	459	
4	5	98	

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Mol	Chain	Length	Quality of chain
5	7	175	
6	8	444	
7	9	217	
8	A	704	
9	B	430	
10	C	228	
11	D	179	
12	E	176	
13	F	75	
14	G	133	
15	H	105	
16	I	96	
17	J	70	
18	K	98	
19	L	83	
20	N	115	
21	O	127	
22	P	112	
23	Q	171	
24	R	345	
25	S	320	
26	T	140	
27	U	145	
28	V	143	
29	M	88	

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Mol	Chain	Length	Quality of chain
29	W	88	
30	X	57	
31	Y	72	
32	Z	97	
33	a	128	
34	b	143	
35	c	127	
36	d	136	
37	f	178	
38	h	125	
39	i	49	
40	j	120	
41	1	318	
42	6	606	
43	g	176	
44	e	158	

2 Entry composition

There are 52 unique types of molecules in this entry. The entry contains 60921 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 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	344	Total	C	N	O	S	0	0
			2582	1707	404	437	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	112	Total	C	N	O	S	0	0
			864	582	127	150	5		

- Molecule 3 is a protein called NADH-ubiquinone oxidoreductase chain 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	458	Total	C	N	O	S	1	0
			3447	2293	548	574	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	96	Total	C	N	O	S	0	0
			697	454	109	124	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	172	Total	C	N	O	S	0	0
			1186	798	179	202	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	427	Total	C	N	O	S	0	0
			2965	1864	552	534	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	9	207	Total	C	N	O	S	0	0
			1535	978	261	286	10		

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	A	688	Total	C	N	O	S	0	0
			5183	3254	915	978	36		

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	B	430	Total	C	N	O	S	0	0
			3410	2178	587	620	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	C	208	Total	C	N	O	S	0	0
			1705	1102	294	306	3		

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	D	152	Total	C	N	O	S	0	0
			1200	769	209	208	14		

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	E	176	Total	C	N	O	S	0	0
			1388	874	239	264	11		

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	F	28	Total	C	N	O	0	0
			183	116	32	35		

- Molecule 14 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	123	Total	C	N	O	S	0	0
			981	619	177	182	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	96	Total	C	N	O	S	0	0
			780	494	147	134	5		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	71	Total	C	N	O	S	0	0
			530	331	99	97	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	J	69	Total	C	N	O	S	0	0
			530	344	96	88	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
18	K	84	Total	C	N	O	0	0
			652	409	125	118		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	L	80	Total	C	N	O	S	0	0
			602	398	97	105	2		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	111	Total	C	N	O	S	0	0
			862	559	149	152	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	O	114	Total	C	N	O	S	0	0
			925	595	170	156	4		

- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	90	Total	C	N	O	S	0	0
			698	442	128	126	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	168	Total	C	N	O	S	0	0
			1345	851	242	243	9		

- Molecule 24 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	319	Total	C	N	O	S	0	0
			2407	1548	431	425	3		

- Molecule 25 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 10, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	S	319	Total	C	N	O	S	0	0
			2299	1457	395	438	9		

- Molecule 26 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	T	138	Total	C	N	O	S	0	0
			942	599	165	172	6		

- Molecule 27 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	U	132	Total	C	N	O	S	0	0
			1019	659	179	178	3		

- Molecule 28 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	V	138	Total	C	N	O	S	0	0
			1093	702	189	193	9		

- Molecule 29 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	W	86	Total	C	N	O	S	0	0
			616	400	98	114	4		
29	M	80	Total	C	N	O	S	0	0
			642	413	96	128	5		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
30	X	49	Total	C	N	O	0	0
			372	243	64	65		

- Molecule 31 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Y	57	Total	C	N	O	S	0	0
			409	277	65	66	1		

- Molecule 32 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Z	74	Total	C	N	O	S	0	0
			493	320	89	82	2		

- Molecule 33 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	a	114	Total	C	N	O	S	0	0
			857	550	159	148			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
34	b	139	Total	C	N	O	S	0	0
			1032	672	190	168	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
35	c	90	Total	C	N	O	S	0	0
			617	391	119	107			

- Molecule 36 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	d	107	Total	C	N	O	S	0	0
			708	445	134	125	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
37	f	167	Total	C	N	O	S	0	0
			1156	739	205	208	4		

- Molecule 38 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	h	91	Total	C	N	O	S	0	0
			721	461	123	135	2		

- Molecule 39 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	i	38	Total	C	N	O		0	0
			277	185	46	46			

- Molecule 40 is a protein called NADH dehydrogenase [ubiquinone] 1 subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	j	113	Total	C	N	O	S	0	0
			892	587	149	153	3		

- Molecule 41 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	1	317	Total	C	N	O	S	0	0
			2500	1676	384	417	23		

- Molecule 42 is a protein called NADH-ubiquinone oxidoreductase chain 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	6	606	Total	C	N	O	S	0	0
			4765	3172	732	819	42		

- Molecule 43 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10.

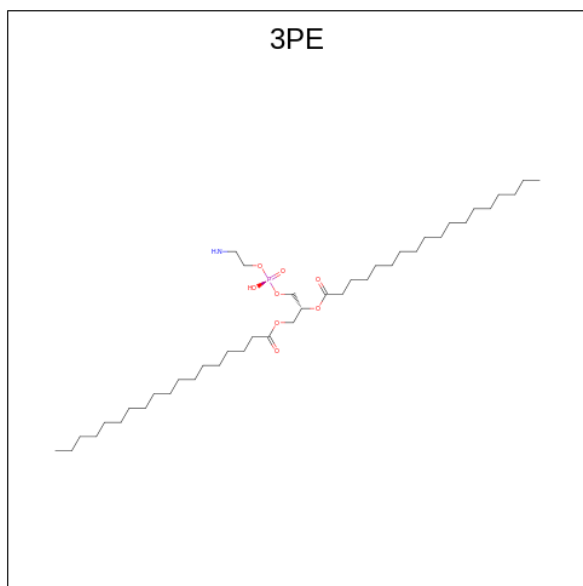
Mol	Chain	Residues	Atoms					AltConf	Trace
43	g	173	Total	C	N	O	S	0	0
			1351	849	246	248	8		

- Molecule 44 is a protein called NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	e	141	Total	C	N	O	S	0	0
			864	539	161	160	4		

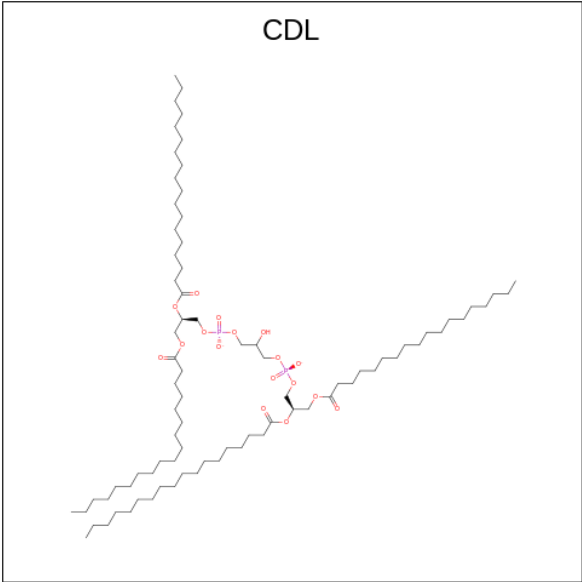
- Molecule 45 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula:

C₄₁H₈₂NO₈P) (labeled as "Ligand of Interest" by depositor).



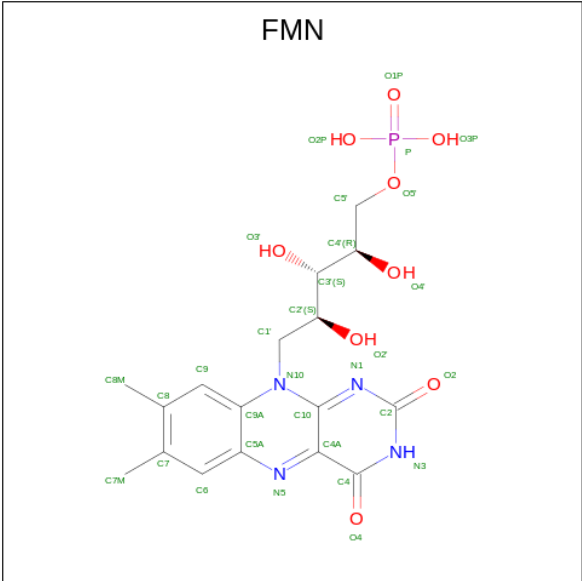
Mol	Chain	Residues	Atoms					AltConf
45	2	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	4	1	Total	C	N	O	P	0
			41	31	1	8	1	
45	B	1	Total	C	N	O	P	0
			51	41	1	8	1	
45	V	1	Total	C	N	O	P	0
			51	41	1	8	1	

- Molecule 46 is CARDIOLIPIN (CCD ID: CDL) (formula: C₈₁H₁₅₆O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



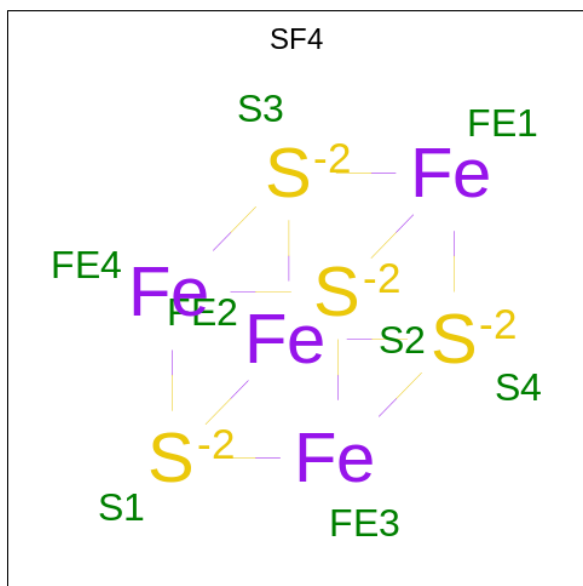
Mol	Chain	Residues	Atoms				AltConf
46	4	1	Total	C	O	P	0
			82	63	17	2	
46	J	1	Total	C	O	P	0
			58	39	17	2	

- Molecule 47 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: C₁₇H₂₁N₄O₉P) (labeled as "Ligand of Interest" by depositor).



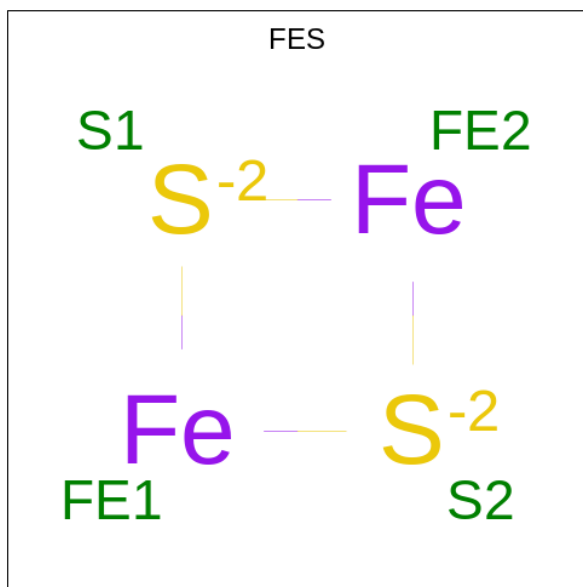
Mol	Chain	Residues	Atoms					AltConf
47	8	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 48 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
48	8	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	
48	A	1	Total	Fe	S	0
			8	4	4	
48	D	1	Total	Fe	S	0
			8	4	4	
48	E	1	Total	Fe	S	0
			8	4	4	
48	E	1	Total	Fe	S	0
			8	4	4	

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

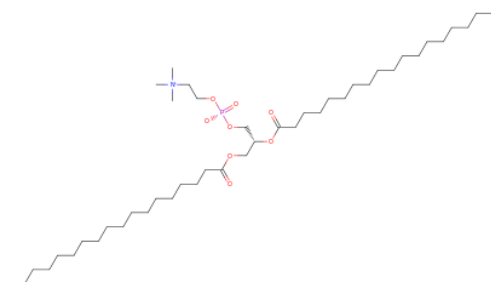


Mol	Chain	Residues	Atoms			AltConf
49	9	1	Total	Fe	S	0
			4	2	2	
49	A	1	Total	Fe	S	0
			4	2	2	

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

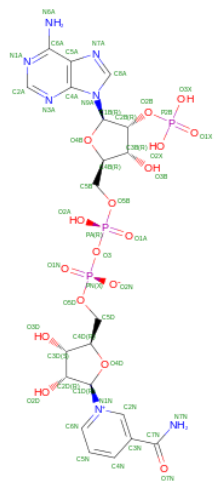
Mol	Chain	Residues	Atoms		AltConf
50	I	1	Total	Zn	0
			1	1	

- Molecule 51 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: C₄₄H₈₈NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
51	L	1	Total 47	C 37	N 1	O 8	P 1	0
51	Q	1	Total 46	C 36	N 1	O 8	P 1	0
51	S	1	Total 47	C 37	N 1	O 8	P 1	0
51	j	1	Total 39	C 29	N 1	O 8	P 1	0

- Molecule 52 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).

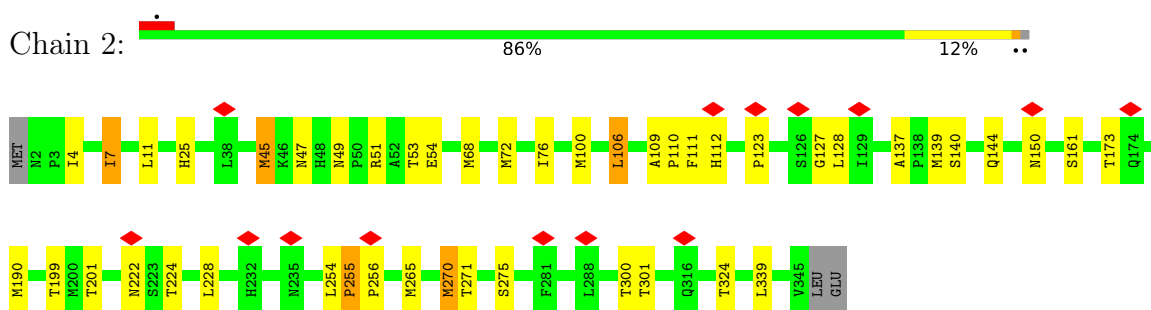


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
52	R	1	48	21	7	17	3	0

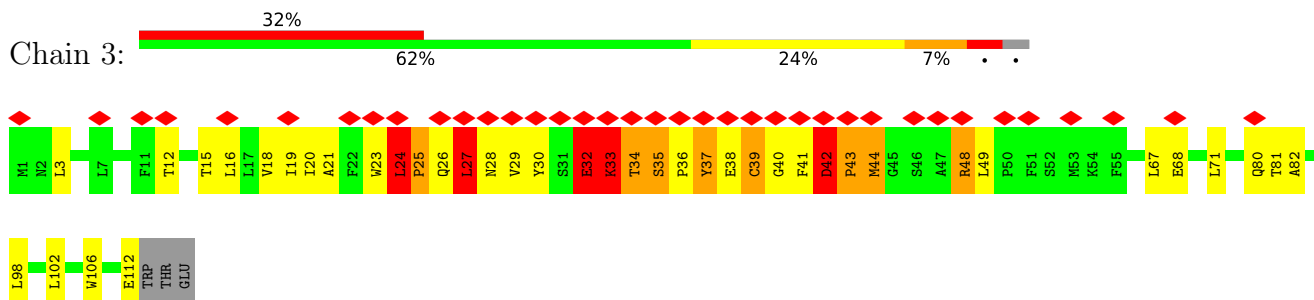
3 Residue-property plots

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

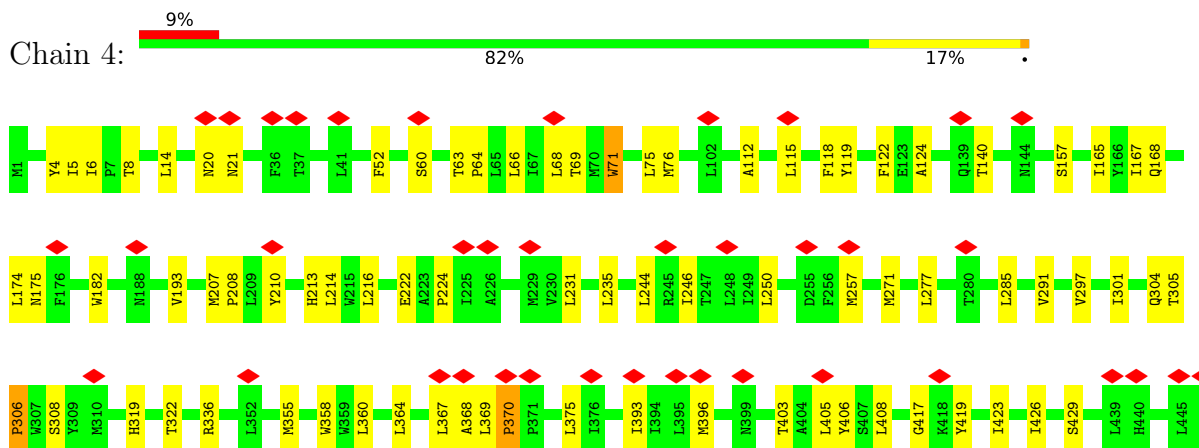
- Molecule 1: NADH-ubiquinone oxidoreductase chain 2

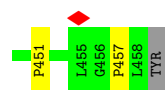


- Molecule 2: NADH-ubiquinone oxidoreductase chain 3

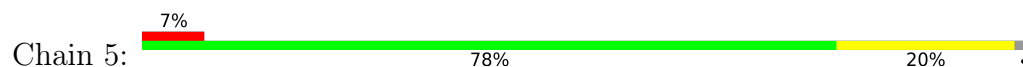


- Molecule 3: NADH-ubiquinone oxidoreductase chain 4

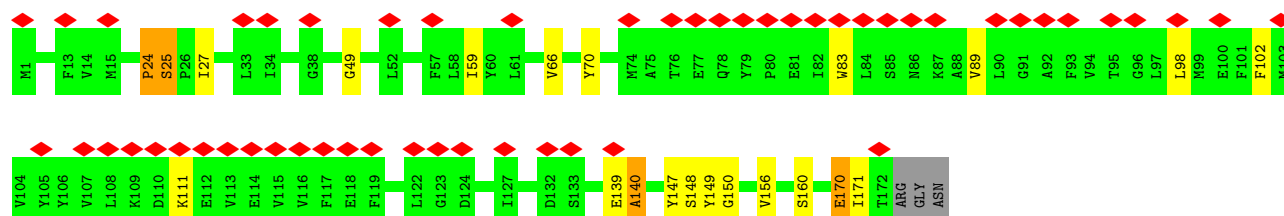
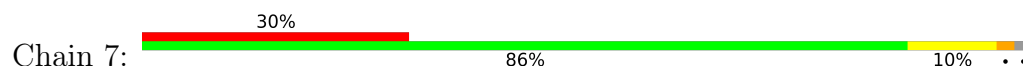




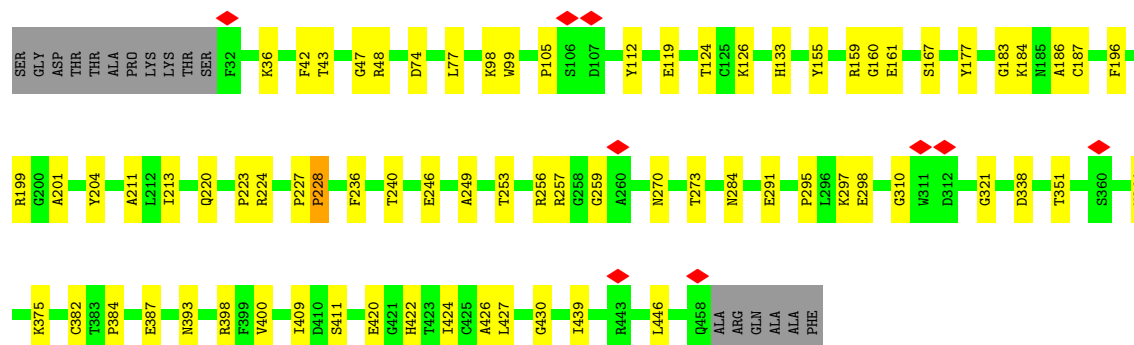
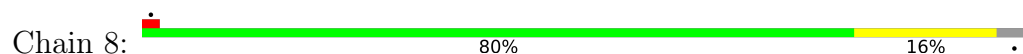
- Molecule 4: NADH-ubiquinone oxidoreductase chain 4L



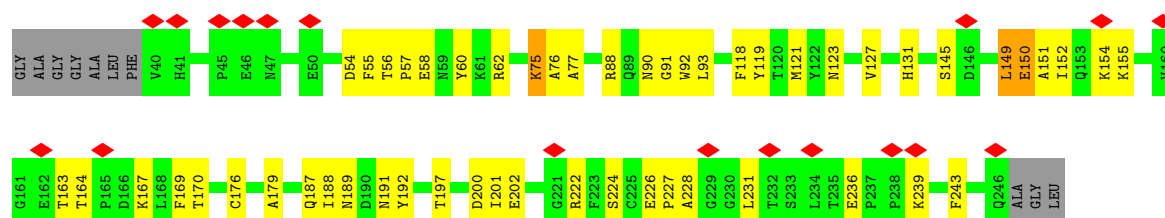
- Molecule 5: NADH-ubiquinone oxidoreductase chain 6



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

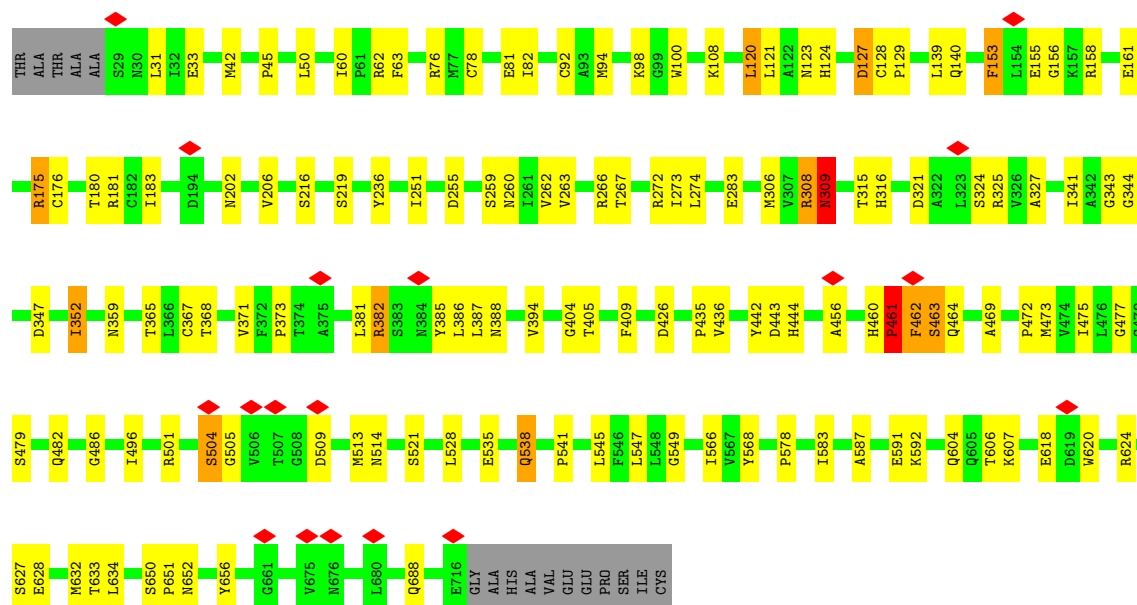


- Molecule 7: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial



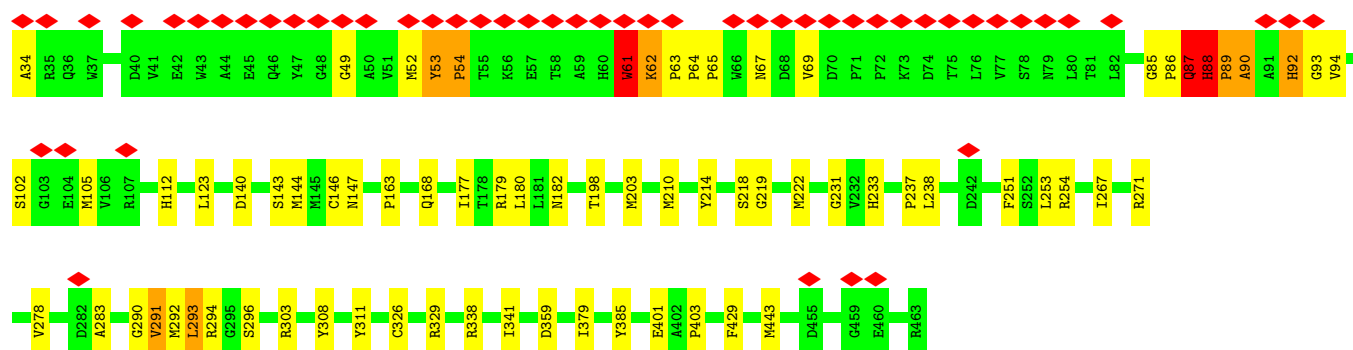
- Molecule 8: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain A: 



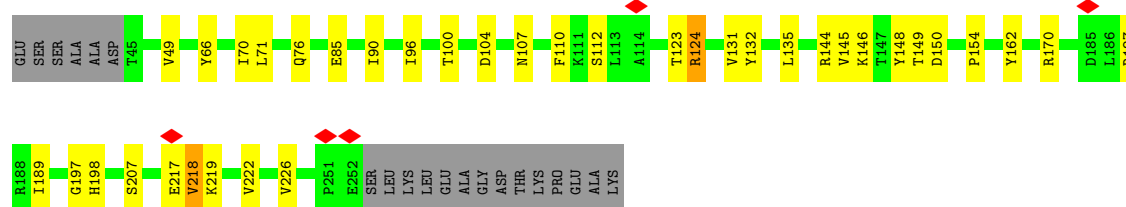
- Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

Chain B: 



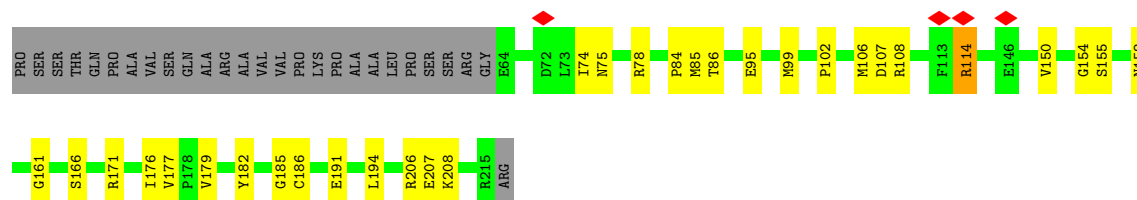
- Molecule 10: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

Chain C: 

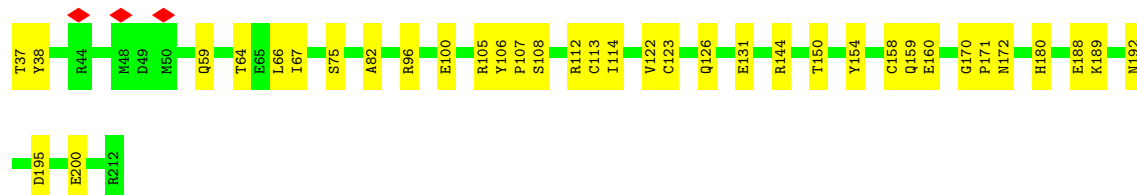
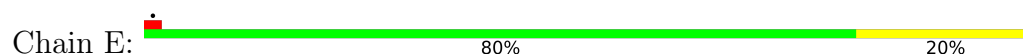


- Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial

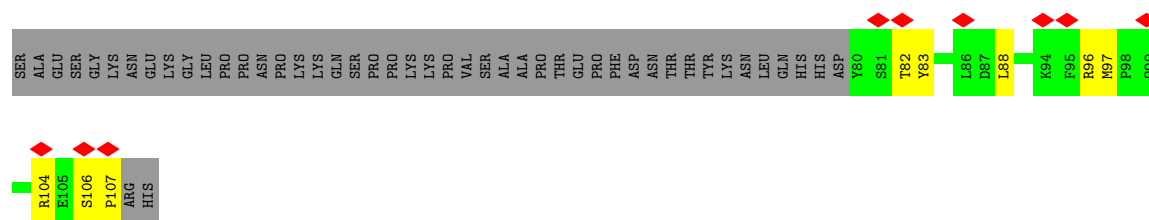
Chain D: 



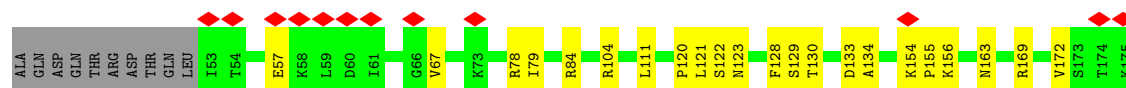
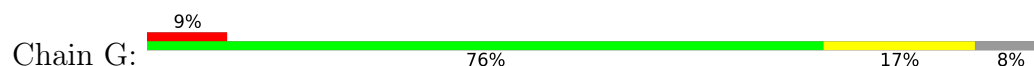
- Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial



- Molecule 13: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial



- Molecule 14: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



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

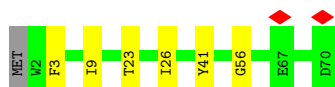
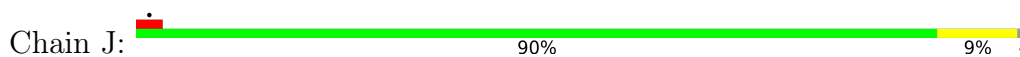


- Molecule 16: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial

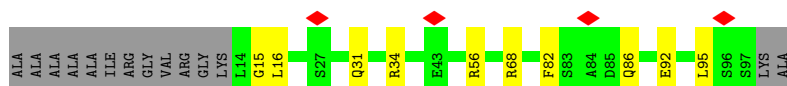
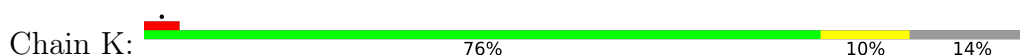




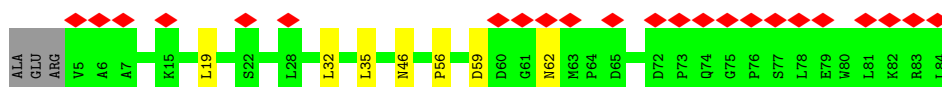
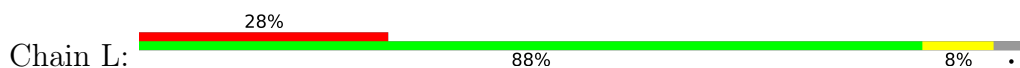
- Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



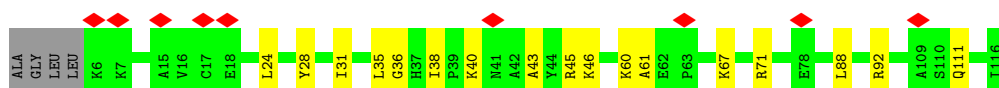
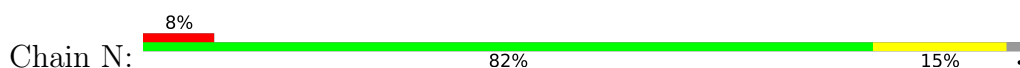
- Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2



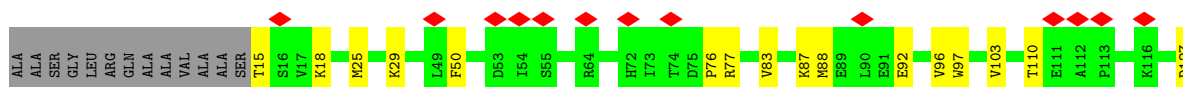
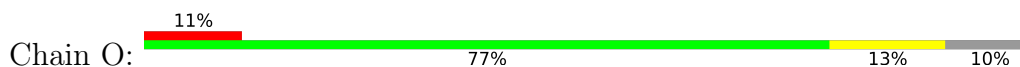
- Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



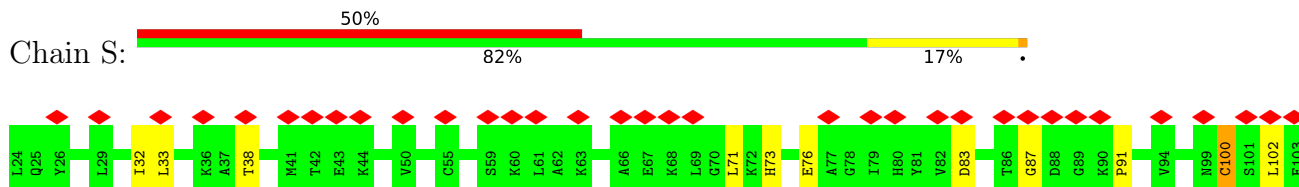
- Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

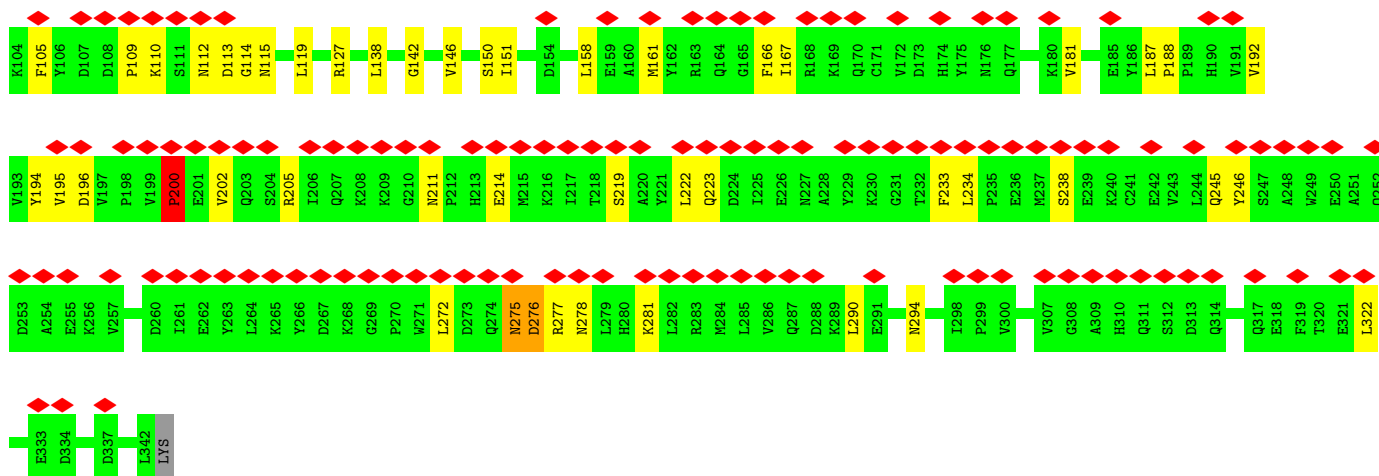


- Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6



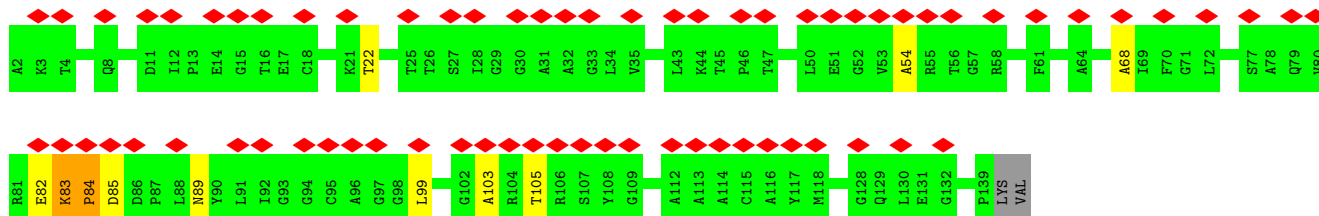
- Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7





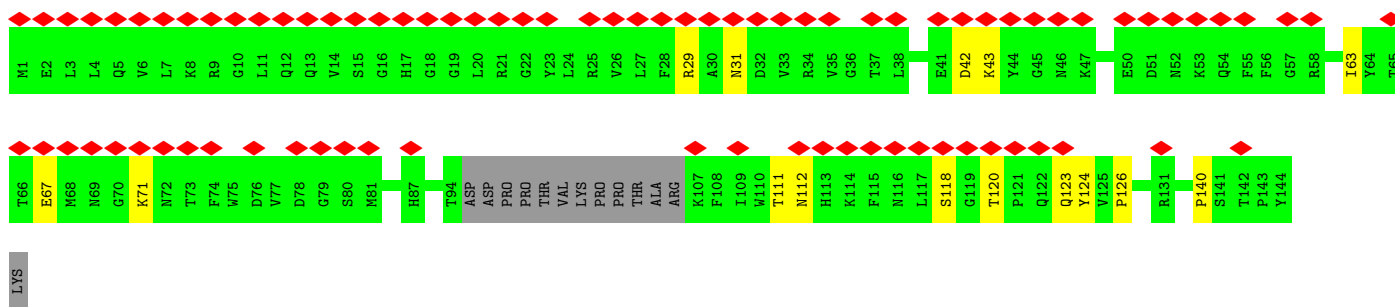
- Molecule 26: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 11

Chain T: 49% 91% 6% ..



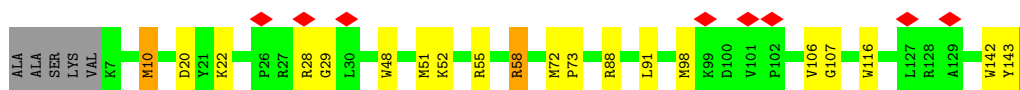
- Molecule 27: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12

Chain U: 57% 81% 10% 9%



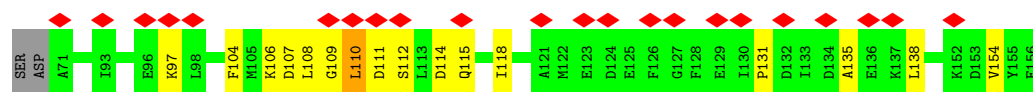
- Molecule 28: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain V: 6% 83% 13% ..

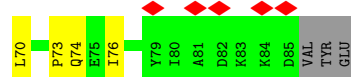
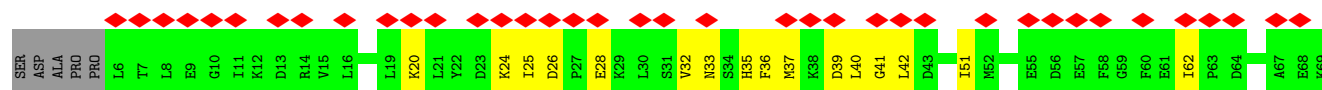


- Molecule 29: Acyl carrier protein, mitochondrial

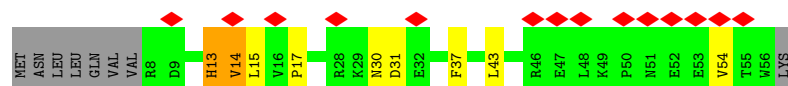
Chain W: 25% 80% 17% ..



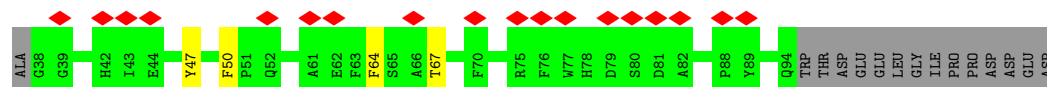
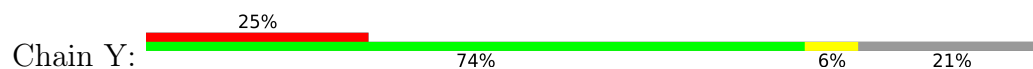
- Molecule 29: Acyl carrier protein, mitochondrial



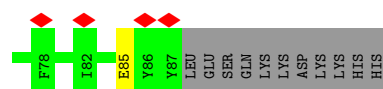
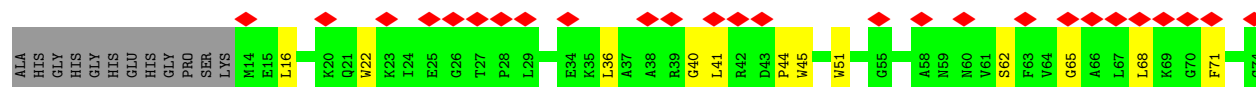
- Molecule 30: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 1



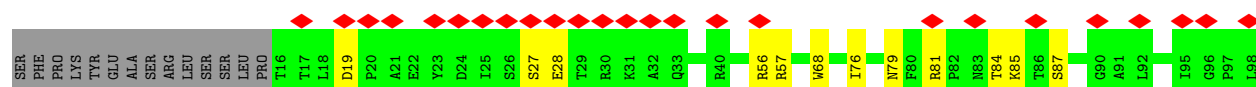
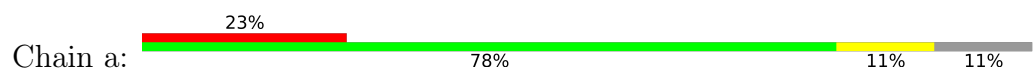
- Molecule 31: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 2, mitochondrial

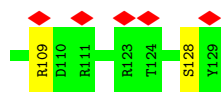


- Molecule 32: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 3

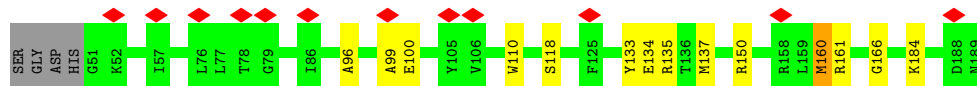
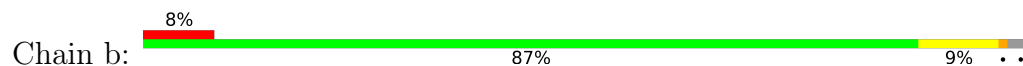


- Molecule 33: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 4

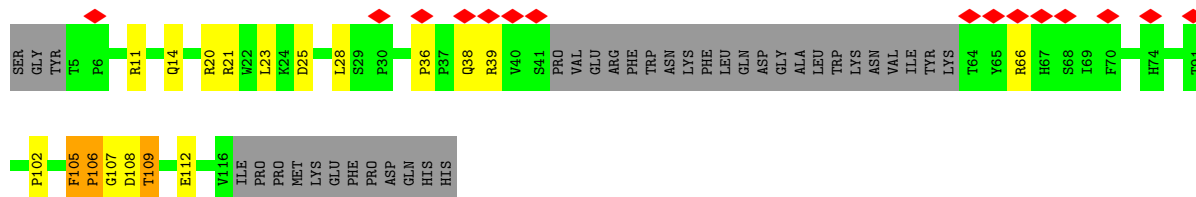




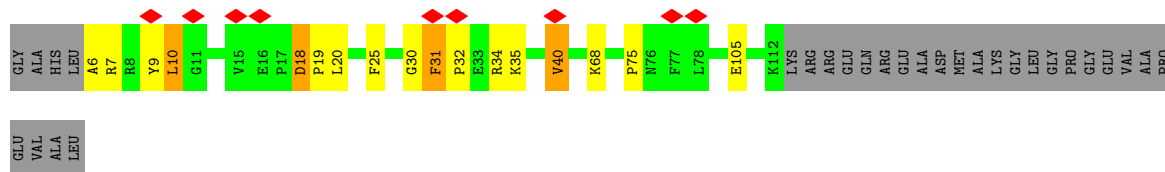
- Molecule 34: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 5, mitochondrial



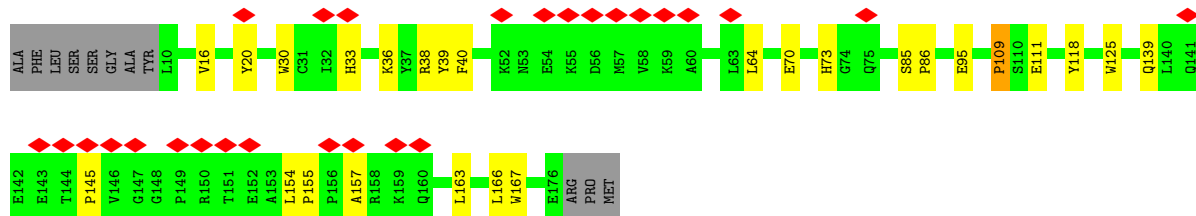
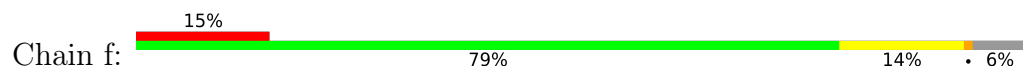
- Molecule 35: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 6



- Molecule 36: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 7

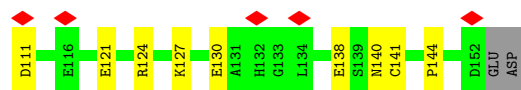


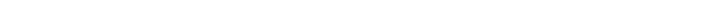
- Molecule 37: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 9

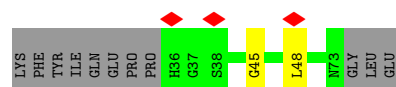


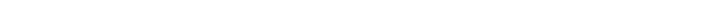
- Molecule 38: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 11, mitochondrial



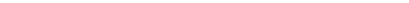


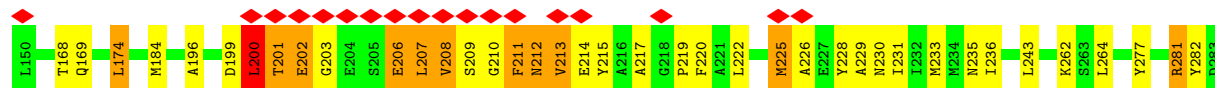
- Chain i:  6% 73% 22%



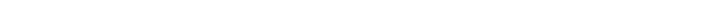
- Chain j:  12% 77% 17% 6%

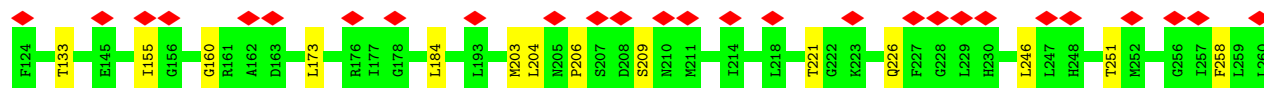


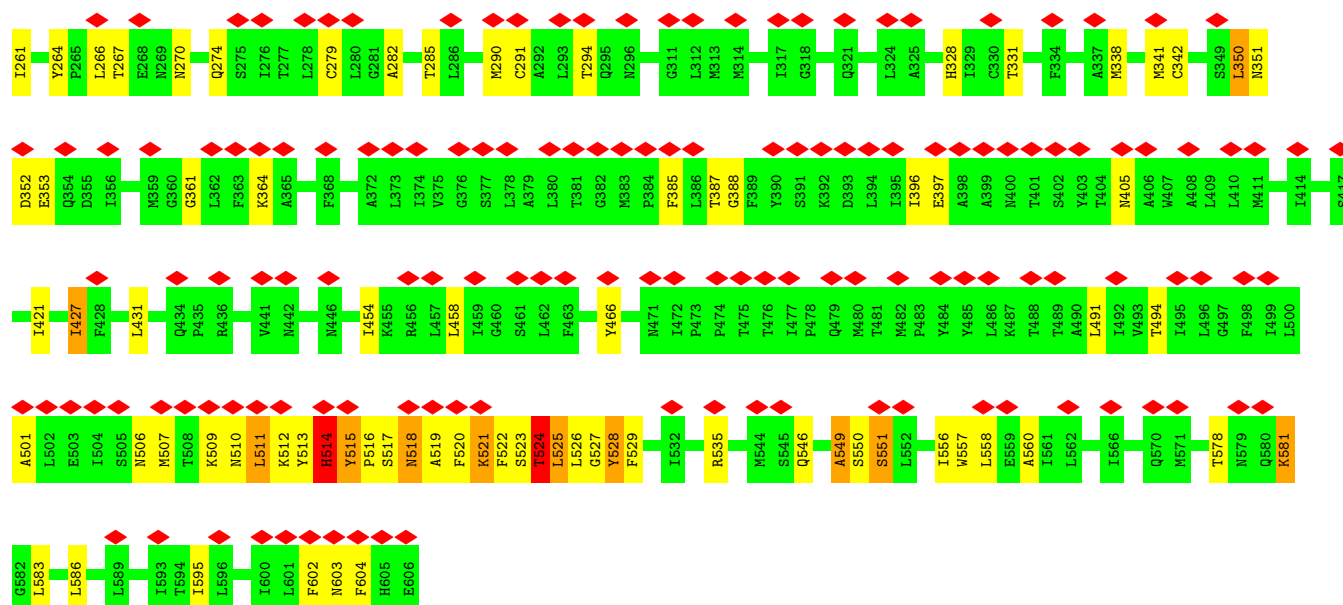
- Chain 1:  12% 76% 20%



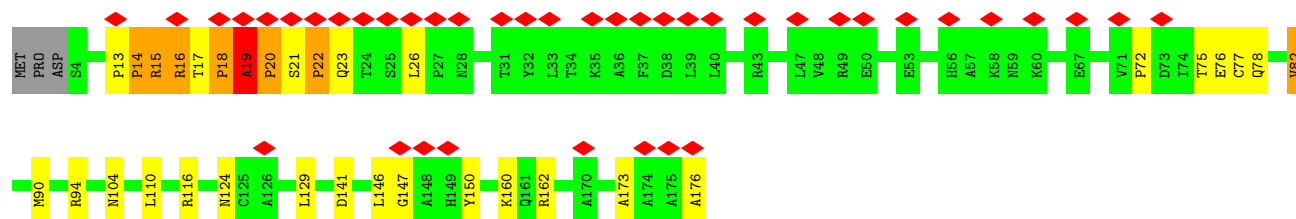
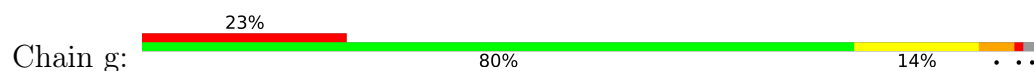
Q284	H287	L288	L289	W290	K291	N292	L310	T311	S312	G313	I314	Q317	THR
------	------	------	------	------	------	------	------	------	------	------	------	------	-----

- Chain 6:  32% 82% 16%

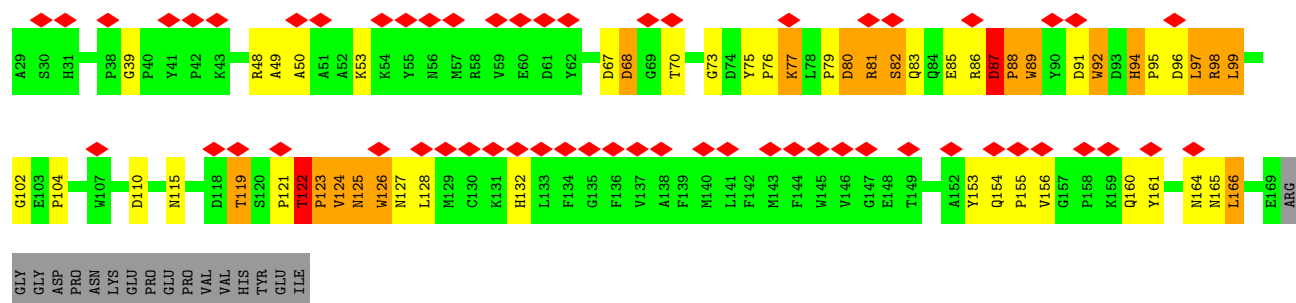




- Molecule 43: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 10



- Molecule 44: NADH dehydrogenase [ubiquinone] 1 beta subcomplex subunit 8, mitochondrial



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	146842	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	1.143	Depositor
Minimum map value	-0.274	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.017	Depositor
Recommended contour level	0.111	Depositor
Map size ($\text{\AA}$)	391.244, 391.244, 391.244	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.3973, 1.3973, 1.3973	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1, FMN, NAP, SF4, CDL, ZN, FES, 3PE

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	2	0.41	0/2646	0.85	3/3618 (0.1%)
2	3	0.51	0/887	0.99	5/1216 (0.4%)
3	4	0.38	0/3538	0.86	10/4845 (0.2%)
4	5	0.36	0/706	0.84	0/960
5	7	0.34	0/1213	0.83	4/1659 (0.2%)
6	8	0.31	0/3035	0.76	6/4130 (0.1%)
7	9	0.29	0/1572	0.76	0/2150
8	A	0.37	0/5269	0.79	12/7152 (0.2%)
9	B	0.46	0/3500	0.88	11/4748 (0.2%)
10	C	0.39	0/1756	0.74	2/2394 (0.1%)
11	D	0.49	0/1231	0.87	1/1669 (0.1%)
12	E	0.45	0/1418	0.83	3/1922 (0.2%)
13	F	0.37	0/188	1.27	5/259 (1.9%)
14	G	0.40	0/1004	0.85	2/1359 (0.1%)
15	H	0.34	0/800	0.82	2/1076 (0.2%)
16	I	0.35	0/538	0.84	1/722 (0.1%)
17	J	0.29	0/545	0.63	0/740
18	K	0.28	0/663	0.72	0/896
19	L	0.33	0/623	0.81	2/862 (0.2%)
20	N	0.27	0/882	0.72	0/1203
21	O	0.31	0/948	0.68	2/1279 (0.2%)
22	P	0.32	0/719	0.80	0/981
23	Q	0.29	0/1381	0.84	2/1869 (0.1%)
24	R	0.32	0/2465	0.85	4/3349 (0.1%)
25	S	0.31	0/2348	0.85	5/3198 (0.2%)
26	T	0.31	0/959	0.83	1/1305 (0.1%)
27	U	0.27	0/1053	0.79	3/1439 (0.2%)
28	V	0.31	0/1121	0.70	0/1515
29	M	0.27	0/651	0.77	2/876 (0.2%)
29	W	0.25	0/624	0.84	0/847
30	X	0.31	0/383	0.94	4/523 (0.8%)
31	Y	0.26	0/428	0.60	0/592

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Z	0.37	0/506	1.04	6/688 (0.9%)
33	a	0.29	0/878	0.82	5/1195 (0.4%)
34	b	0.32	0/1058	0.83	5/1434 (0.3%)
35	c	0.34	0/632	1.03	6/871 (0.7%)
36	d	0.31	0/724	0.79	2/989 (0.2%)
37	f	0.24	0/1191	0.77	2/1639 (0.1%)
38	h	0.34	0/743	0.87	0/1013
39	i	0.22	0/286	0.48	0/392
40	j	0.31	0/922	0.83	5/1254 (0.4%)
41	l	0.40	0/2572	0.86	7/3513 (0.2%)
42	6	0.30	0/4892	0.74	6/6660 (0.1%)
43	g	0.27	0/1380	0.88	7/1872 (0.4%)
44	e	0.36	0/888	1.22	19/1234 (1.5%)
All	All	0.35	0/61766	0.83	162/84107 (0.2%)

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	2	0	9
3	4	0	6
4	5	0	3
5	7	0	5
6	8	0	1
7	9	0	4
8	A	0	12
9	B	0	3
10	C	0	1
11	D	0	3
12	E	0	1
15	H	0	1
16	I	0	1
20	N	0	1
22	P	0	2
23	Q	0	1
24	R	0	4
25	S	0	4
26	T	0	3
27	U	0	1
28	V	0	3

Continued on next page...

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Mol	Chain	#Chirality outliers	#Planarity outliers
29	M	0	1
29	W	0	1
34	b	0	3
36	d	0	1
37	f	0	1
38	h	0	2
40	j	0	2
41	1	0	1
42	6	0	5
43	g	0	1
44	e	0	3
All	All	0	90

There are no bond length outliers.

The worst 5 of 162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	g	19	ALA	CA-C-N	11.74	134.52	119.84
43	g	19	ALA	C-N-CA	11.74	134.52	119.84
8	A	176	CYS	N-CA-C	8.82	122.05	111.02
37	f	163	LEU	CA-C-N	8.70	147.89	127.00
37	f	163	LEU	C-N-CA	8.70	147.89	127.00

There are no chirality outliers.

5 of 90 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	106	LEU	Peptide
1	2	111	PHE	Peptide
1	2	128	LEU	Peptide
1	2	199	THR	Peptide
1	2	45	MET	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	2	2582	0	2612	30	0
2	3	864	0	866	65	0
3	4	3447	0	3442	46	0
4	5	697	0	708	13	0
5	7	1186	0	1123	14	0
6	8	2965	0	2596	46	0
7	9	1535	0	1491	34	0
8	A	5183	0	5179	77	0
9	B	3410	0	3318	86	0
10	C	1705	0	1645	27	0
11	D	1200	0	1195	31	0
12	E	1388	0	1340	22	0
13	F	183	0	132	5	0
14	G	981	0	965	14	0
15	H	780	0	753	21	0
16	I	530	0	508	8	0
17	J	530	0	503	5	0
18	K	652	0	636	6	0
19	L	602	0	592	5	0
20	N	862	0	868	10	0
21	O	925	0	907	16	0
22	P	698	0	659	13	0
23	Q	1345	0	1282	19	0
24	R	2407	0	2296	52	0
25	S	2299	0	2028	34	0
26	T	942	0	890	4	0
27	U	1019	0	900	9	0
28	V	1093	0	1048	28	0
29	M	642	0	642	13	0
29	W	616	0	579	22	0
30	X	372	0	314	4	0
31	Y	409	0	318	3	0
32	Z	493	0	395	6	0
33	a	857	0	765	29	0
34	b	1032	0	954	8	0
35	c	617	0	492	28	0
36	d	708	0	513	30	0
37	f	1156	0	892	45	0
38	h	721	0	632	60	0
39	i	277	0	240	1	0
40	j	892	0	835	12	0
41	1	2500	0	2615	119	0
42	6	4765	0	4893	109	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	g	1351	0	1262	48	0
44	e	864	0	567	56	0
45	2	41	0	59	1	0
45	4	41	0	59	1	0
45	B	51	0	82	2	0
45	V	51	0	82	0	0
46	4	82	0	114	1	0
46	J	58	0	60	1	0
47	8	31	0	19	2	0
48	8	8	0	0	0	0
48	A	16	0	0	1	0
48	D	8	0	0	0	0
48	E	16	0	0	0	0
49	9	4	0	0	0	0
49	A	4	0	0	0	0
50	I	1	0	0	0	0
51	L	47	0	71	2	0
51	Q	46	0	66	1	0
51	S	47	0	71	2	0
51	j	39	0	55	0	0
52	R	48	0	23	3	0
All	All	60921	0	58151	1081	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 9.

The worst 5 of 1081 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)
41:1:17:VAL:HG21	41:1:225:MET:CE	1.21	1.61
41:1:131:GLY:CA	41:1:207:LEU:CD1	1.75	1.58
36:d:6:ALA:CB	36:d:31:PHE:N	1.68	1.54
35:c:109:THR:CB	43:g:18:PRO:HA	1.15	1.53
41:1:200:LEU:CD1	41:1:206:GLU:HG2	1.37	1.51

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	342/347 (99%)	298 (87%)	44 (13%)	0	100	100
2	3	110/115 (96%)	78 (71%)	18 (16%)	14 (13%)	0	4
3	4	457/459 (100%)	374 (82%)	77 (17%)	6 (1%)	9	38
4	5	94/98 (96%)	80 (85%)	14 (15%)	0	100	100
5	7	170/175 (97%)	135 (79%)	31 (18%)	4 (2%)	4	29
6	8	425/444 (96%)	344 (81%)	79 (19%)	2 (0%)	24	57
7	9	205/217 (94%)	165 (80%)	39 (19%)	1 (0%)	24	57
8	A	686/704 (97%)	563 (82%)	118 (17%)	5 (1%)	18	51
9	B	428/430 (100%)	353 (82%)	65 (15%)	10 (2%)	5	30
10	C	206/228 (90%)	175 (85%)	31 (15%)	0	100	100
11	D	150/179 (84%)	131 (87%)	19 (13%)	0	100	100
12	E	174/176 (99%)	148 (85%)	25 (14%)	1 (1%)	21	54
13	F	26/75 (35%)	17 (65%)	9 (35%)	0	100	100
14	G	121/133 (91%)	99 (82%)	20 (16%)	2 (2%)	7	34
15	H	94/105 (90%)	73 (78%)	21 (22%)	0	100	100
16	I	69/96 (72%)	56 (81%)	11 (16%)	2 (3%)	3	25
17	J	67/70 (96%)	63 (94%)	3 (4%)	1 (2%)	8	36
18	K	82/98 (84%)	62 (76%)	20 (24%)	0	100	100
19	L	78/83 (94%)	68 (87%)	10 (13%)	0	100	100
20	N	109/115 (95%)	91 (84%)	18 (16%)	0	100	100
21	O	112/127 (88%)	98 (88%)	14 (12%)	0	100	100
22	P	86/112 (77%)	66 (77%)	20 (23%)	0	100	100
23	Q	166/171 (97%)	117 (70%)	47 (28%)	2 (1%)	10	40
24	R	315/345 (91%)	249 (79%)	64 (20%)	2 (1%)	21	54
25	S	317/320 (99%)	249 (78%)	65 (20%)	3 (1%)	14	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	T	136/140 (97%)	113 (83%)	22 (16%)	1 (1%)	18	51
27	U	128/145 (88%)	101 (79%)	27 (21%)	0	100	100
28	V	136/143 (95%)	119 (88%)	15 (11%)	2 (2%)	8	36
29	M	78/88 (89%)	62 (80%)	16 (20%)	0	100	100
29	W	84/88 (96%)	65 (77%)	19 (23%)	0	100	100
30	X	47/57 (82%)	37 (79%)	8 (17%)	2 (4%)	2	19
31	Y	55/72 (76%)	44 (80%)	11 (20%)	0	100	100
32	Z	72/97 (74%)	49 (68%)	23 (32%)	0	100	100
33	a	112/128 (88%)	87 (78%)	25 (22%)	0	100	100
34	b	137/143 (96%)	117 (85%)	20 (15%)	0	100	100
35	c	86/127 (68%)	63 (73%)	19 (22%)	4 (5%)	2	18
36	d	105/136 (77%)	74 (70%)	26 (25%)	5 (5%)	2	17
37	f	165/178 (93%)	126 (76%)	38 (23%)	1 (1%)	21	54
38	h	89/125 (71%)	60 (67%)	24 (27%)	5 (6%)	1	15
39	i	36/49 (74%)	34 (94%)	2 (6%)	0	100	100
40	j	111/120 (92%)	95 (86%)	16 (14%)	0	100	100
41	1	315/318 (99%)	267 (85%)	42 (13%)	6 (2%)	6	32
42	6	604/606 (100%)	513 (85%)	81 (13%)	10 (2%)	7	34
43	g	171/176 (97%)	138 (81%)	28 (16%)	5 (3%)	3	25
44	e	139/158 (88%)	74 (53%)	45 (32%)	20 (14%)	0	3
All	All	7895/8516 (93%)	6390 (81%)	1389 (18%)	116 (2%)	11	36

5 of 116 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	3	24	LEU
2	3	30	TYR
2	3	33	LYS
2	3	34	THR
2	3	35	SER

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	2	274/316 (87%)	273 (100%)	1 (0%)	84	83
2	3	90/101 (89%)	81 (90%)	9 (10%)	7	28
3	4	351/413 (85%)	350 (100%)	1 (0%)	86	84
4	5	75/86 (87%)	75 (100%)	0	100	100
5	7	104/142 (73%)	104 (100%)	0	100	100
6	8	236/353 (67%)	236 (100%)	0	100	100
7	9	160/183 (87%)	158 (99%)	2 (1%)	61	71
8	A	551/588 (94%)	548 (100%)	3 (0%)	81	81
9	B	359/371 (97%)	352 (98%)	7 (2%)	50	66
10	C	183/204 (90%)	182 (100%)	1 (0%)	81	81
11	D	126/150 (84%)	124 (98%)	2 (2%)	55	68
12	E	145/151 (96%)	145 (100%)	0	100	100
13	F	13/69 (19%)	13 (100%)	0	100	100
14	G	105/119 (88%)	105 (100%)	0	100	100
15	H	80/95 (84%)	78 (98%)	2 (2%)	42	61
16	I	52/79 (66%)	49 (94%)	3 (6%)	18	44
17	J	50/59 (85%)	50 (100%)	0	100	100
18	K	66/81 (82%)	66 (100%)	0	100	100
19	L	63/71 (89%)	63 (100%)	0	100	100
20	N	88/101 (87%)	88 (100%)	0	100	100
21	O	95/113 (84%)	95 (100%)	0	100	100
22	P	72/96 (75%)	72 (100%)	0	100	100
23	Q	142/154 (92%)	139 (98%)	3 (2%)	47	64
24	R	232/298 (78%)	229 (99%)	3 (1%)	61	71
25	S	205/283 (72%)	203 (99%)	2 (1%)	68	74
26	T	79/101 (78%)	79 (100%)	0	100	100
27	U	95/131 (72%)	95 (100%)	0	100	100
28	V	107/120 (89%)	106 (99%)	1 (1%)	70	74
29	M	73/81 (90%)	73 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
29	W	57/81 (70%)	55 (96%)	2 (4%)	32	54
30	X	32/54 (59%)	32 (100%)	0	100	100
31	Y	29/62 (47%)	29 (100%)	0	100	100
32	Z	28/75 (37%)	28 (100%)	0	100	100
33	a	70/114 (61%)	70 (100%)	0	100	100
34	b	85/124 (68%)	85 (100%)	0	100	100
35	c	45/121 (37%)	45 (100%)	0	100	100
36	d	42/119 (35%)	42 (100%)	0	100	100
37	f	80/160 (50%)	79 (99%)	1 (1%)	61	71
38	h	70/112 (62%)	63 (90%)	7 (10%)	7	28
39	i	23/45 (51%)	23 (100%)	0	100	100
40	j	88/106 (83%)	88 (100%)	0	100	100
41	1	274/275 (100%)	265 (97%)	9 (3%)	33	56
42	6	523/534 (98%)	512 (98%)	11 (2%)	47	64
43	g	130/157 (83%)	128 (98%)	2 (2%)	57	69
44	e	44/141 (31%)	39 (89%)	5 (11%)	5	23
All	All	5891/7389 (80%)	5814 (99%)	77 (1%)	59	71

5 of 77 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
41	1	228	TYR
43	g	16	ARG
42	6	155	ILE
42	6	520	PHE
44	e	160	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
38	h	70	ASN
42	6	226	GLN
40	j	88	HIS
41	1	292	ASN
42	6	479	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 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	$\# Z > 2$
45	3PE	V	201	-	50,50,50	0.85	4 (8%)	53,55,55	1.10	2 (3%)
48	SF4	E	301	-	0,12,12	-	-	-		
51	PC1	L	200	-	46,46,53	1.01	4 (8%)	52,54,61	1.06	2 (3%)
49	FES	9	301	-	0,4,4	-	-	-		
46	CDL	J	101	-	57,57,99	1.14	7 (12%)	63,69,111	1.19	4 (6%)
51	PC1	Q	201	-	45,45,53	1.00	4 (8%)	51,53,61	1.07	2 (3%)
48	SF4	A	802	-	0,12,12	-	-	-		
48	SF4	8	502	-	0,12,12	-	-	-		
45	3PE	4	502	-	40,40,50	0.92	3 (7%)	43,45,55	1.37	3 (6%)
48	SF4	A	801	-	0,12,12	-	-	-		
52	NAP	R	601	-	49,52,52	4.36	22 (44%)	69,80,80	1.86	15 (21%)
51	PC1	S	401	-	46,46,53	1.00	4 (8%)	52,54,61	1.00	2 (3%)
47	FMN	8	501	-	33,33,33	1.10	2 (6%)	48,50,50	1.62	11 (22%)
46	CDL	4	501	-	81,81,99	0.97	7 (8%)	87,93,111	1.11	5 (5%)
45	3PE	2	401	-	40,40,50	0.95	4 (10%)	43,45,55	1.18	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	SF4	E	302	-	0,12,12	-	-	-		
48	SF4	D	301	-	0,12,12	-	-	-		
49	FES	A	803	-	0,4,4	-	-	-		
51	PC1	j	201	-	38,38,53	1.12	4 (10%)	44,46,61	1.09	2 (4%)
45	3PE	B	501	9	50,50,50	0.85	4 (8%)	53,55,55	1.13	2 (3%)

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
45	3PE	V	201	-	-	21/54/54/54	-
48	SF4	E	301	-	-	-	0/6/5/5
51	PC1	L	200	-	-	23/50/50/57	-
49	FES	9	301	-	-	-	0/1/1/1
46	CDL	J	101	-	-	31/68/68/110	-
51	PC1	Q	201	-	-	20/49/49/57	-
48	SF4	A	802	-	-	-	0/6/5/5
48	SF4	8	502	-	-	-	0/6/5/5
45	3PE	4	502	-	-	24/44/44/54	-
48	SF4	A	801	-	-	-	0/6/5/5
52	NAP	R	601	-	-	16/35/67/67	0/5/5/5
51	PC1	S	401	-	-	32/50/50/57	-
47	FMN	8	501	-	-	10/18/18/18	0/3/3/3
46	CDL	4	501	-	-	39/92/92/110	-
45	3PE	2	401	-	-	21/44/44/54	-
48	SF4	E	302	-	-	-	0/6/5/5
48	SF4	D	301	-	-	-	0/6/5/5
51	PC1	j	201	-	-	23/42/42/57	-
49	FES	A	803	-	-	-	0/1/1/1
45	3PE	B	501	9	-	26/54/54/54	-

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	R	601	NAP	O4D-C1D	16.10	1.63	1.41
52	R	601	NAP	C2D-C1D	-14.38	1.31	1.53
52	R	601	NAP	C2B-C1B	-9.13	1.29	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	R	601	NAP	O4B-C1B	8.27	1.61	1.42
52	R	601	NAP	C7N-N7N	6.91	1.46	1.33

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	R	601	NAP	N3A-C2A-N1A	-6.03	119.17	128.60
52	R	601	NAP	C5A-C4A-N3A	-5.14	120.04	126.75
45	4	502	3PE	O21-C21-C22	4.88	122.02	111.50
52	R	601	NAP	N6A-C6A-N1A	-4.80	107.84	118.35
51	L	200	PC1	O21-C21-C22	4.60	121.42	111.50

There are no chirality outliers.

5 of 286 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	2	401	3PE	C11-O13-P-O12
45	2	401	3PE	C11-O13-P-O14
45	2	401	3PE	C22-C21-O21-C2
45	4	502	3PE	C1-O11-P-O12
45	4	502	3PE	C1-O11-P-O13

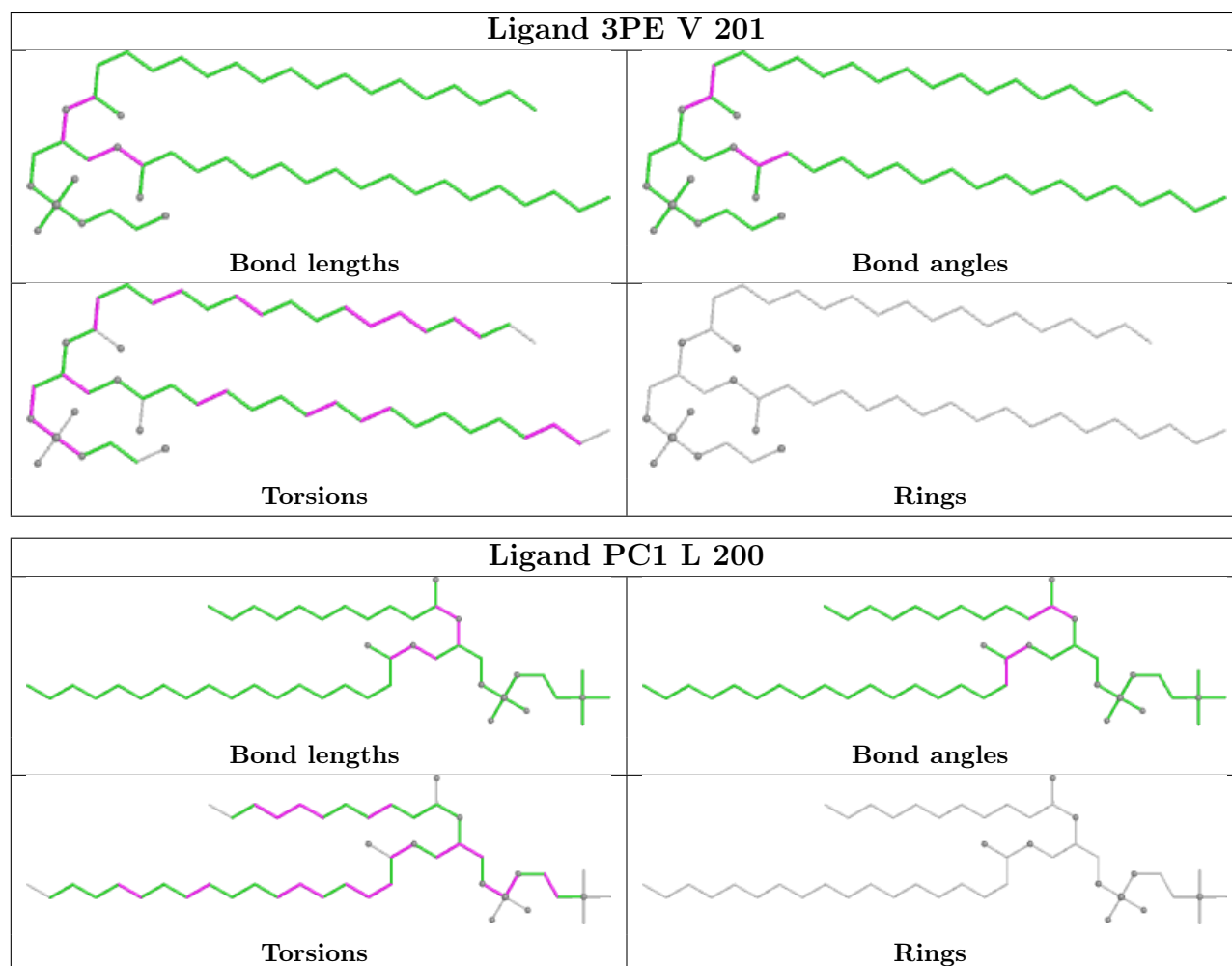
There are no ring outliers.

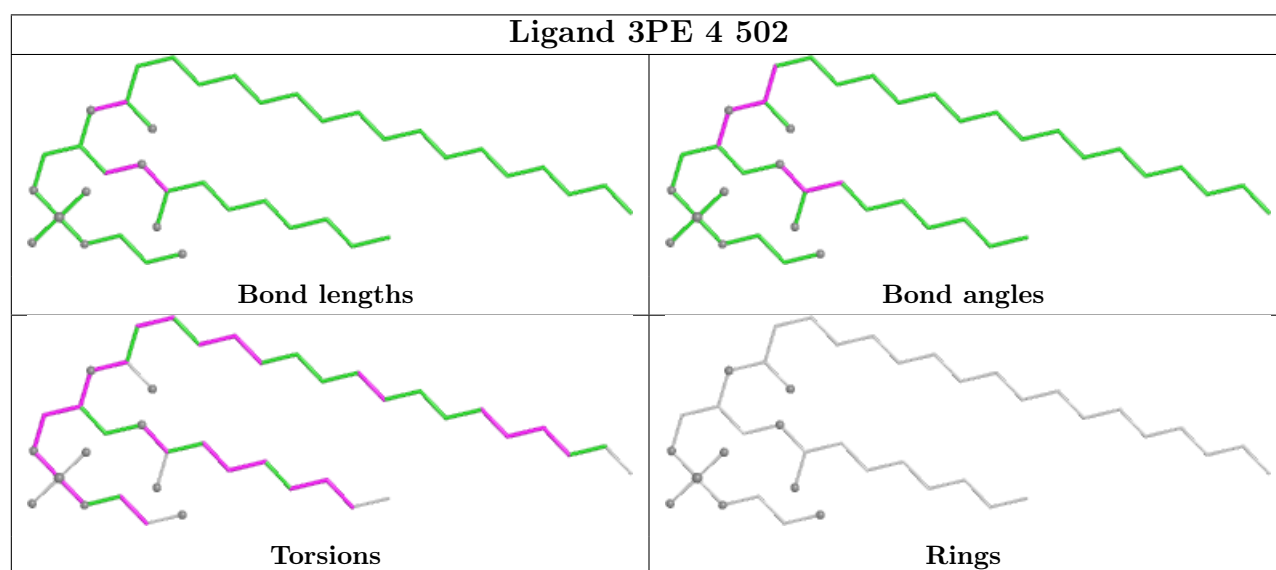
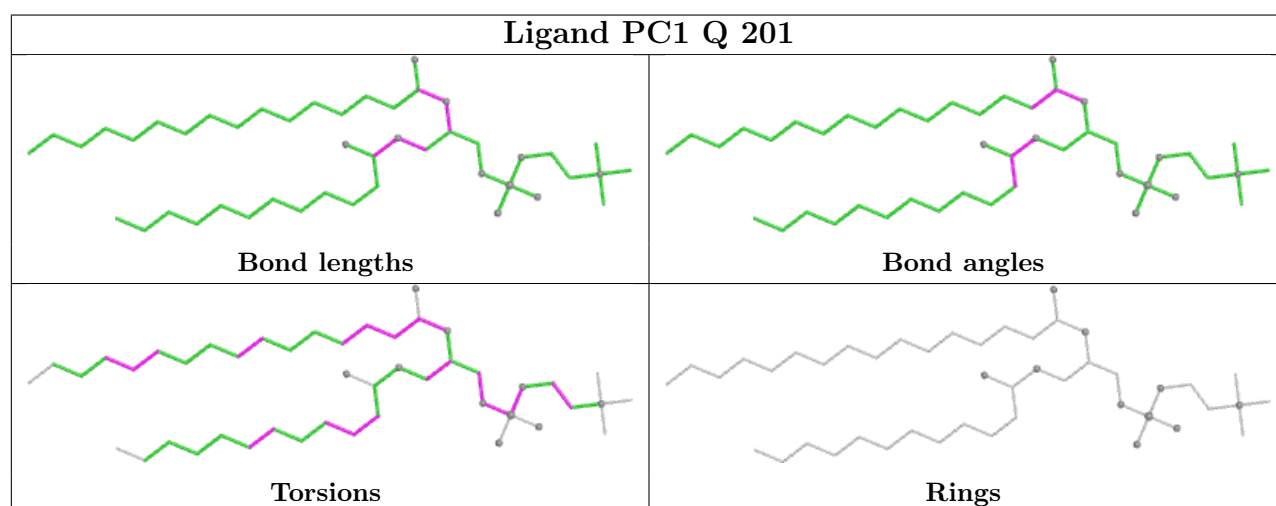
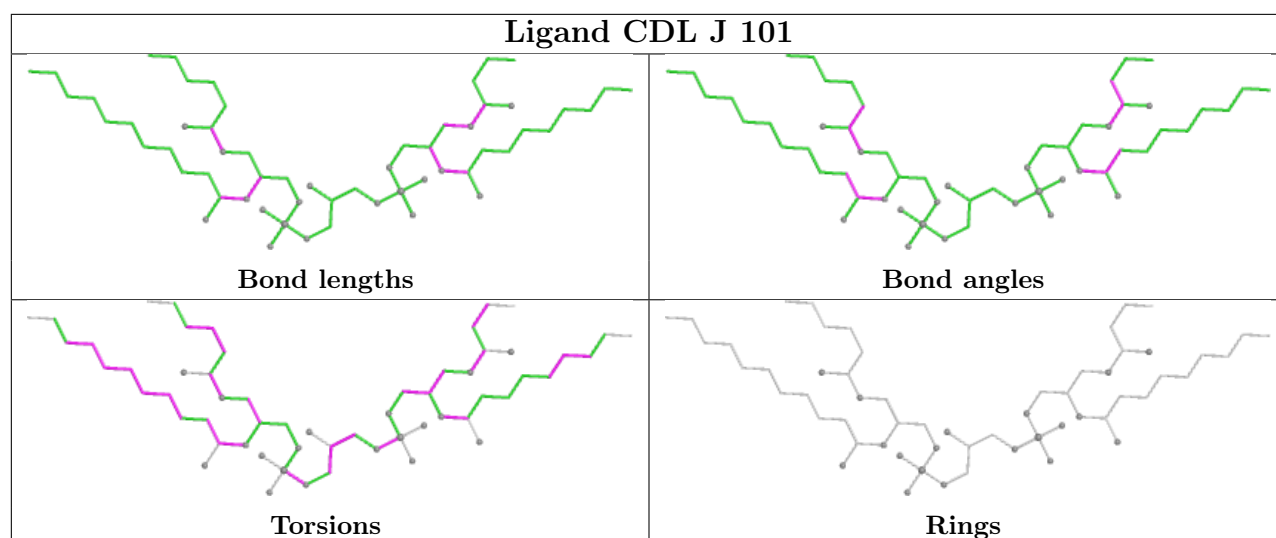
11 monomers are involved in 17 short contacts:

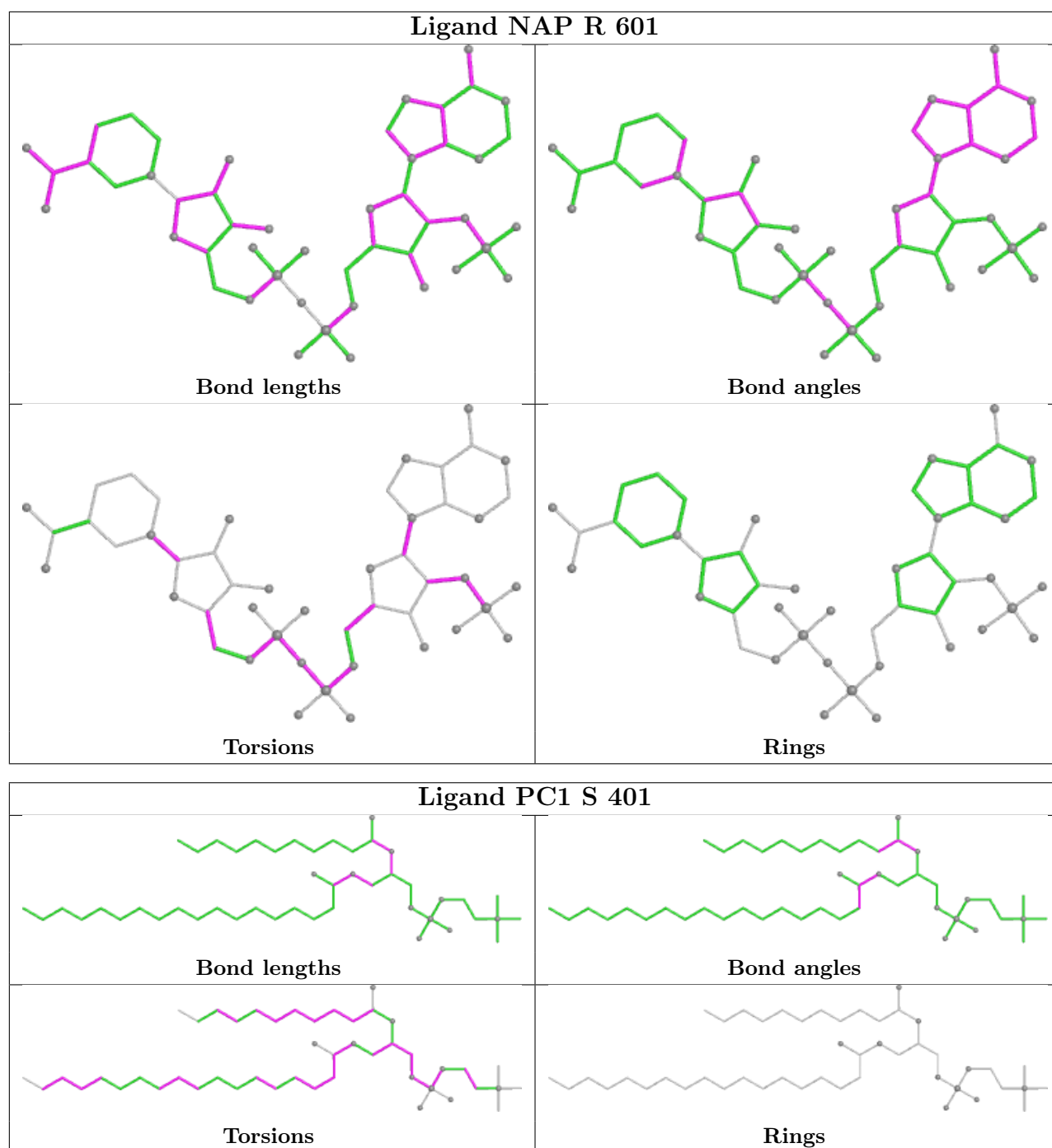
Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	L	200	PC1	2	0
46	J	101	CDL	1	0
51	Q	201	PC1	1	0
45	4	502	3PE	1	0
48	A	801	SF4	1	0
52	R	601	NAP	3	0
51	S	401	PC1	2	0
47	8	501	FMN	2	0
46	4	501	CDL	1	0
45	2	401	3PE	1	0
45	B	501	3PE	2	0

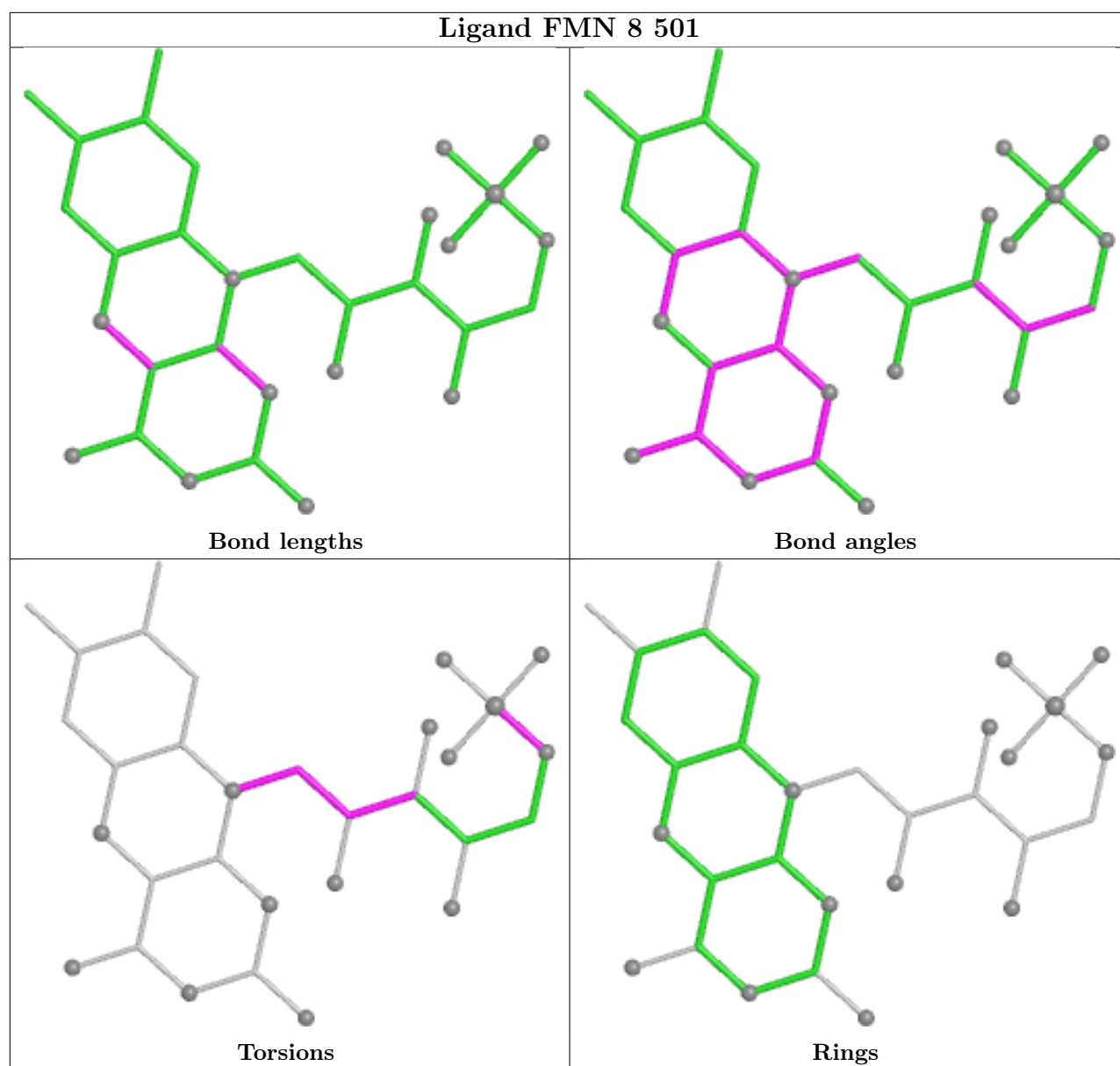
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

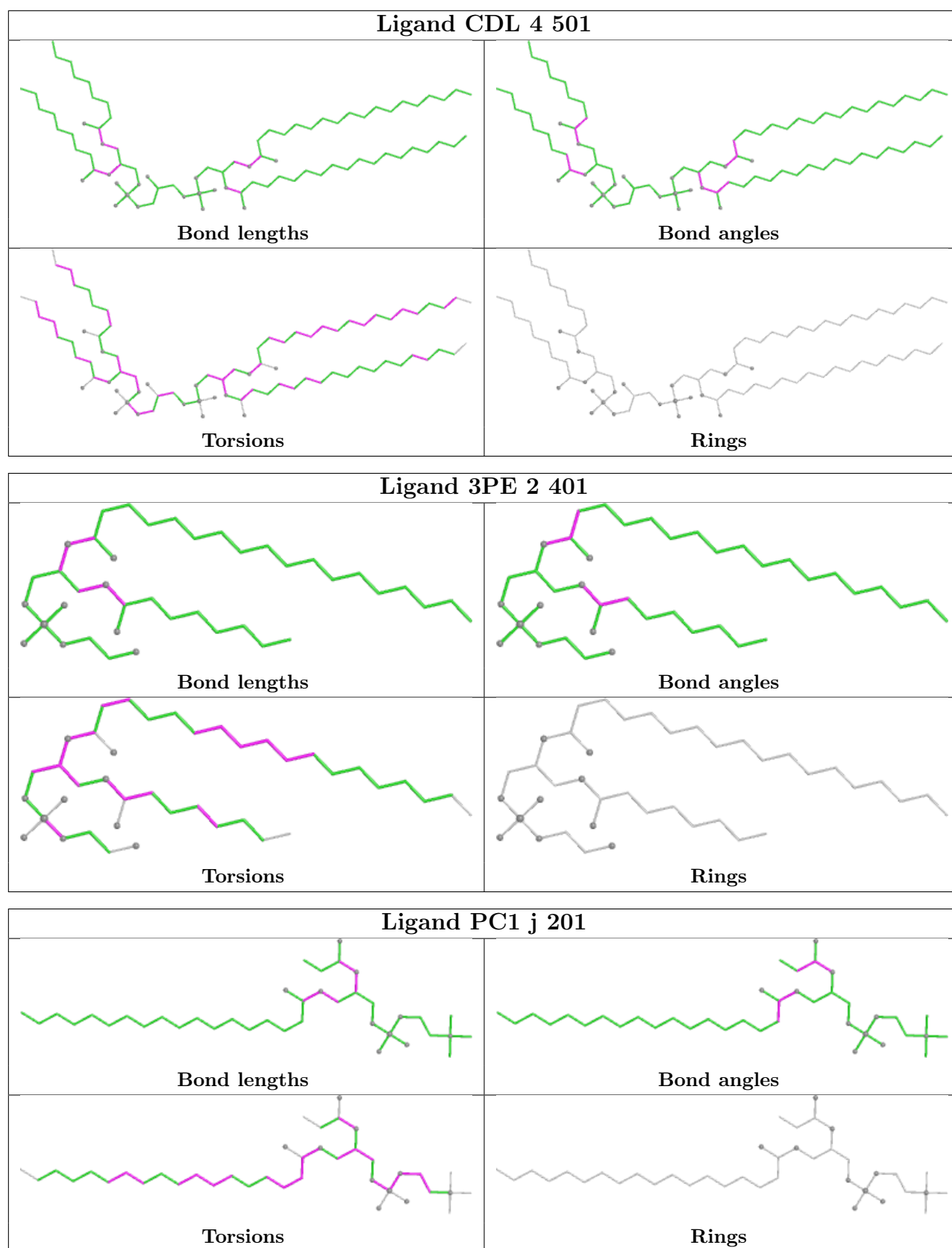
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

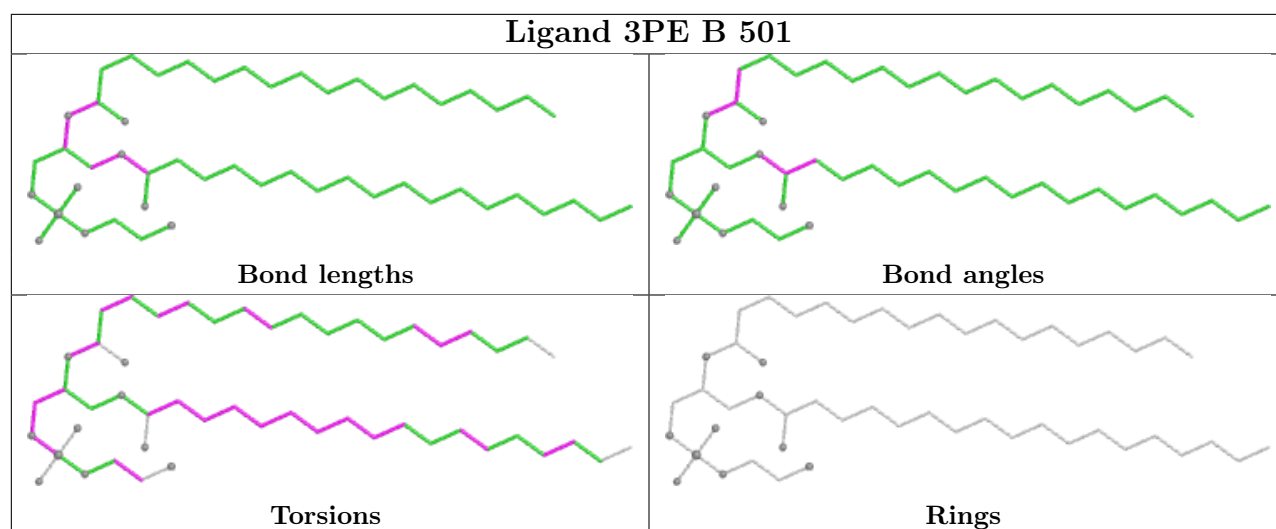












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

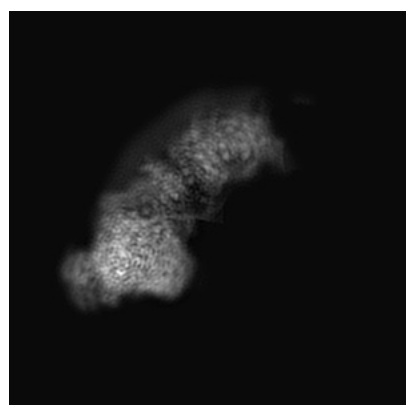
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30676. These allow visual inspection of the internal detail of the map and identification of artifacts.

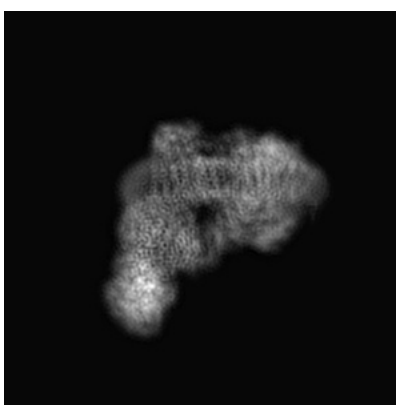
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

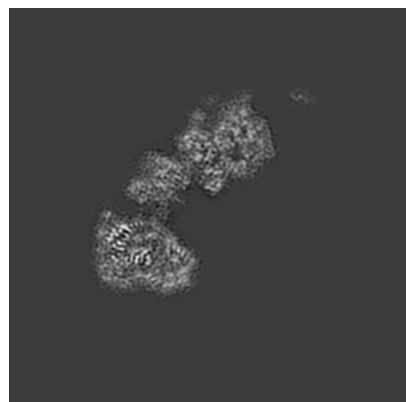


Z

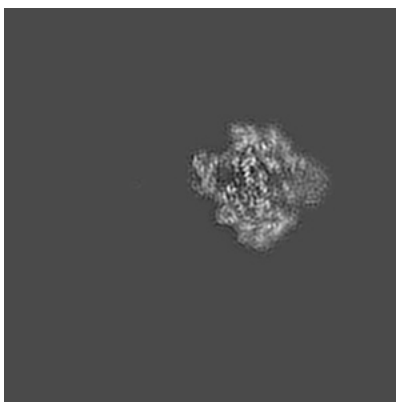
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

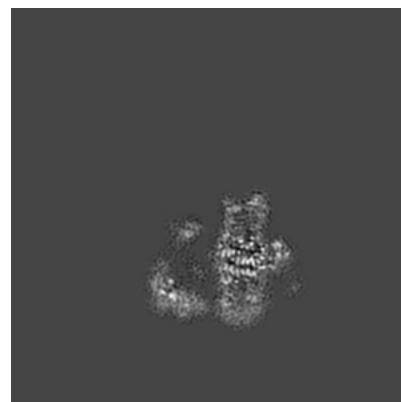
6.2.1 Primary map



X Index: 140



Y Index: 140

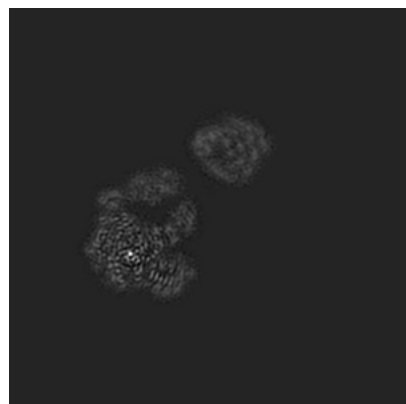


Z Index: 140

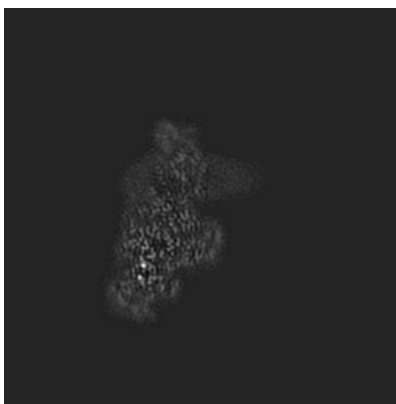
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

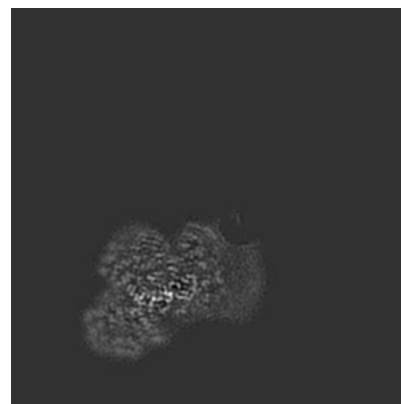
6.3.1 Primary map



X Index: 124



Y Index: 76

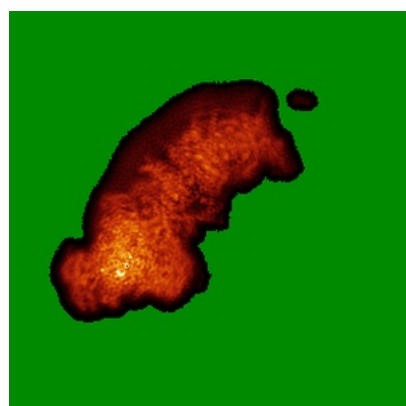


Z Index: 96

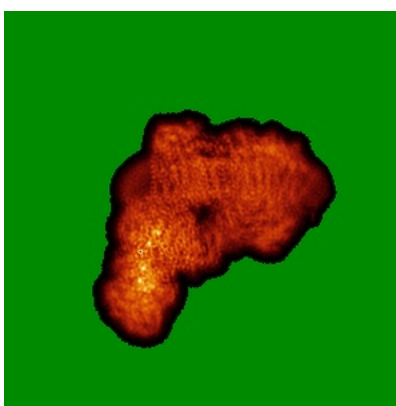
The images above show the largest variance slices of the map in three orthogonal directions.

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

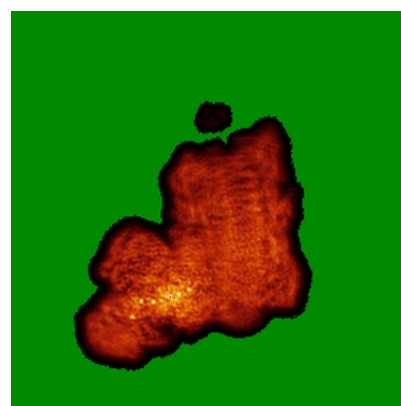
6.4.1 Primary map



X



Y



Z

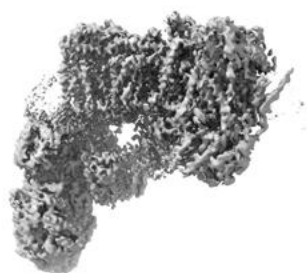
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.111. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

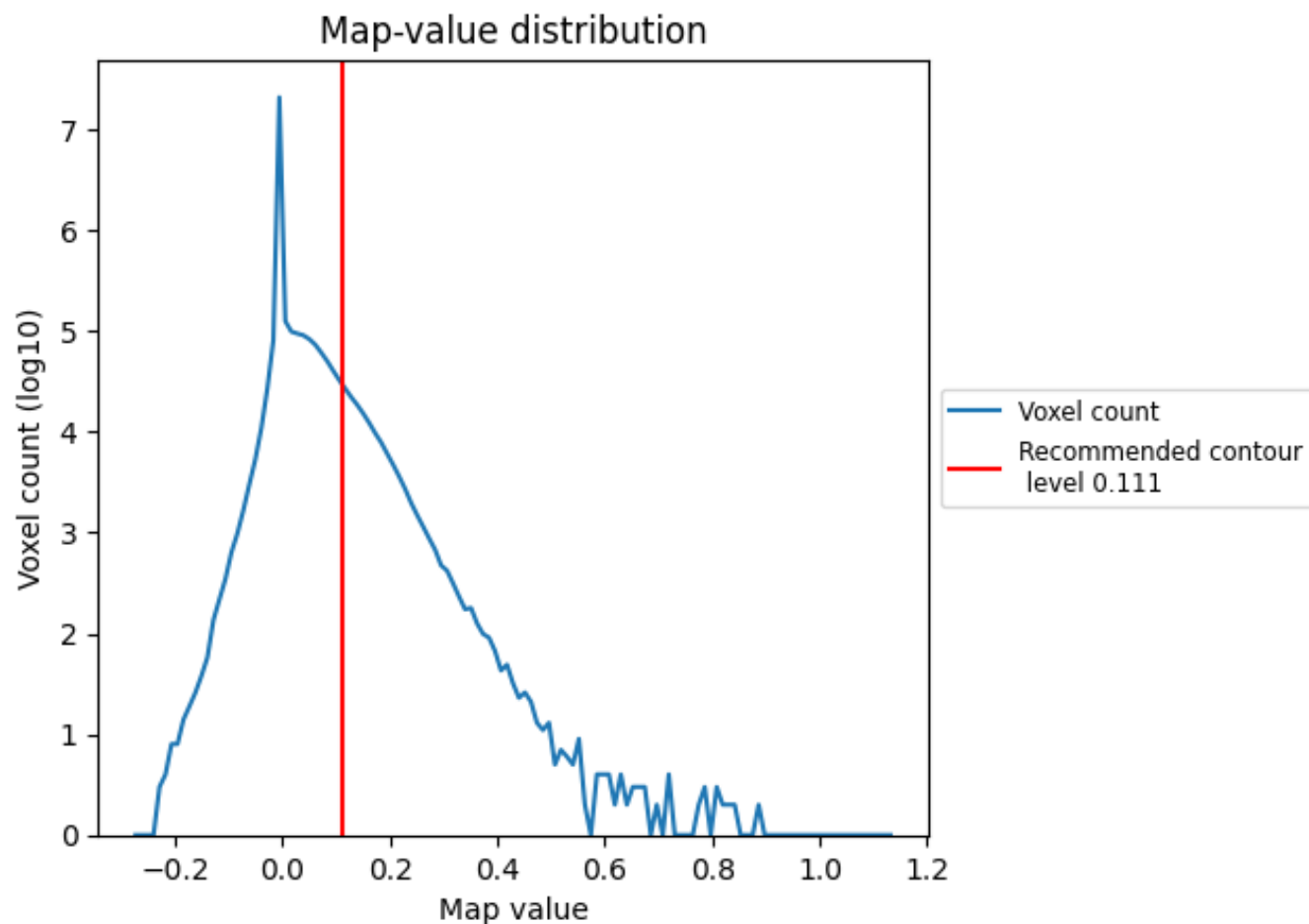
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

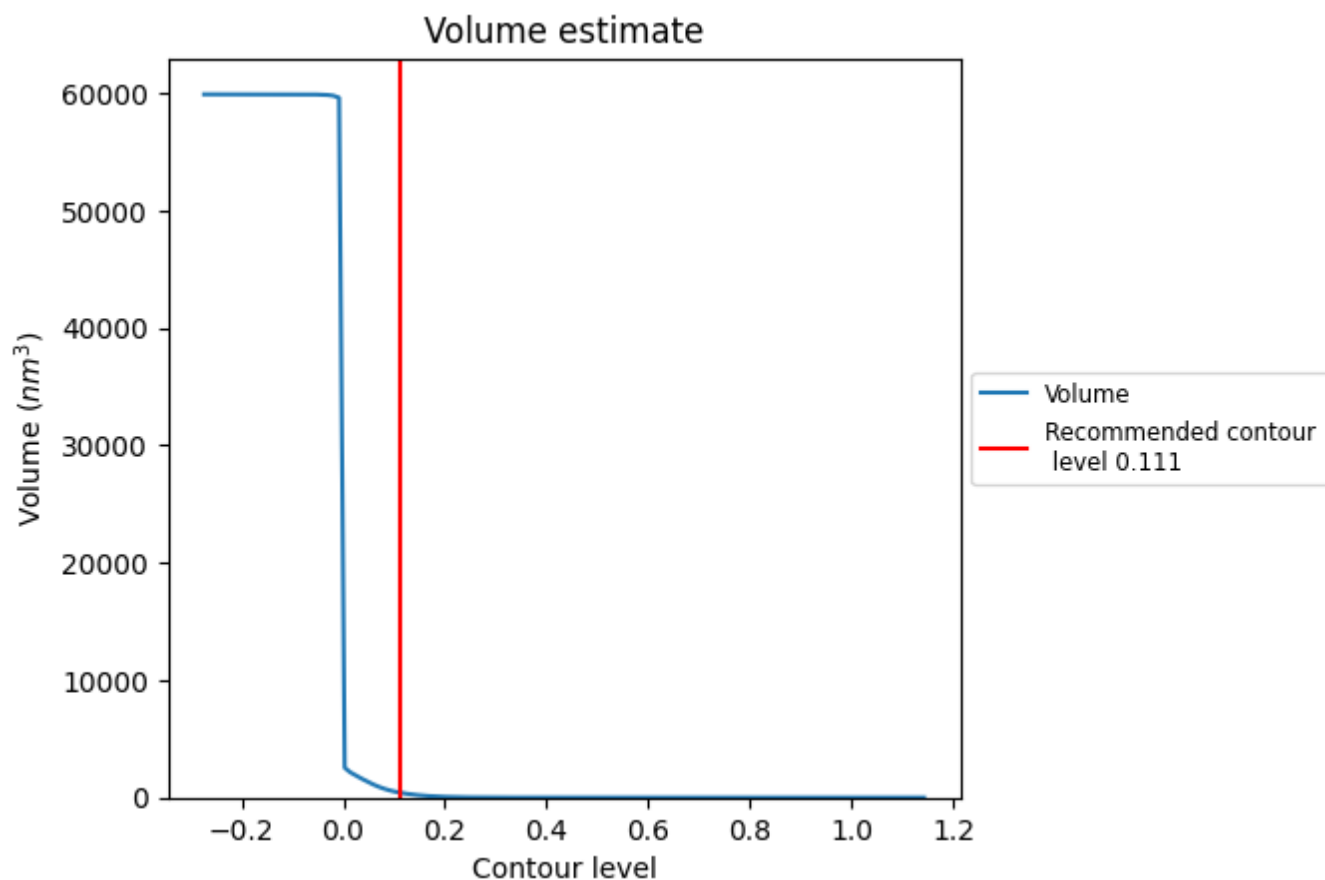
This section contains the results of statistical analysis of the map.

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.

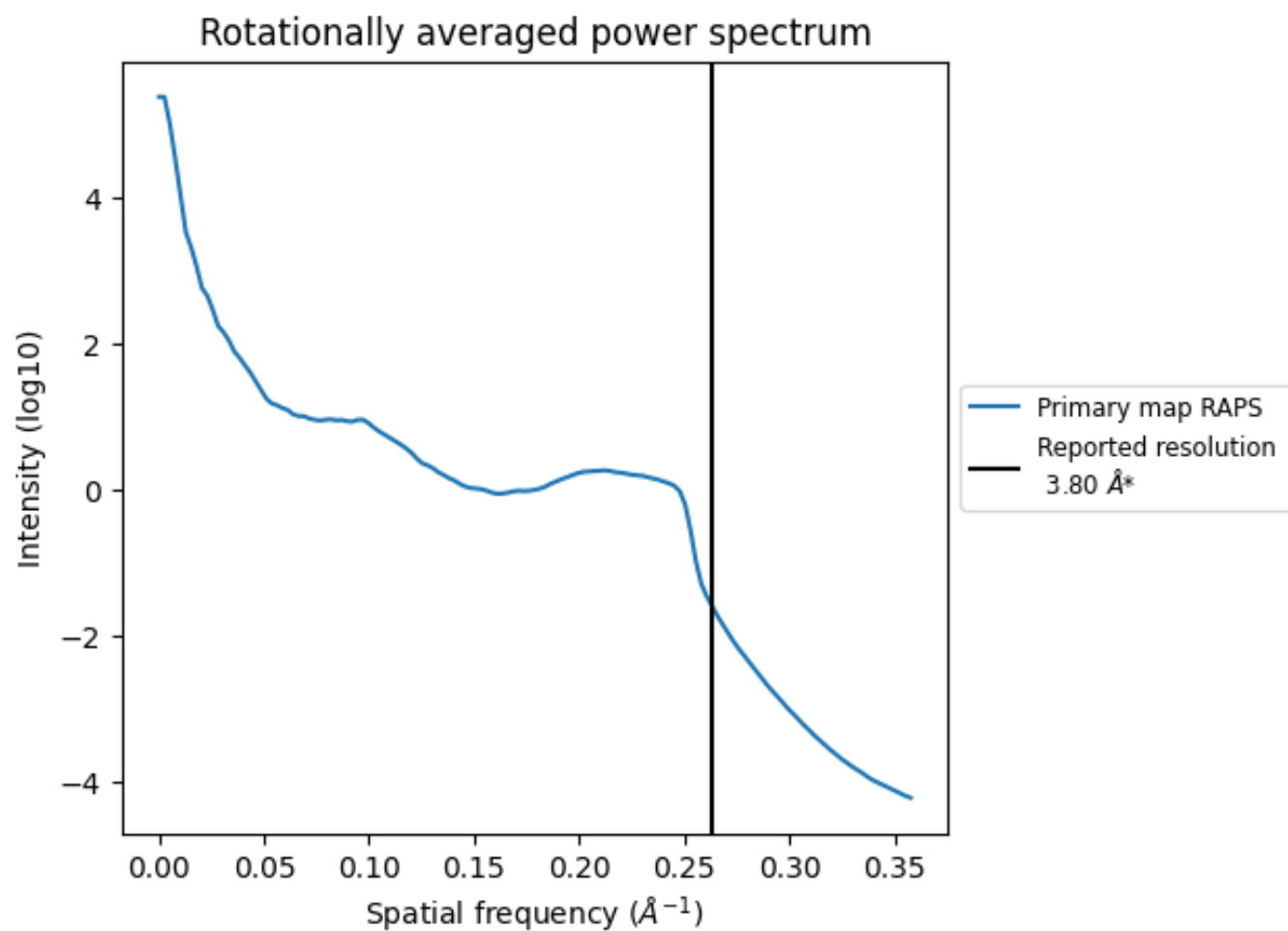
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 422 nm³; this corresponds to an approximate mass of 381 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

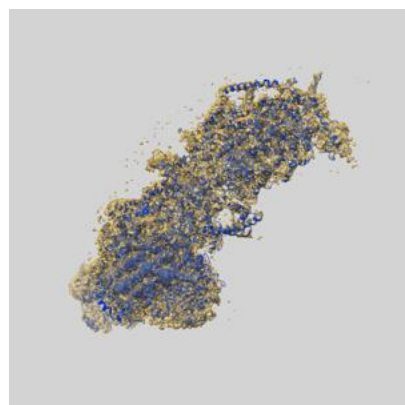
8 Fourier-Shell correlation ⓘ

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

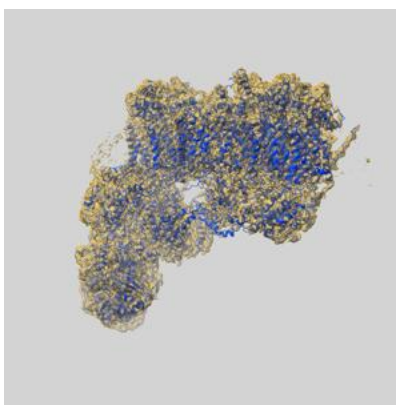
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-30676 and PDB model 7DGZ. Per-residue inclusion information can be found in section 3 on page 18.

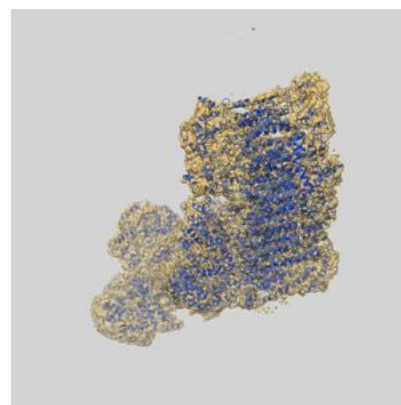
9.1 Map-model overlay [i](#)



X



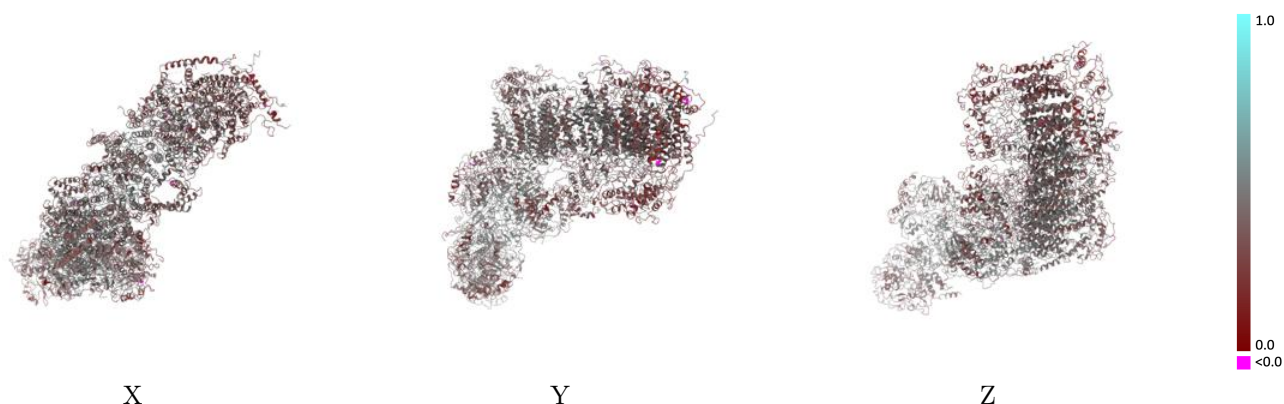
Y



Z

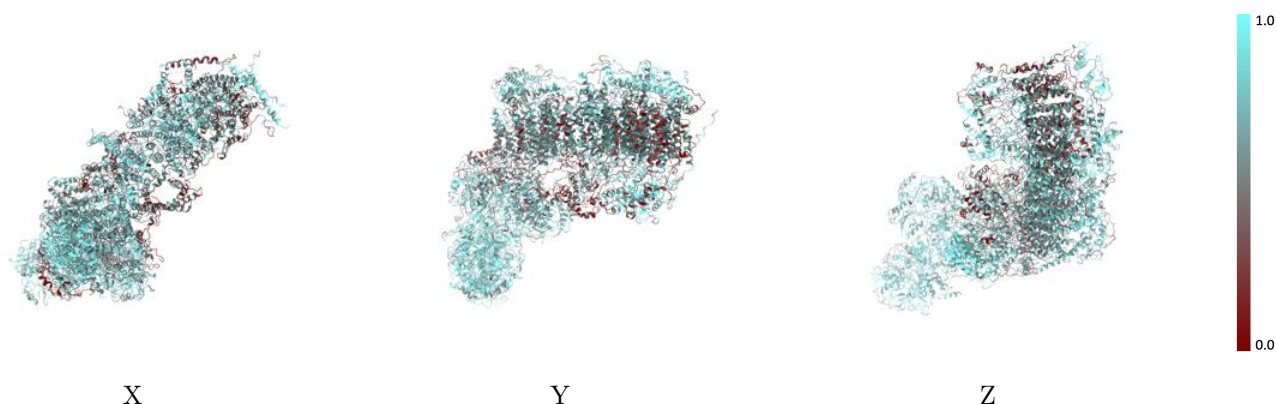
The images above show the 3D surface view of the map at the recommended contour level 0.111 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



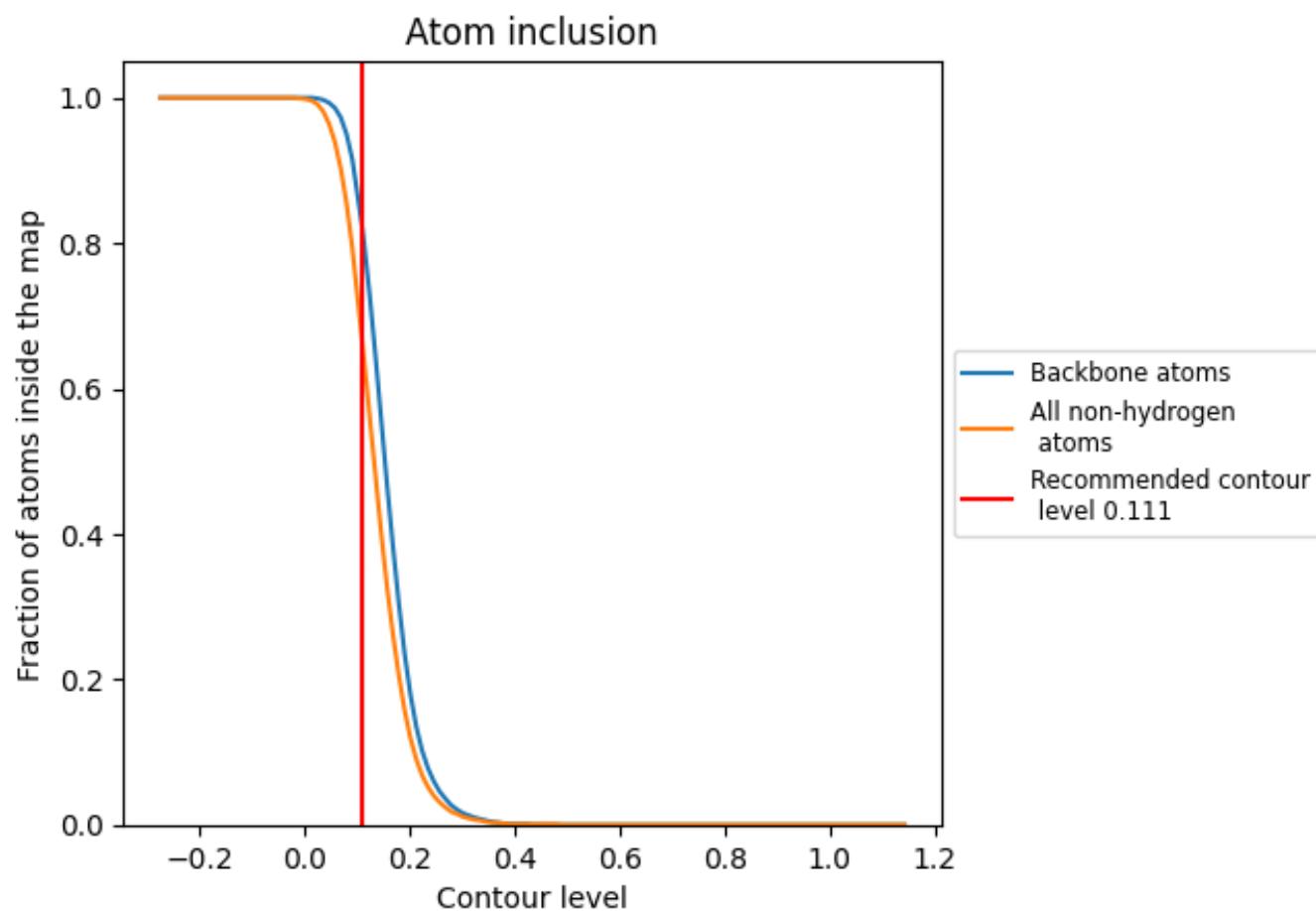
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.111).

9.4 Atom inclusion ⓘ



At the recommended contour level, 82% of all backbone atoms, 66% 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 (0.111) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6580	 0.3970
1	 0.6540	 0.4450
2	 0.7030	 0.4400
3	 0.4720	 0.3970
4	 0.6490	 0.4310
5	 0.6520	 0.4170
6	 0.5000	 0.3600
7	 0.5220	 0.3890
8	 0.8220	 0.3680
9	 0.7550	 0.3410
A	 0.8070	 0.4290
B	 0.7360	 0.4640
C	 0.8110	 0.4650
D	 0.7850	 0.4690
E	 0.8440	 0.4640
F	 0.5470	 0.2900
G	 0.7300	 0.4560
H	 0.7210	 0.4280
I	 0.5480	 0.4010
J	 0.6890	 0.4240
K	 0.7460	 0.3520
L	 0.5670	 0.3910
M	 0.3970	 0.2920
N	 0.7400	 0.3910
O	 0.6880	 0.4050
P	 0.5360	 0.3740
Q	 0.7160	 0.3820
R	 0.6200	 0.3730
S	 0.4020	 0.3490
T	 0.4500	 0.3680
U	 0.3600	 0.3690
V	 0.6960	 0.3990
W	 0.5870	 0.2980
X	 0.5380	 0.3400
Y	 0.5730	 0.3310



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Chain	Atom inclusion	Q-score
Z	 0.5330	 0.3110
a	 0.6220	 0.3860
b	 0.7390	 0.4150
c	 0.6590	 0.3290
d	 0.7850	 0.2910
e	 0.5590	 0.3690
f	 0.6880	 0.3400
g	 0.6150	 0.3390
h	 0.6310	 0.3680
i	 0.6590	 0.3650
j	 0.6680	 0.4040