



# Full wwPDB EM Validation Report ⓘ

Nov 10, 2024 – 03:55 am GMT

PDB ID : 7A23  
EMDB ID : EMD-11614  
Title : Plant mitochondrial respiratory complex I  
Authors : Soufari, H.; Waltz, F.; Hashem, Y.  
Deposited on : 2020-08-15  
Resolution : 3.70 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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:

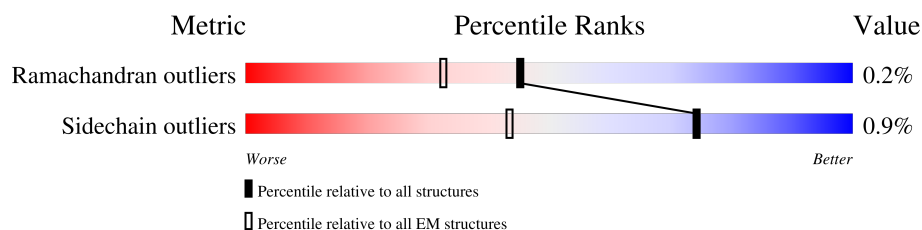
EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 3.70 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.







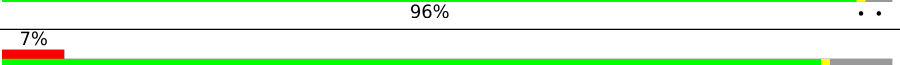
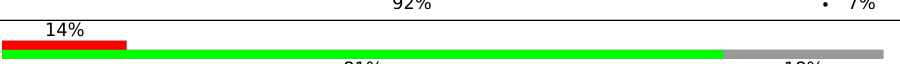
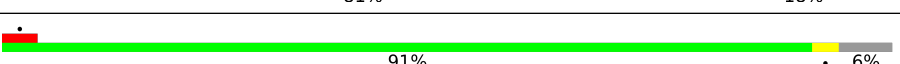
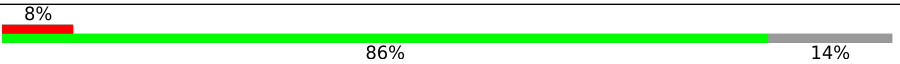


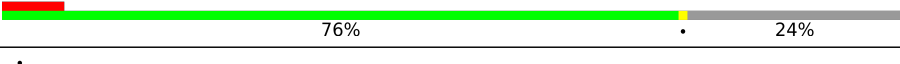
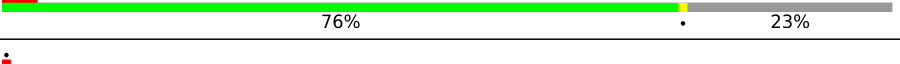

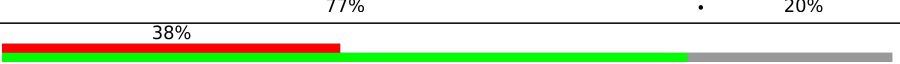
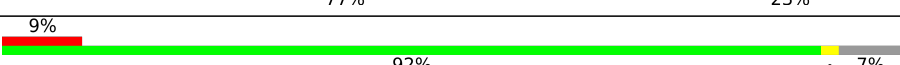
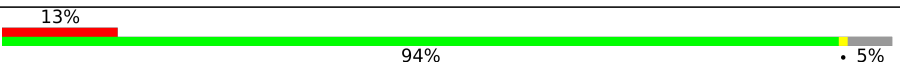

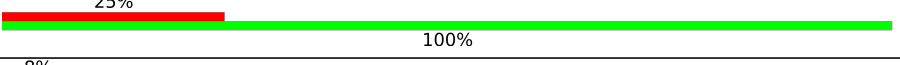




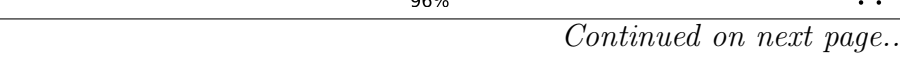


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	486	<div> <div>5%</div> <div>88%</div> <div>12%</div> </div>
2	I	499	<div> <div>14%</div> <div>95%</div> <div>• •</div> </div>
3	J	119	<div> <div>32%</div> <div>81%</div> <div>19%</div> </div>
4	N	205	<div> <div>20%</div> <div>72%</div> <div>27%</div> </div>
5	H	325	<div> <div>16%</div> <div>96%</div> <div>• •</div> </div>
6	K	100	<div> <div>12%</div> <div>84%</div> <div>• 15%</div> </div>
7	Y	106	<div> <div>10%</div> <div>92%</div> <div>• 8%</div> </div>
8	Z	143	<div> <div>13%</div> <div>98%</div> <div>•</div> </div>
9	V	65	<div> <div>14%</div> <div>88%</div> <div>12%</div> </div>

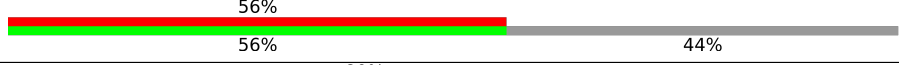
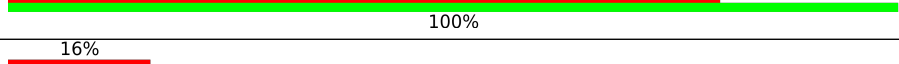
*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	W	65	
11	S	131	
12	i	81	
13	j	83	
14	G	394	
15	C	748	
16	T	402	
17	F	190	
18	B	255	
19	O	154	
20	P	110	
21	R	169	
22	U	159	
23	E	218	
24	D	222	
25	X	133	
26	c	106	
27	Q	97	
28	k	122	
29	r	24	
30	n	113	
31	o	252	
32	p	275	
32	q	275	
33	M	495	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
34	f	107	
35	g	114	
36	d	117	
37	a	669	
38	b	103	
39	h	69	
40	e	126	
41	l	71	
42	s	20	
43	m	98	
44	t	73	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	T7X	I	501	X	-	-	-

## 2 Entry composition

There are 54 unique types of molecules in this entry. The entry contains 57959 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 51kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	429	Total	C	N	O	S	0	0
			3328	2100	593	610	25		

- Molecule 2 is a protein called Nad2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	I	481	Total	C	N	O	S	0	0
			3754	2525	569	633	27		

- Molecule 3 is a protein called Nad3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	96	Total	C	N	O	S	0	0
			800	559	112	126	3		

- Molecule 4 is a protein called Nad6m.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	149	Total	C	N	O	S	0	0
			1201	810	194	189	8		

- Molecule 5 is a protein called Nad1m.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	318	Total	C	N	O	S	0	0
			2493	1691	378	409	15		

- Molecule 6 is a protein called Nad4Lm.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	85	Total	C	N	O	S	0	0
			667	450	101	110	6		

- Molecule 7 is a protein called PGIV.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	Y	98	Total	C	N	O	S	0	0
			774	484	133	145	12		

- Molecule 8 is a protein called B16.6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Z	140	Total	C	N	O	S	0	0
			1103	701	195	199	8		

- Molecule 9 is a protein called MWFE.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	57	Total	C	N	O	S	0	0
			461	296	82	78	5		

- Molecule 10 is a protein called B9.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	W	37	Total	C	N	O	S	0	0
			273	179	45	46	3		

- Molecule 11 is a protein called B14.5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	101	Total	C	N	O	S	0	0
			821	513	143	161	4		

- Molecule 12 is a protein called B14.5b.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	i	66	Total	C	N	O	S	0	0
			514	331	91	87	5		

- Molecule 13 is a protein called 15kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	j	68	Total	C	N	O	S	0	0
			582	359	113	103	7		

- Molecule 14 is a protein called Nad7m.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	G	382	Total	C	N	O	S	0	0
			3049	1939	535	551	24		

- Molecule 15 is a protein called 75kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	C	693	Total	C	N	O	S	0	0
			5288	3315	926	1008	39		

- Molecule 16 is a protein called 39kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	328	Total	C	N	O	S	0	0
			2535	1628	433	459	15		

- Molecule 17 is a protein called Nad9m.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	F	178	Total	C	N	O	S	0	0
			1518	979	262	272	5		

- Molecule 18 is a protein called 24kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B	219	Total	C	N	O	S	0	0
			1702	1081	286	323	12		

- Molecule 19 is a protein called 18kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	O	111	Total	C	N	O	S	0	0
			874	561	150	162	1		

- Molecule 20 is a protein called 13kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	P	71	Total	C	N	O	S	0	0
			554	348	97	103	6		

- Molecule 21 is a protein called B13.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	R	129	Total	C	N	O	S	0	0
			1039	656	174	204	5		

- Molecule 22 is a protein called B17.2.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	U	122	Total	C	N	O	S	0	0
			1011	643	184	183	1		

- Molecule 23 is a protein called PSST.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	153	Total	C	N	O	S	0	0
			1215	779	212	210	14		

- Molecule 24 is a protein called TYKY.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	D	177	Total	C	N	O	S	0	0
			1438	901	239	287	11		

- Molecule 25 is a protein called B14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	X	103	Total	C	N	O	S	0	0
			843	537	151	152	3		

- Molecule 26 is a protein called 20.9kDa.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	99	Total	C	N	O	S	0	0
			744	479	121	140	4		

- Molecule 27 is a protein called B8.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	Q	92	Total	C	N	O	S	0	0
			722	456	128	132	6		

- Molecule 28 is a protein called ACPM1.



Mol	Chain	Residues	Atoms					AltConf	Trace
28	k	78	Total	C	N	O	S	0	0
			614	390	94	127	3		

- Molecule 29 is a protein called Unk1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	r	24	Total	C	N	O		0	0
			120	72	24	24			

- Molecule 30 is a protein called P2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	n	27	Total	C	N	O		0	0
			205	133	35	37			

- Molecule 31 is a protein called CAL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	o	202	Total	C	N	O	S	0	0
			1568	1006	270	287	5		

- Molecule 32 is a protein called CA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	q	228	Total	C	N	O	S	0	0
			1736	1088	318	324	6		
32	p	224	Total	C	N	O	S	0	0
			1705	1068	311	320	6		

- Molecule 33 is a protein called Nad4m.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	M	482	Total	C	N	O	S	0	0
			3825	2579	593	630	23		

- Molecule 34 is a protein called PDSW.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	f	76	Total	C	N	O	S	0	0
			640	407	116	113	4		

- Molecule 35 is a protein called ESSS.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	g	47	Total	C	N	O	S	0	0
			386	253	60	71	2		

- Molecule 36 is a protein called B22.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	d	66	Total	C	N	O	0	0
			329	197	66	66		

- Molecule 37 is a protein called Nad5m.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	a	600	Total	C	N	O	S	0	0
			4677	3106	725	813	33		

- Molecule 38 is a protein called B18.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	b	63	Total	C	N	O	S	0	0
			519	327	89	94	9		

- Molecule 39 is a protein called AGGG.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	h	28	Total	C	N	O	S	0	0
			232	155	40	35	2		

- Molecule 40 is a protein called ACPM2.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	e	84	Total	C	N	O	0	0
			417	249	84	84		

- Molecule 41 is a protein called B15.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	l	23	Total	C	N	O	0	0
			112	66	23	23		

- Molecule 42 is a protein called Unk2.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	s	20	Total	C	N	O	0	0
			100	60	20	20		

- Molecule 43 is a protein called P1.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	m	69	Total	C	N	O	S	0	0
			605	385	112	103	5		

- Molecule 44 is a protein called B12-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	t	31	Total	C	N	O	S	0	0
			232	149	42	38	3		

- Molecule 45 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ).



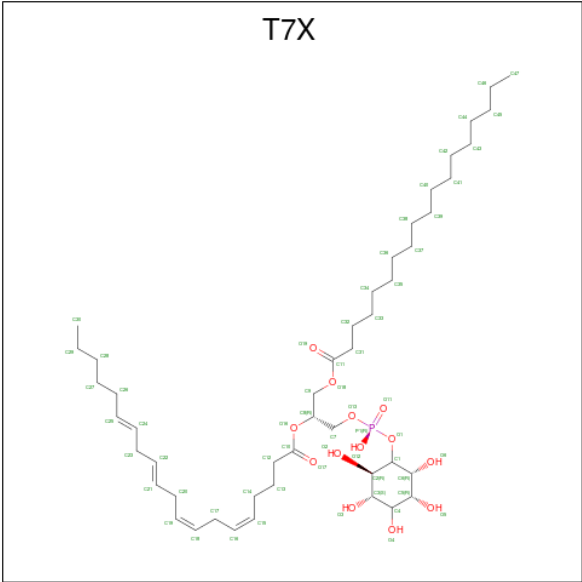
Mol	Chain	Residues	Atoms			AltConf
45	A	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	C	1	Total	Fe	S	0
			8	4	4	
45	E	1	Total	Fe	S	0
			8	4	4	

*Continued on next page...*

Mol	Chain	Residues	Atoms			AltConf
45	D	1	Total	Fe	S	0
			8	4	4	
45	D	1	Total	Fe	S	0
			8	4	4	

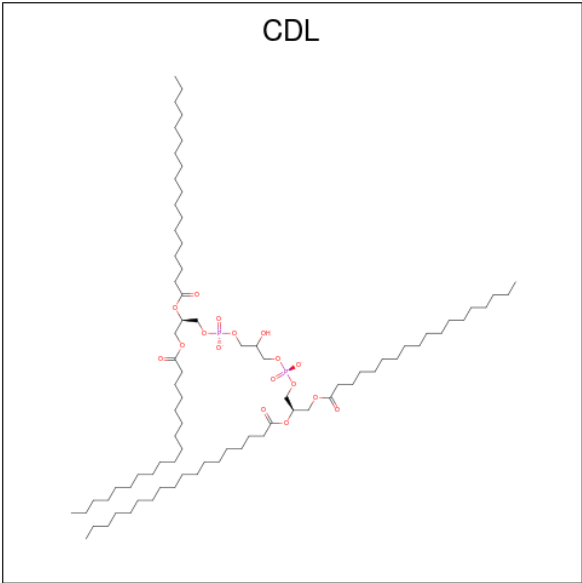
- 
- The image displays the chemical structure of Flavin Mononucleotide (FMN). It features an isoalloxazine ring system, which is a tricyclic aromatic heterocycle consisting of a benzene ring fused to two pyrimidine rings. The ring atoms are labeled: N1, N3, N5, N9, C2, C4, C6, C7, C8, C9, C10, C12, C13, C14, C15, C16, C17, C18, C19, C20, C21, C22, C23, C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34, C35, C36, C37, C38, C39, C40, C41, C42, C43, C44, C45, C46, C47, C48, C49, C50, C51, C52, C53, C54, C55, C56, C57, C58, C59, C60, C61, C62, C63, C64, C65, C66, C67, C68, C69, C70, C71, C72, C73, C74, C75, C76, C77, C78, C79, C80, C81, C82, C83, C84, C85, C86, C87, C88, C89, C90, C91, C92, C93, C94, C95, C96, C97, C98, C99, C100. The ribityl chain is attached to the N1 position of the isoalloxazine ring. The ribityl chain consists of three carbon atoms (C1, C2, C3) and a phosphate group (P, O1P, O2P, O3P). The ribityl chain is shown in a 3D representation with wedged and dashed bonds indicating stereochemistry. The phosphate group is shown in a 2D representation with red oxygen atoms and a purple phosphorus atom. The overall structure is colored with blue for the ring system, red for the ribityl chain, and purple for the phosphate group.

- Molecule 47 is Phosphatidylinositol (three-letter code: T7X) (formula:  $C_{47}H_{83}O_{13}P$ ).



Mol	Chain	Residues	Atoms				AltConf
47	I	1	Total	C	O	P	0
			54	40	13	1	
47	p	1	Total	C	O	P	0
			61	47	13	1	

- Molecule 48 is CARDIOLIPIN (three-letter code: CDL) (formula: C<sub>81</sub>H<sub>156</sub>O<sub>17</sub>P<sub>2</sub>).



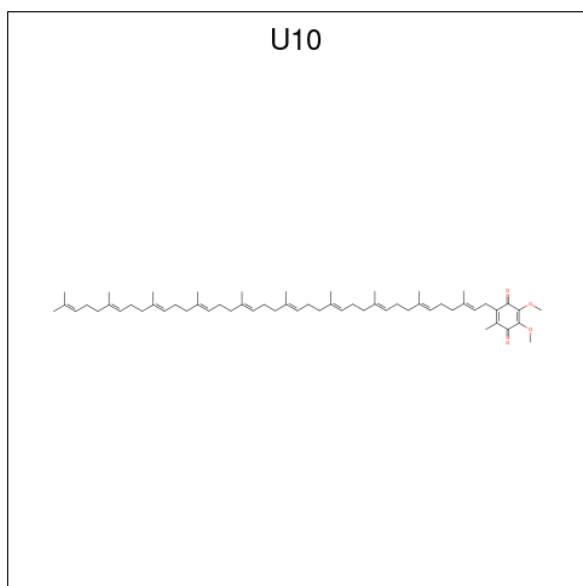
Mol	Chain	Residues	Atoms				AltConf
48	I	1	Total	C	O	P	0
			100	81	17	2	
48	I	1	Total	C	O	P	0
			98	79	17	2	

Continued on next page...

*Continued from previous page...*

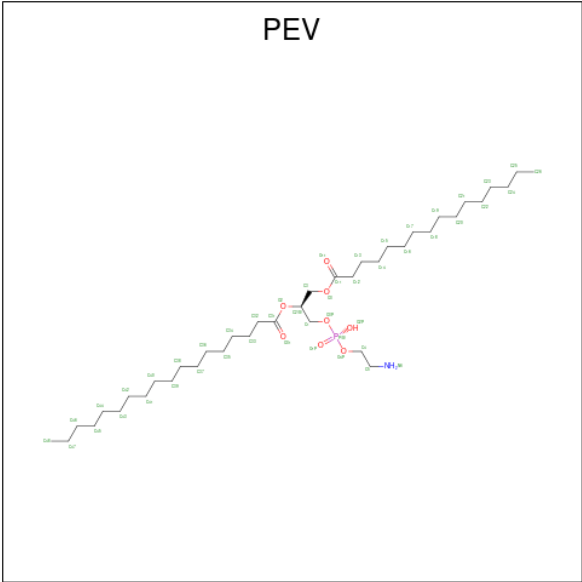
Mol	Chain	Residues	Atoms				AltConf
48	J	1	Total	C	O	P	0
			87	68	17	2	

- Molecule 49 is UBIQUINONE-10 (three-letter code: U10) (formula:  $C_{59}H_{90}O_4$ ).



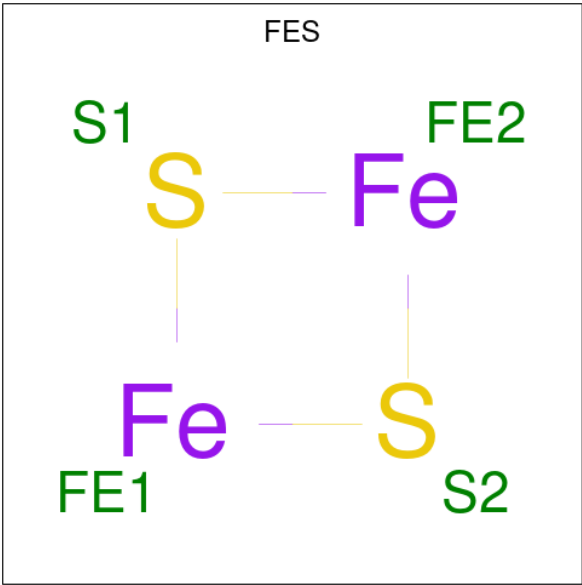
Mol	Chain	Residues	Atoms				AltConf
49	H	1	Total	C	O		0
			44	40	4		

- Molecule 50 is (1S)-2-{[(2-AMINOETHOXY)(HYDROXY)PHOSPHORYL]OXY}-1-[(PALMITOYLOXY)METHYL]ETHYL STEARATE (three-letter code: PEV) (formula:  $C_{39}H_{78}NO_8P$ ).



Mol	Chain	Residues	Atoms					AltConf
50	H	1	Total	C	N	O	P	0
			49	39	1	8	1	

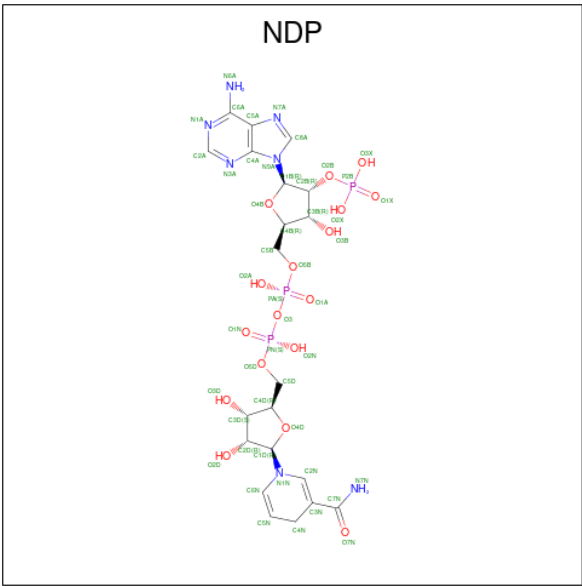
- Molecule 51 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
51	C	1	Total	Fe	S	0
			4	2	2	
51	B	1	Total	Fe	S	0
			4	2	2	

- Molecule 52 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE

PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).



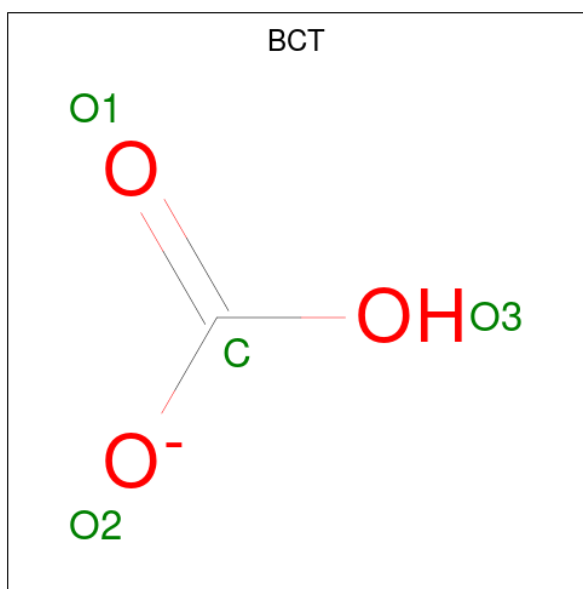
Mol	Chain	Residues	Atoms					AltConf
52	T	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 53 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
53	P	1	Total	Zn	0
			1	1	
53	q	1	Total	Zn	0
			1	1	

- Molecule 54 is BICARBONATE ION (three-letter code: BCT) (formula: CHO<sub>3</sub>).






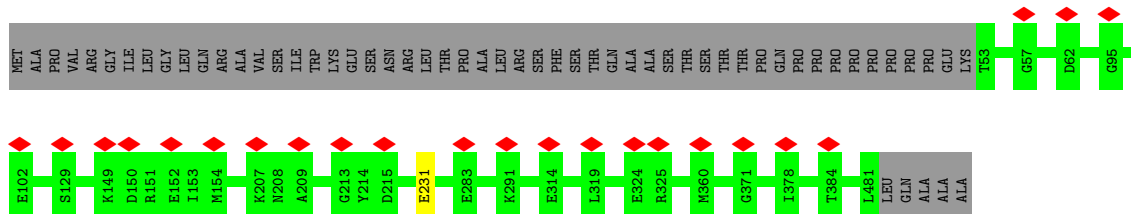
Mol	Chain	Residues	Atoms			AltConf
54	q	1	Total	C	O	0
			4	1	3	

### 3 Residue-property plots [i](#)

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

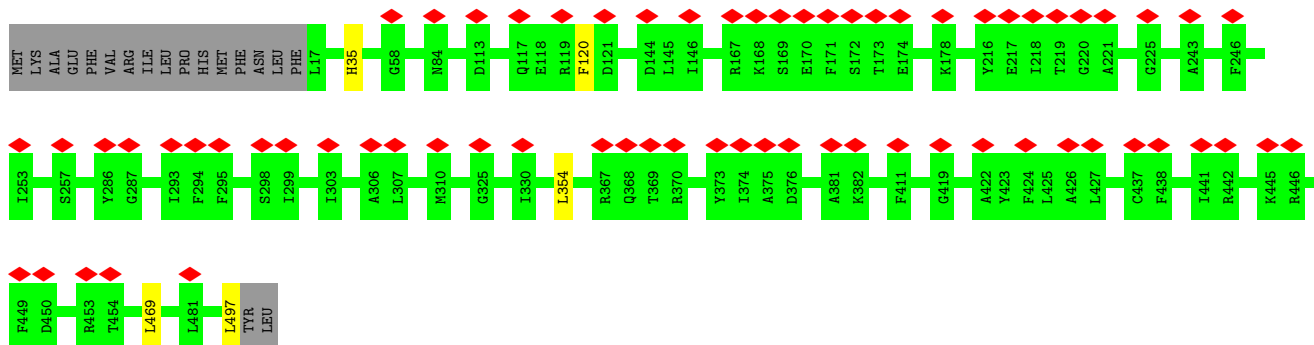
#### • Molecule 1: 51kDa

Chain A: 




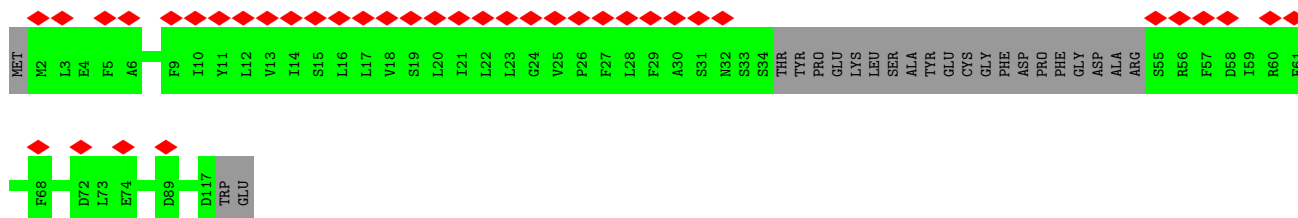
#### • Molecule 2: Nad2m

Chain I: 

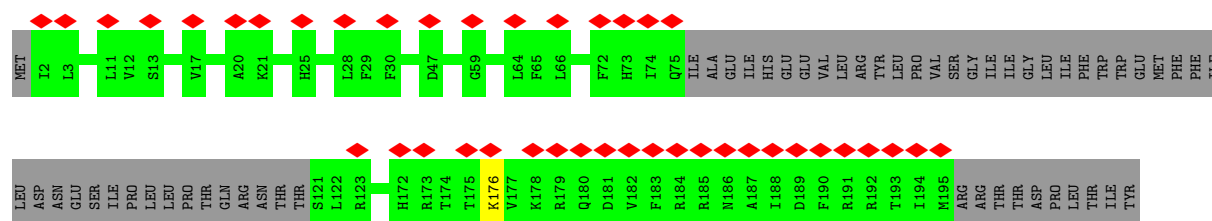
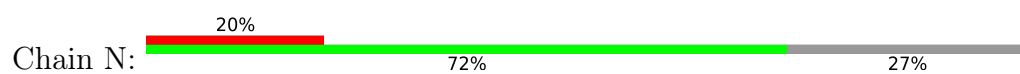


#### • Molecule 3: Nad3m

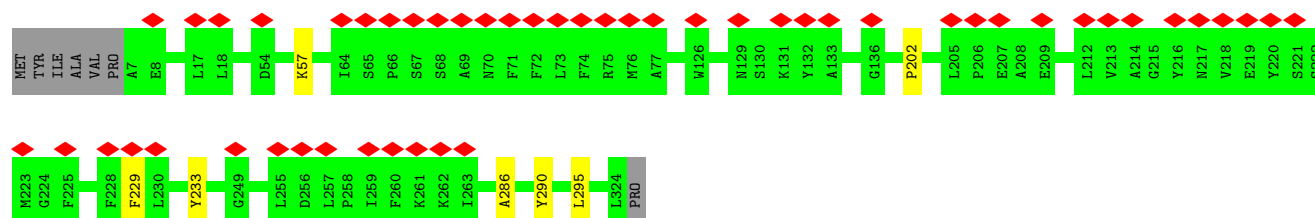
Chain J: 



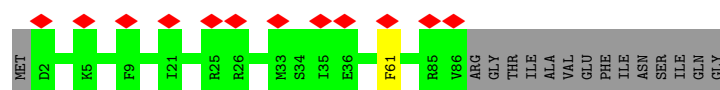
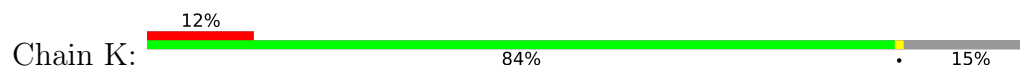
#### • Molecule 4: Nad6m



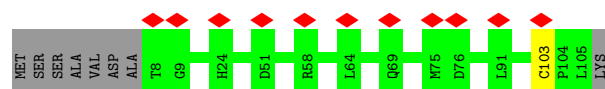
- Molecule 5: Nad1m



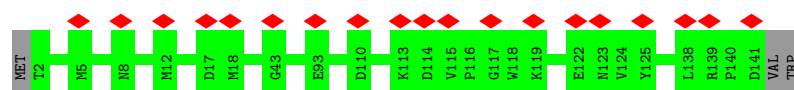
- Molecule 6: Nad4Lm



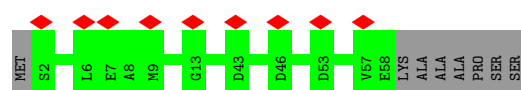
- Molecule 7: PGIV



- Molecule 8: B16.6

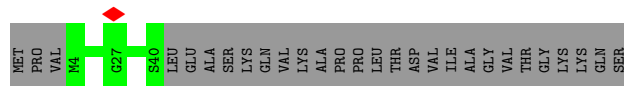


- Molecule 9: MWFE



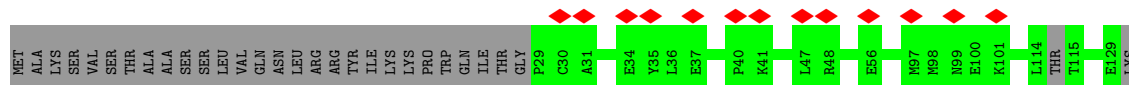
- Molecule 10: B9

Chain W:  57% 43%




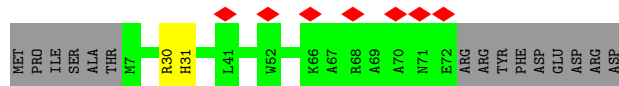
- Molecule 11: B14.5a

Chain S:  10% 77% 23%




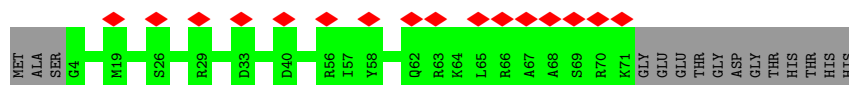
- Molecule 12: B14.5b

Chain i:  9% 79% 19%



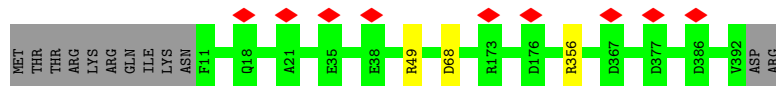
- Molecule 13: 15kDa

Chain j:  19% 82% 18%



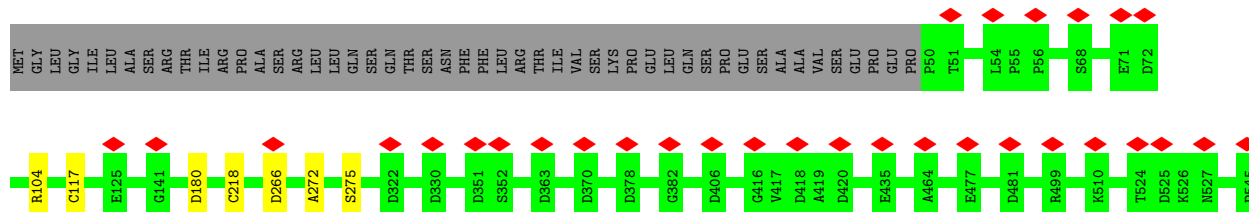
- Molecule 14: Nad7m

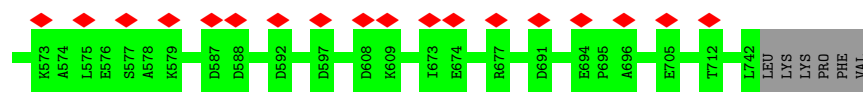
Chain G:  96% ..



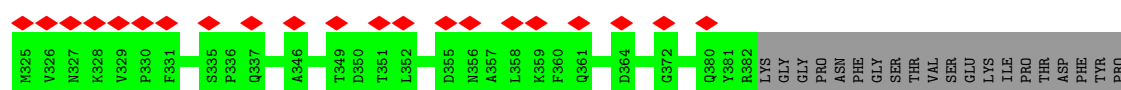
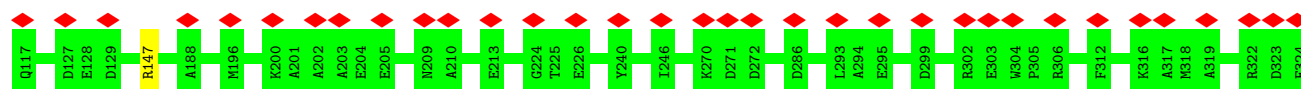
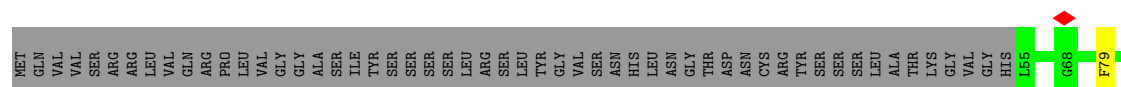
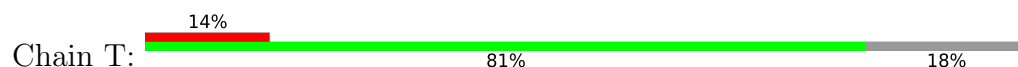
- Molecule 15: 75kDa

Chain C:  7% 92% 7%

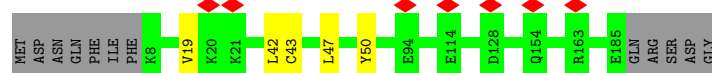




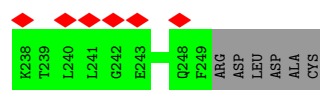
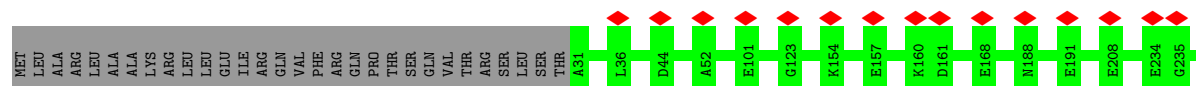
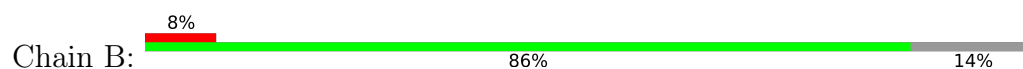
• Molecule 16: 39kDa



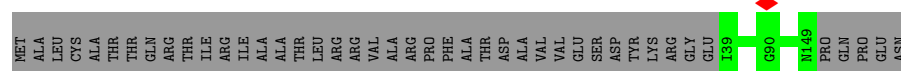
• Molecule 17: Nad9m



• Molecule 18: 24kDa

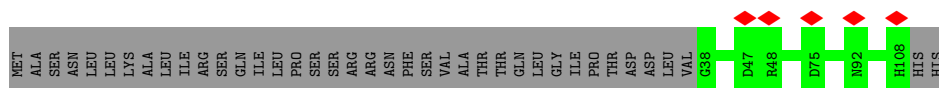


• Molecule 19: 18kDa

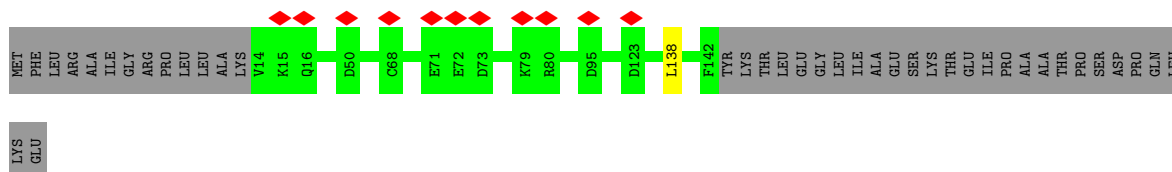
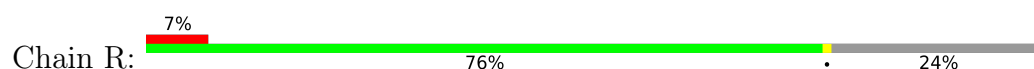


• Molecule 20: 13kDa

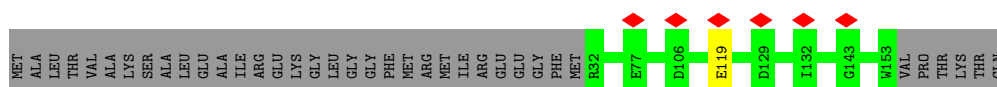
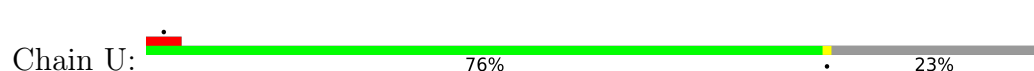




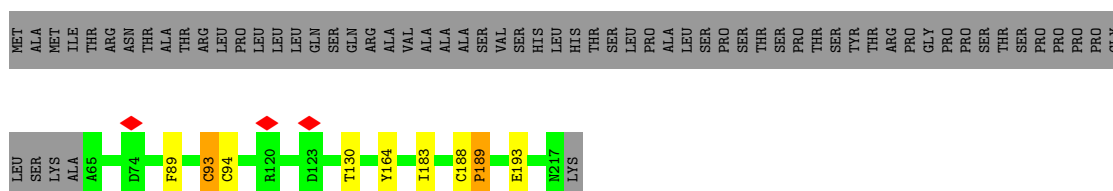
## • Molecule 21: B13



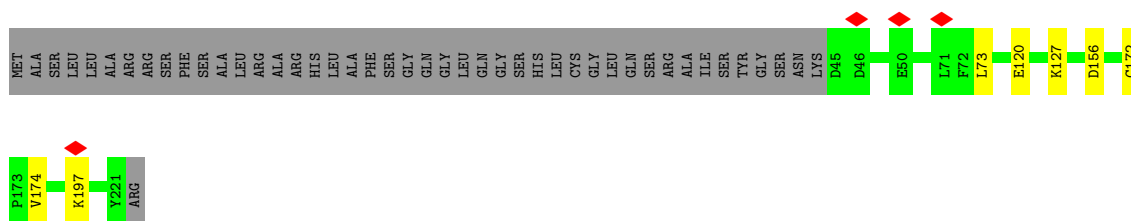
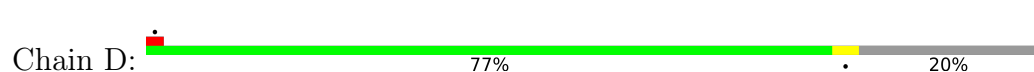
## • Molecule 22: B17.2



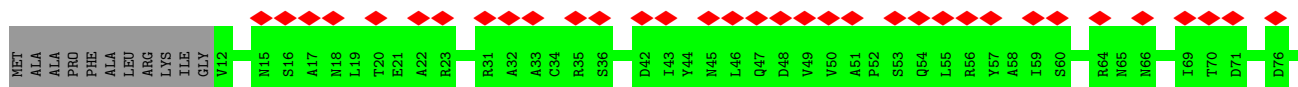
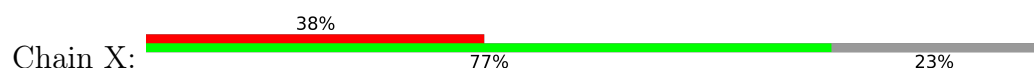
## • Molecule 23: PSST

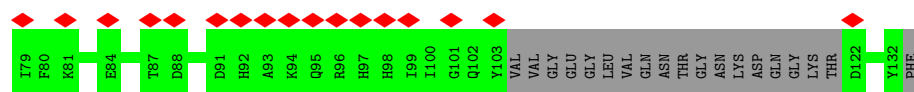


## • Molecule 24: TYKY

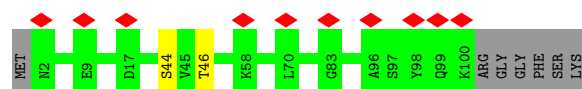


## • Molecule 25: B14

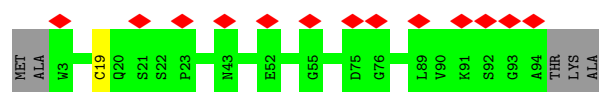




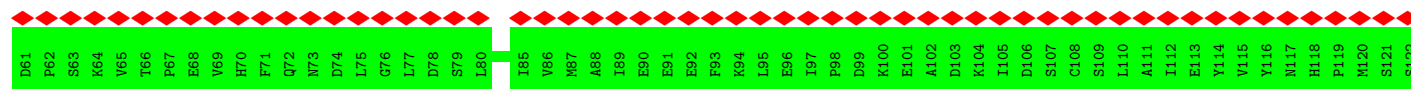
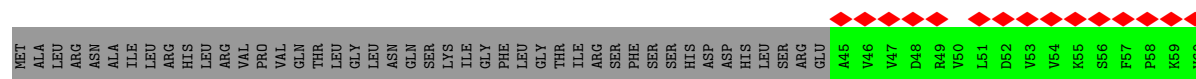
• Molecule 26: 20.9kDa



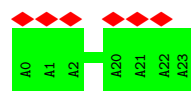
• Molecule 27: B8



• Molecule 28: ACPM1



• Molecule 29: Unk1

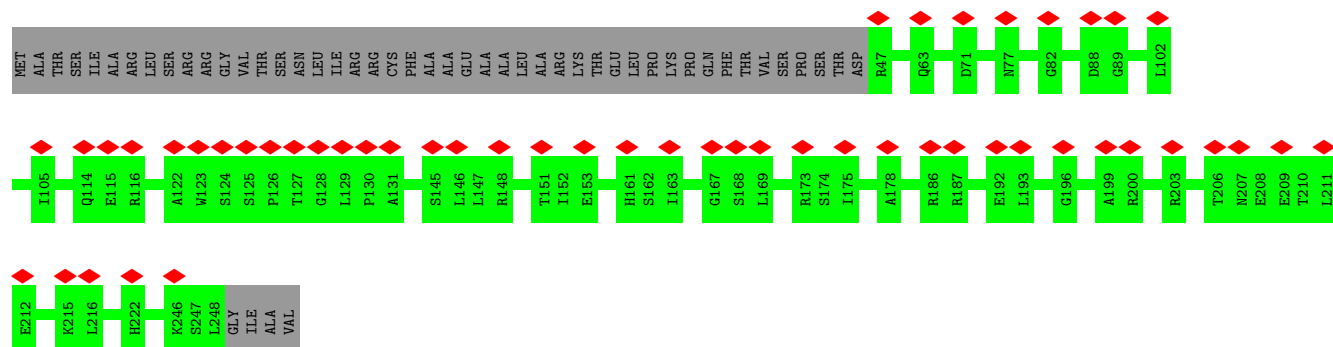


• Molecule 30: P2

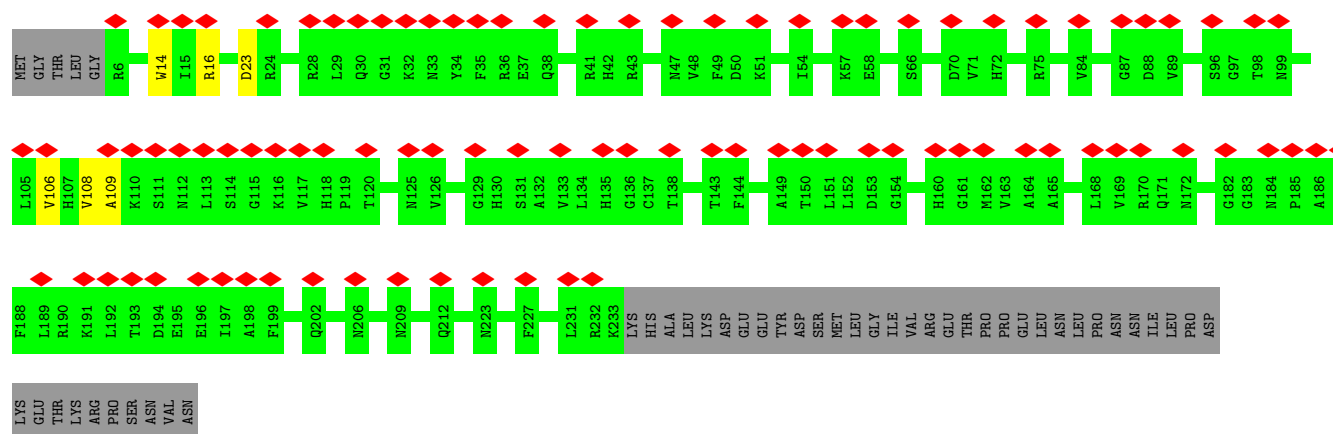
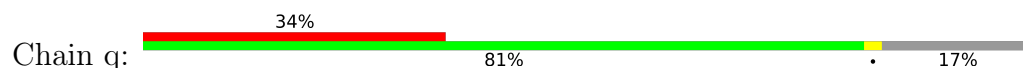


• Molecule 31: CAL1

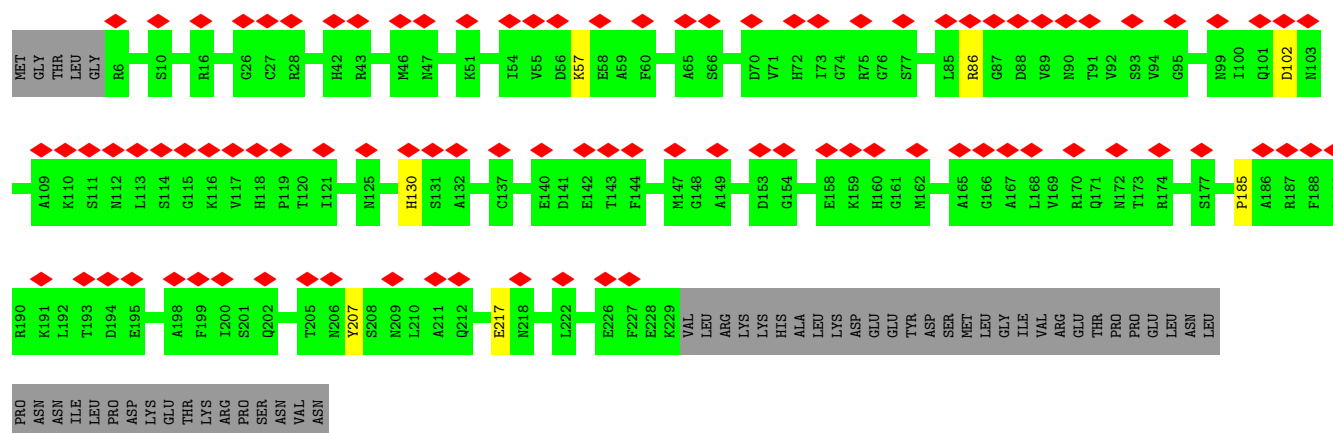
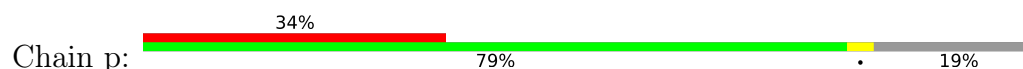




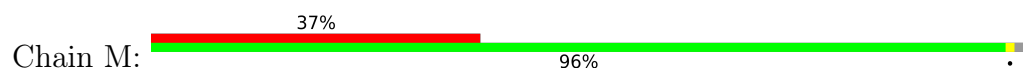
## • Molecule 32: CA1



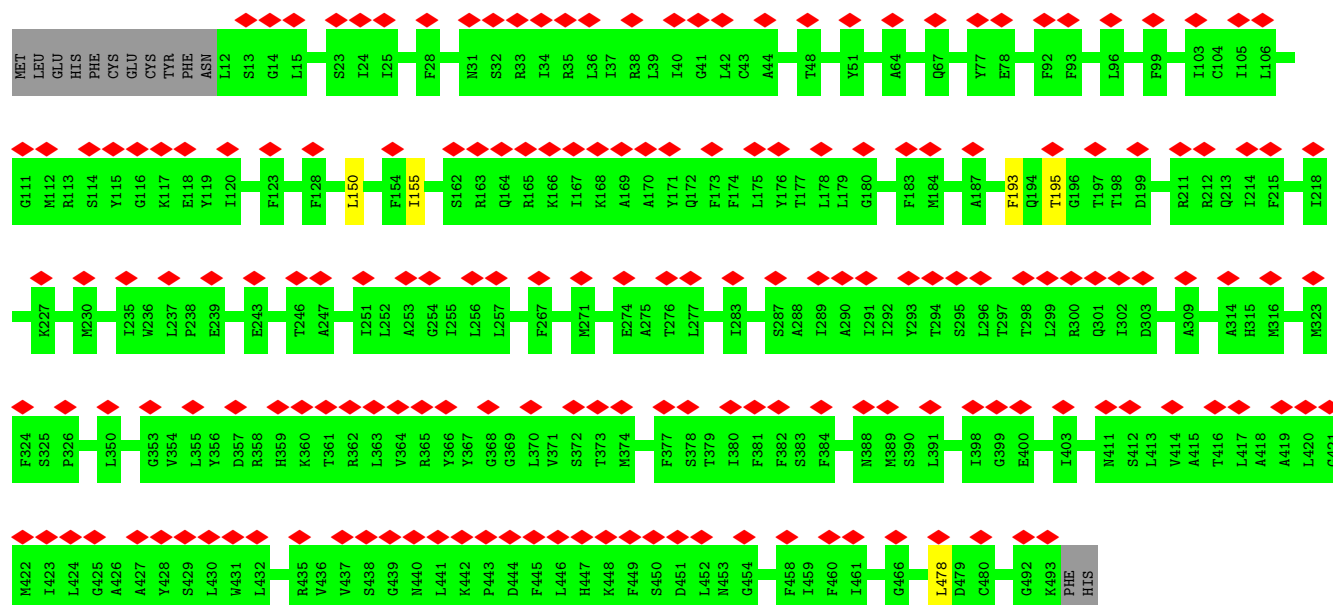
## • Molecule 32: CA1



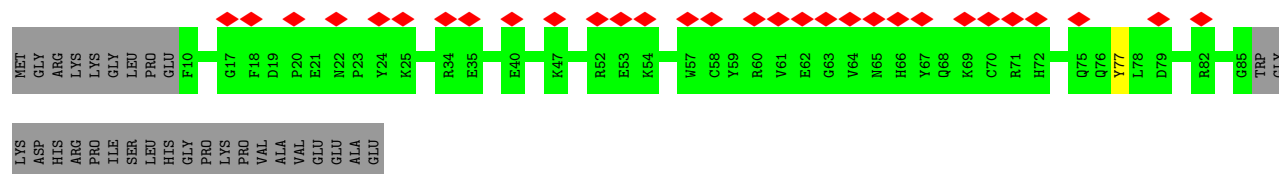
## • Molecule 33: Nad4m



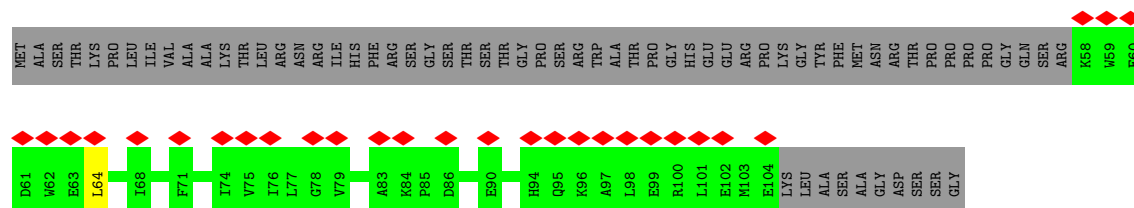




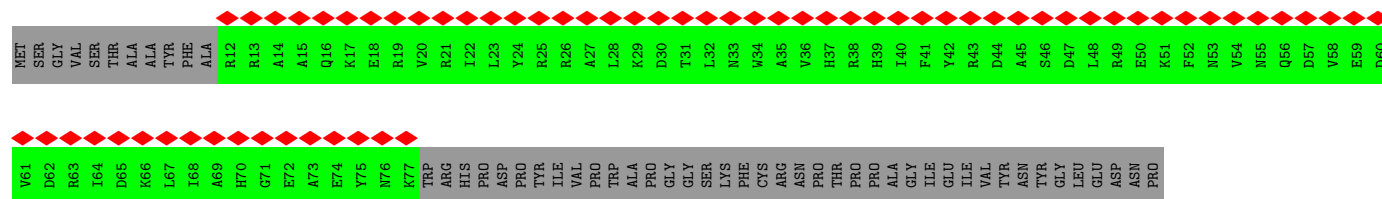
- Molecule 34: PDSW



- Molecule 35: ESSS

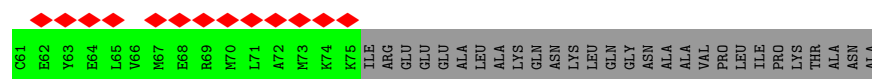


- Molecule 36: B22

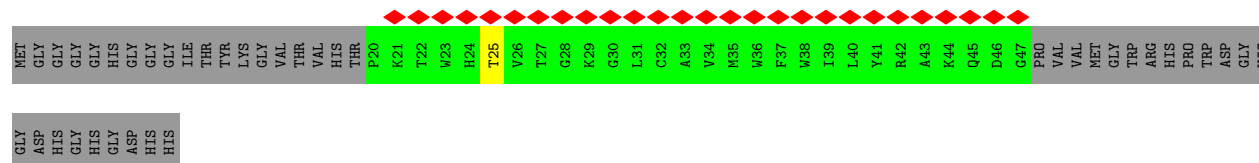


- Molecule 37: Nad5m

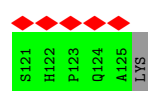
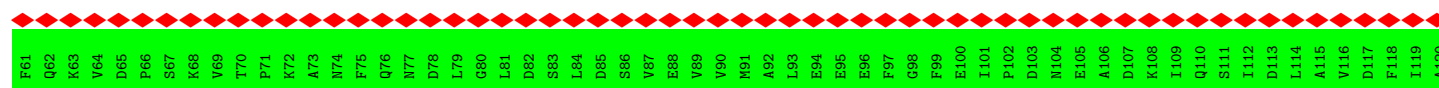
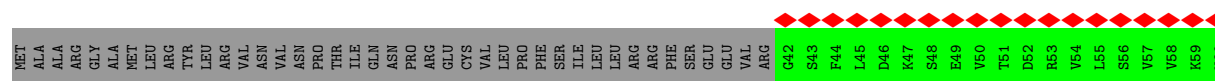




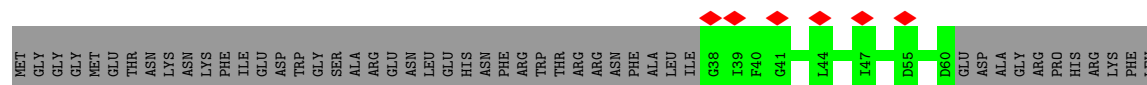
• Molecule 39: AGGG



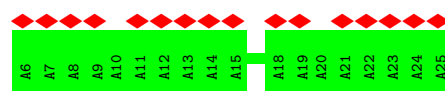
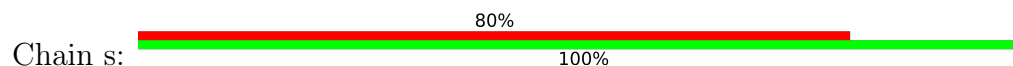
• Molecule 40: ACPM2



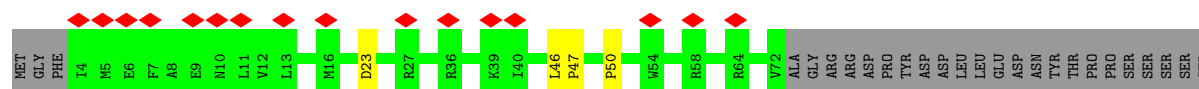
• Molecule 41: B15



• Molecule 42: Unk2



• Molecule 43: P1



SER  
SER  
ASP

● Molecule 44: B12-1



MET	ALA	LYS	PRO	LEU	GLY	THR	THR	GLY	PHE	PHE	ARG	ARG	ASP	GLU	TRP	ARG	K20	H21	P22	M23	L24	S25	N26	Q27	M28	R29	H30	A31	L32	P33	G34	L35	G36	I37	G38	V39	A40	A41	F42	C43	V44	Y45	L46	V47	G48	E49	Q50	ILE	TYR	ASN	LYS	ALA	LEU	ALA	PRO	SER	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

SER  
SER  
HIS  
HIS  
HIS  
GLN  
GLU  
GLN  
THR  
ALA  
PRO  
SER  
HIS

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	65018	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.257	Depositor
Minimum map value	-0.079	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0235	Depositor
Map size (Å)	399.6, 399.6, 399.6	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FES, CDL, PEV, SF4, BCT, NDP, U10, ZN, FMN, T7X

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.40	0/3401	0.51	0/4588
2	I	0.41	0/3855	0.56	0/5234
3	J	0.42	0/826	0.49	0/1120
4	N	0.39	0/1227	0.50	0/1664
5	H	0.49	0/2565	0.64	5/3492 (0.1%)
6	K	0.37	0/677	0.47	0/916
7	Y	0.40	0/788	0.49	0/1059
8	Z	0.35	0/1132	0.52	0/1530
9	V	0.33	0/473	0.43	0/636
10	W	0.50	0/277	0.63	0/375
11	S	0.36	0/840	0.49	0/1141
12	i	0.44	0/524	0.70	0/706
13	j	0.34	0/595	0.49	0/791
14	G	0.51	0/3120	0.56	0/4221
15	C	0.43	0/5386	0.54	1/7299 (0.0%)
16	T	0.40	0/2591	0.52	0/3509
17	F	0.47	0/1564	0.57	1/2120 (0.0%)
18	B	0.38	0/1743	0.49	0/2364
19	O	0.45	0/899	0.48	0/1215
20	P	0.41	0/567	0.52	0/768
21	R	0.44	0/1061	0.64	0/1441
22	U	0.42	0/1044	0.50	0/1413
23	E	0.50	0/1250	0.67	3/1697 (0.2%)
24	D	0.53	0/1467	0.62	0/1981
25	X	0.29	0/861	0.40	0/1166
26	c	0.46	1/760 (0.1%)	0.51	0/1028
27	Q	0.32	0/734	0.46	0/989
28	k	0.25	0/625	0.43	0/848
29	r	0.25	0/119	0.46	0/165
30	n	0.40	0/208	0.59	0/282
31	o	0.32	0/1606	0.48	0/2192
32	p	0.38	0/1737	0.63	2/2353 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
32	q	0.33	0/1768	0.56	0/2395
33	M	0.37	0/3930	0.57	0/5344
34	f	0.28	0/657	0.46	0/885
35	g	0.32	0/396	0.59	1/539 (0.2%)
36	d	0.24	0/328	0.39	0/457
37	a	0.29	0/4802	0.51	0/6520
38	b	0.25	0/528	0.50	0/705
39	h	0.60	0/241	0.60	0/326
40	e	0.24	0/416	0.42	0/579
41	l	0.25	0/111	0.37	0/152
42	s	0.25	0/99	0.31	0/137
43	m	0.30	0/621	0.60	2/834 (0.2%)
44	t	0.63	0/237	0.64	0/319
All	All	0.40	1/58656 (0.0%)	0.54	15/79495 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
32	q	0	1
33	M	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	44	SER	CA-CB	-5.43	1.44	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	229	PHE	CB-CA-C	7.53	125.45	110.40
23	E	94	CYS	CB-CA-C	6.69	123.78	110.40
35	g	64	LEU	CA-CB-CG	5.69	128.40	115.30
43	m	47	PRO	N-CA-CB	5.68	110.12	103.30
23	E	189	PRO	N-CA-C	-5.50	97.81	112.10
23	E	93	CYS	CA-CB-SG	-5.35	104.37	114.00
5	H	286	ALA	N-CA-CB	-5.29	102.70	110.10
43	m	23	ASP	CB-CG-OD1	5.26	123.03	118.30
32	p	185	PRO	N-CA-C	-5.25	98.46	112.10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	295	LEU	CA-CB-CG	5.24	127.35	115.30
5	H	202	PRO	N-CA-C	-5.19	98.61	112.10
32	p	130	HIS	CB-CA-C	-5.18	100.04	110.40
17	F	50	TYR	CB-CA-C	5.17	120.73	110.40
15	C	117	CYS	CA-CB-SG	-5.12	104.78	114.00
5	H	233	TYR	CB-CA-C	5.09	120.58	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
33	M	478	LEU	Peptide
32	q	109	ALA	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	427/486 (88%)	381 (89%)	46 (11%)	0	100	100
2	I	479/499 (96%)	440 (92%)	39 (8%)	0	100	100
3	J	92/119 (77%)	86 (94%)	6 (6%)	0	100	100
4	N	145/205 (71%)	125 (86%)	20 (14%)	0	100	100
5	H	316/325 (97%)	283 (90%)	33 (10%)	0	100	100
6	K	83/100 (83%)	81 (98%)	2 (2%)	0	100	100
7	Y	96/106 (91%)	87 (91%)	8 (8%)	1 (1%)	13	44
8	Z	138/143 (96%)	112 (81%)	26 (19%)	0	100	100

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	55/65 (85%)	52 (94%)	3 (6%)	0	100	100
10	W	35/65 (54%)	31 (89%)	4 (11%)	0	100	100
11	S	99/131 (76%)	86 (87%)	13 (13%)	0	100	100
12	i	64/81 (79%)	59 (92%)	4 (6%)	1 (2%)	8	37
13	j	66/83 (80%)	63 (96%)	3 (4%)	0	100	100
14	G	380/394 (96%)	348 (92%)	32 (8%)	0	100	100
15	C	691/748 (92%)	618 (89%)	72 (10%)	1 (0%)	48	78
16	T	326/402 (81%)	281 (86%)	45 (14%)	0	100	100
17	F	176/190 (93%)	151 (86%)	25 (14%)	0	100	100
18	B	217/255 (85%)	184 (85%)	33 (15%)	0	100	100
19	O	109/154 (71%)	102 (94%)	7 (6%)	0	100	100
20	P	69/110 (63%)	64 (93%)	5 (7%)	0	100	100
21	R	127/169 (75%)	119 (94%)	8 (6%)	0	100	100
22	U	120/159 (76%)	98 (82%)	22 (18%)	0	100	100
23	E	151/218 (69%)	134 (89%)	16 (11%)	1 (1%)	19	51
24	D	175/222 (79%)	160 (91%)	14 (8%)	1 (1%)	22	54
25	X	99/133 (74%)	92 (93%)	7 (7%)	0	100	100
26	c	97/106 (92%)	91 (94%)	6 (6%)	0	100	100
27	Q	90/97 (93%)	81 (90%)	9 (10%)	0	100	100
28	k	76/122 (62%)	74 (97%)	2 (3%)	0	100	100
29	r	22/24 (92%)	18 (82%)	4 (18%)	0	100	100
30	n	25/113 (22%)	22 (88%)	3 (12%)	0	100	100
31	o	200/252 (79%)	172 (86%)	28 (14%)	0	100	100
32	p	222/275 (81%)	190 (86%)	30 (14%)	2 (1%)	14	47
32	q	226/275 (82%)	195 (86%)	28 (12%)	3 (1%)	10	40
33	M	480/495 (97%)	433 (90%)	47 (10%)	0	100	100
34	f	74/107 (69%)	67 (90%)	7 (10%)	0	100	100
35	g	45/114 (40%)	39 (87%)	6 (13%)	0	100	100
36	d	64/117 (55%)	60 (94%)	4 (6%)	0	100	100
37	a	592/669 (88%)	524 (88%)	66 (11%)	2 (0%)	37	67
38	b	61/103 (59%)	50 (82%)	11 (18%)	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	h	26/69 (38%)	26 (100%)	0	0	100	100
40	e	82/126 (65%)	80 (98%)	2 (2%)	0	100	100
41	l	21/71 (30%)	21 (100%)	0	0	100	100
42	s	18/20 (90%)	18 (100%)	0	0	100	100
43	m	67/98 (68%)	48 (72%)	17 (25%)	2 (3%)	3	27
44	t	29/73 (40%)	28 (97%)	1 (3%)	0	100	100
All	All	7252/8888 (82%)	6474 (89%)	764 (10%)	14 (0%)	45	72

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
12	i	30	ARG
32	q	108	VAL
15	C	272	ALA
24	D	120	GLU
32	q	23	ASP
32	q	106	VAL
32	p	102	ASP
32	p	217	GLU
37	a	509	SER
7	Y	103	CYS
23	E	189	PRO
37	a	511	PHE
43	m	46	LEU
43	m	50	PRO

### 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	349/396 (88%)	348 (100%)	1 (0%)	91	94
2	I	399/416 (96%)	394 (99%)	5 (1%)	65	77
3	J	87/106 (82%)	87 (100%)	0	100	100

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	N	133/186 (72%)	132 (99%)	1 (1%)	79	85
5	H	266/272 (98%)	264 (99%)	2 (1%)	79	85
6	K	74/86 (86%)	73 (99%)	1 (1%)	62	76
7	Y	88/94 (94%)	88 (100%)	0	100	100
8	Z	112/115 (97%)	112 (100%)	0	100	100
9	V	48/53 (91%)	48 (100%)	0	100	100
10	W	30/53 (57%)	30 (100%)	0	100	100
11	S	92/118 (78%)	92 (100%)	0	100	100
12	i	52/66 (79%)	51 (98%)	1 (2%)	52	70
13	j	62/73 (85%)	62 (100%)	0	100	100
14	G	328/340 (96%)	325 (99%)	3 (1%)	75	84
15	C	576/625 (92%)	571 (99%)	5 (1%)	75	84
16	T	271/334 (81%)	269 (99%)	2 (1%)	81	88
17	F	168/179 (94%)	164 (98%)	4 (2%)	44	63
18	B	188/220 (86%)	188 (100%)	0	100	100
19	O	93/128 (73%)	93 (100%)	0	100	100
20	P	62/97 (64%)	62 (100%)	0	100	100
21	R	115/148 (78%)	114 (99%)	1 (1%)	75	84
22	U	104/133 (78%)	103 (99%)	1 (1%)	73	82
23	E	129/184 (70%)	122 (95%)	7 (5%)	18	46
24	D	157/191 (82%)	151 (96%)	6 (4%)	28	53
25	X	92/114 (81%)	92 (100%)	0	100	100
26	c	79/84 (94%)	78 (99%)	1 (1%)	65	77
27	Q	82/85 (96%)	81 (99%)	1 (1%)	67	79
28	k	73/112 (65%)	73 (100%)	0	100	100
30	n	21/84 (25%)	21 (100%)	0	100	100
31	o	171/211 (81%)	171 (100%)	0	100	100
32	p	181/228 (79%)	178 (98%)	3 (2%)	56	73
32	q	184/228 (81%)	182 (99%)	2 (1%)	70	80
33	M	421/434 (97%)	417 (99%)	4 (1%)	73	82
34	f	68/93 (73%)	67 (98%)	1 (2%)	60	75

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	g	42/96 (44%)	42 (100%)	0	100	100
37	a	504/568 (89%)	503 (100%)	1 (0%)	92	96
38	b	56/87 (64%)	56 (100%)	0	100	100
39	h	23/51 (45%)	22 (96%)	1 (4%)	25	50
43	m	63/90 (70%)	63 (100%)	0	100	100
44	t	24/60 (40%)	23 (96%)	1 (4%)	25	51
All	All	6067/7238 (84%)	6012 (99%)	55 (1%)	74	84

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	231	GLU
2	I	35	HIS
2	I	120	PHE
2	I	354	LEU
2	I	469	LEU
2	I	497	LEU
4	N	176	LYS
5	H	57	LYS
5	H	290	TYR
6	K	61	PHE
12	i	31	HIS
14	G	49	ARG
14	G	68	ASP
14	G	356	ARG
15	C	104	ARG
15	C	180	ASP
15	C	218	CYS
15	C	266	ASP
15	C	275	SER
16	T	79	PHE
16	T	147	ARG
17	F	19	VAL
17	F	42	LEU
17	F	43	CYS
17	F	47	LEU
21	R	138	LEU
22	U	119	GLU
23	E	89	PHE
23	E	93	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
23	E	130	THR
23	E	164	TYR
23	E	183	ILE
23	E	188	CYS
23	E	193	GLU
24	D	73	LEU
24	D	127	LYS
24	D	156	ASP
24	D	172	CYS
24	D	174	VAL
24	D	197	LYS
26	c	46	THR
27	Q	19	CYS
32	q	14	TRP
32	q	16	ARG
32	p	57	LYS
32	p	86	ARG
32	p	207	TYR
33	M	150	LEU
33	M	155	ILE
33	M	193	PHE
33	M	195	THR
34	f	77	TYR
37	a	511	PHE
39	h	25	THR
44	t	37	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (104) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	426	ASN
1	A	441	GLN
2	I	80	HIS
2	I	84	ASN
2	I	276	ASN
2	I	292	GLN
2	I	312	GLN
2	I	326	HIS
2	I	464	ASN
4	N	25	HIS
4	N	73	HIS
5	H	174	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
5	H	322	GLN
6	K	27	ASN
6	K	43	ASN
6	K	45	ASN
7	Y	45	ASN
7	Y	87	ASN
8	Z	63	GLN
8	Z	126	ASN
9	V	30	HIS
9	V	34	HIS
9	V	39	HIS
9	V	42	HIS
12	i	17	GLN
14	G	23	HIS
14	G	113	ASN
14	G	212	GLN
14	G	277	GLN
15	C	116	ASN
15	C	165	ASN
15	C	182	GLN
15	C	184	GLN
15	C	284	ASN
15	C	428	ASN
15	C	522	ASN
15	C	538	GLN
15	C	569	GLN
15	C	605	HIS
15	C	606	HIS
15	C	716	GLN
16	T	117	GLN
16	T	153	ASN
16	T	182	GLN
16	T	209	ASN
16	T	291	HIS
16	T	340	ASN
17	F	27	HIS
17	F	125	ASN
18	B	84	ASN
18	B	126	HIS
18	B	196	ASN
19	O	49	HIS
19	O	77	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
20	P	92	ASN
21	R	129	HIS
22	U	41	GLN
22	U	46	ASN
22	U	69	GLN
22	U	134	HIS
22	U	138	HIS
22	U	141	ASN
23	E	100	HIS
24	D	111	HIS
24	D	190	HIS
25	X	15	ASN
25	X	98	HIS
25	X	131	ASN
27	Q	35	ASN
27	Q	88	ASN
30	n	81	ASN
30	n	83	ASN
31	o	77	ASN
31	o	94	ASN
31	o	114	GLN
31	o	120	HIS
32	q	33	ASN
32	q	47	ASN
32	q	72	HIS
32	q	90	ASN
32	q	184	ASN
32	q	206	ASN
32	q	209	ASN
32	q	218	ASN
32	q	223	ASN
32	p	99	ASN
32	p	130	HIS
32	p	160	HIS
32	p	214	HIS
32	p	223	ASN
33	M	67	GLN
33	M	201	GLN
33	M	241	HIS
33	M	301	GLN
33	M	317	ASN
33	M	491	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
34	f	36	HIS
34	f	66	HIS
37	a	135	GLN
37	a	171	ASN
37	a	417	ASN
37	a	495	ASN
37	a	541	GLN
38	b	56	HIS

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 2 are monoatomic - leaving 18 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	SF4	D	301	24	0,12,12	-	-	-		
45	SF4	C	802	15	0,12,12	-	-	-		
48	CDL	I	503	-	97,97,99	0.27	0	103,109,111	0.34	0
51	FES	C	803	15	0,4,4	-	-	-		
52	NDP	T	501	-	45,52,52	0.62	0	53,80,80	0.83	2 (3%)
45	SF4	C	801	15	0,12,12	-	-	-		



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
45	SF4	A	501	1	0,12,12	-	-	-		
45	SF4	D	302	24	0,12,12	-	-	-		
47	T7X	I	501	-	54,54,61	0.28	0	64,66,73	0.77	3 (4%)
50	PEV	H	502	-	48,48,48	0.38	0	51,53,53	0.39	0
49	U10	H	501	-	44,44,63	0.72	2 (4%)	53,56,79	0.57	0
45	SF4	E	301	23	0,12,12	-	-	-		
47	T7X	p	301	-	61,61,61	0.26	0	71,73,73	0.39	0
54	BCT	q	802	53	2,3,3	0.60	0	2,3,3	0.26	0
51	FES	B	301	-	0,4,4	-	-	-		
48	CDL	J	401	-	86,86,99	0.31	0	92,98,111	0.52	1 (1%)
46	FMN	A	502	-	33,33,33	0.62	0	48,50,50	0.72	1 (2%)
48	CDL	I	502	-	99,99,99	0.27	0	105,111,111	0.43	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CDL	I	503	-	-	32/108/108/110	-
52	NDP	T	501	-	-	6/30/77/77	0/5/5/5
45	SF4	C	802	15	-	-	0/6/5/5
45	SF4	D	301	24	-	-	0/6/5/5
51	FES	C	803	15	-	-	0/1/1/1
45	SF4	C	801	15	-	-	0/6/5/5
45	SF4	A	501	1	-	-	0/6/5/5
47	T7X	I	501	-	1/1/10/18	16/49/73/80	0/1/1/1
45	SF4	D	302	24	-	-	0/6/5/5
50	PEV	H	502	-	-	25/52/52/52	-
49	U10	H	501	-	-	18/41/65/87	0/1/1/1
47	T7X	p	301	-	-	16/56/80/80	0/1/1/1
45	SF4	E	301	23	-	-	0/6/5/5
51	FES	B	301	-	-	-	0/1/1/1
48	CDL	J	401	-	-	33/97/97/110	-
46	FMN	A	502	-	-	6/18/18/18	0/3/3/3
48	CDL	I	502	-	-	33/110/110/110	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	H	501	U10	C4-C5	-2.41	1.41	1.48
49	H	501	U10	C3-C2	-2.38	1.42	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	I	501	T7X	C4-C3-C2	3.29	116.58	110.82
48	J	401	CDL	OA6-CA4-CA6	2.84	118.69	108.40
47	I	501	T7X	O3-C3-C4	2.55	116.24	110.35
47	I	501	T7X	O3-C3-C2	2.41	115.92	110.35
52	T	501	NDP	O4D-C1D-C2D	-2.39	101.42	106.64
52	T	501	NDP	C5A-C6A-N6A	2.31	123.87	120.35
46	A	502	FMN	C4-N3-C2	-2.09	121.78	125.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
47	I	501	T7X	C3

All (185) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	502	FMN	N10-C1'-C2'-C3'
46	A	502	FMN	O3'-C3'-C4'-C5'
47	I	501	T7X	C2-C1-O1-P1
47	I	501	T7X	C6-C1-O1-P1
47	I	501	T7X	C8-C7-O13-P1
47	I	501	T7X	C12-C10-O16-C8
47	I	501	T7X	O17-C10-O16-C8
48	I	502	CDL	CA2-OA2-PA1-OA3
48	I	502	CDL	OA7-CA5-OA6-CA4
48	I	502	CDL	C11-CA5-OA6-CA4
48	I	502	CDL	CB3-OB5-PB2-OB3
48	I	502	CDL	CB4-CB3-OB5-PB2
48	I	503	CDL	C1-CA2-OA2-PA1
48	I	503	CDL	CA2-OA2-PA1-OA3
48	I	503	CDL	OB9-CB7-OB8-CB6
48	I	503	CDL	C71-CB7-OB8-CB6
48	J	401	CDL	OA7-CA5-OA6-CA4
48	J	401	CDL	C1-CB2-OB2-PB2
48	J	401	CDL	CB3-OB5-PB2-OB2
48	J	401	CDL	CB4-CB3-OB5-PB2
49	H	501	U10	C12-C11-C9-C10

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
49	H	501	U10	C17-C18-C19-C20
49	H	501	U10	C17-C18-C19-C21
49	H	501	U10	C21-C22-C23-C24
49	H	501	U10	C26-C27-C28-C29
49	H	501	U10	C35-C34-C36-C37
50	H	502	PEV	C1-O3P-P-O1P
50	H	502	PEV	C1-O3P-P-O4P
50	H	502	PEV	C4-O4P-P-O1P
50	H	502	PEV	C5-C4-O4P-P
48	J	401	CDL	C11-CA5-OA6-CA4
49	H	501	U10	C12-C11-C9-C8
48	I	502	CDL	O1-C1-CA2-OA2
49	H	501	U10	C14-C16-C17-C18
49	H	501	U10	C24-C26-C27-C28
46	A	502	FMN	C2'-C3'-C4'-C5'
50	H	502	PEV	C16-C17-C18-C19
50	H	502	PEV	C11-C12-C13-C14
46	A	502	FMN	O3'-C3'-C4'-O4'
46	A	502	FMN	C2'-C3'-C4'-O4'
49	H	501	U10	C4-C3-O3-C3M
48	I	502	CDL	CA2-OA2-PA1-OA5
48	I	502	CDL	CA7-C31-C32-C33
52	T	501	NDP	C2D-C1D-N1N-C6N
48	I	502	CDL	C79-C80-C81-C82
47	p	301	T7X	C12-C10-O16-C8
50	H	502	PEV	C22-C23-C24-C25
49	H	501	U10	C3-C4-O4-C4M
48	I	503	CDL	C34-C35-C36-C37
47	p	301	T7X	O17-C10-O16-C8
48	J	401	CDL	C35-C36-C37-C38
48	I	503	CDL	CB2-OB2-PB2-OB5
52	T	501	NDP	C2D-C1D-N1N-C2N
48	I	503	CDL	C1-CB2-OB2-PB2
48	I	502	CDL	CA5-C11-C12-C13
49	H	501	U10	C7-C8-C9-C11
50	H	502	PEV	C23-C24-C25-C26
50	H	502	PEV	C35-C36-C37-C38
47	I	501	T7X	C39-C40-C41-C42
48	J	401	CDL	CA6-CA4-OA6-CA5
48	I	503	CDL	C36-C37-C38-C39
48	I	502	CDL	C77-C78-C79-C80
48	I	503	CDL	OB6-CB4-CB6-OB8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	I	503	CDL	C53-C54-C55-C56
48	J	401	CDL	C19-C20-C21-C22
48	I	502	CDL	CB2-C1-CA2-OA2
48	J	401	CDL	C17-C18-C19-C20
50	H	502	PEV	O3P-C1-C2-C3
48	J	401	CDL	C51-C52-C53-C54
47	p	301	T7X	C31-C11-O18-C9
48	I	502	CDL	C1-CA2-OA2-PA1
48	J	401	CDL	CA4-CA3-OA5-PA1
48	I	502	CDL	C15-C16-C17-C18
48	I	503	CDL	CB3-CB4-CB6-OB8
47	I	501	T7X	C15-C16-C17-C18
47	I	501	T7X	C18-C19-C20-C21
47	p	301	T7X	C19-C20-C21-C22
47	p	301	T7X	C22-C23-C24-C25
50	H	502	PEV	O3P-C1-C2-O2
50	H	502	PEV	C2-C1-O3P-P
48	I	502	CDL	C75-C76-C77-C78
48	I	502	CDL	C18-C19-C20-C21
48	J	401	CDL	OA5-CA3-CA4-CA6
48	I	503	CDL	C73-C74-C75-C76
48	J	401	CDL	C21-C22-C23-C24
47	I	501	T7X	C7-C8-C9-O18
48	J	401	CDL	OA5-CA3-CA4-OA6
47	I	501	T7X	O16-C8-C9-O18
48	I	503	CDL	C80-C81-C82-C83
48	J	401	CDL	C51-CB5-OB6-CB4
48	I	503	CDL	C20-C21-C22-C23
48	J	401	CDL	C72-C73-C74-C75
48	I	503	CDL	C57-C58-C59-C60
48	I	503	CDL	CB5-C51-C52-C53
48	I	502	CDL	CA2-OA2-PA1-OA4
48	J	401	CDL	CB3-OB5-PB2-OB4
48	J	401	CDL	C53-C54-C55-C56
49	H	501	U10	C25-C24-C26-C27
48	J	401	CDL	CB7-C71-C72-C73
52	T	501	NDP	O4D-C1D-N1N-C6N
48	I	502	CDL	C33-C34-C35-C36
48	I	503	CDL	C72-C73-C74-C75
48	I	503	CDL	C31-CA7-OA8-CA6
47	p	301	T7X	O19-C11-O18-C9
46	A	502	FMN	C5'-O5'-P-O1P

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
48	I	503	CDL	CA4-CA6-OA8-CA7
47	I	501	T7X	C7-O13-P1-O1
48	I	502	CDL	CB3-OB5-PB2-OB2
48	I	503	CDL	CA2-OA2-PA1-OA5
48	I	503	CDL	CB3-OB5-PB2-OB2
48	J	401	CDL	CA2-OA2-PA1-OA5
50	H	502	PEV	C36-C37-C38-C39
48	J	401	CDL	C16-C17-C18-C19
47	p	301	T7X	C24-C25-C26-C27
48	I	502	CDL	C59-C60-C61-C62
48	J	401	CDL	C31-C32-C33-C34
48	I	503	CDL	C17-C18-C19-C20
48	I	502	CDL	CA2-C1-CB2-OB2
48	I	503	CDL	C16-C17-C18-C19
47	p	301	T7X	C13-C14-C15-C16
50	H	502	PEV	C33-C34-C35-C36
48	I	503	CDL	OA9-CA7-OA8-CA6
50	H	502	PEV	O2-C2-C3-O3
50	H	502	PEV	C13-C14-C15-C16
49	H	501	U10	C23-C24-C26-C27
48	I	502	CDL	C11-C12-C13-C14
48	I	502	CDL	CB3-CB4-CB6-OB8
48	J	401	CDL	OB7-CB5-OB6-CB4
49	H	501	U10	C7-C8-C9-C10
47	p	301	T7X	C36-C37-C38-C39
48	J	401	CDL	C33-C34-C35-C36
47	p	301	T7X	C1-O1-P1-O12
47	p	301	T7X	C37-C38-C39-C40
48	J	401	CDL	C34-C35-C36-C37
48	J	401	CDL	CB6-CB4-OB6-CB5
50	H	502	PEV	C3-C2-O2-C31
47	p	301	T7X	C43-C44-C45-C46
47	I	501	T7X	C21-C22-C23-C24
52	T	501	NDP	O4D-C1D-N1N-C2N
48	J	401	CDL	C58-C59-C60-C61
50	H	502	PEV	C41-C42-C43-C44
52	T	501	NDP	PN-O3-PA-O1A
48	I	502	CDL	C57-C58-C59-C60
48	I	503	CDL	C75-C76-C77-C78
48	J	401	CDL	C75-C76-C77-C78
50	H	502	PEV	C21-C22-C23-C24
48	I	502	CDL	C31-CA7-OA8-CA6

*Continued on next page...*

*Continued from previous page...*

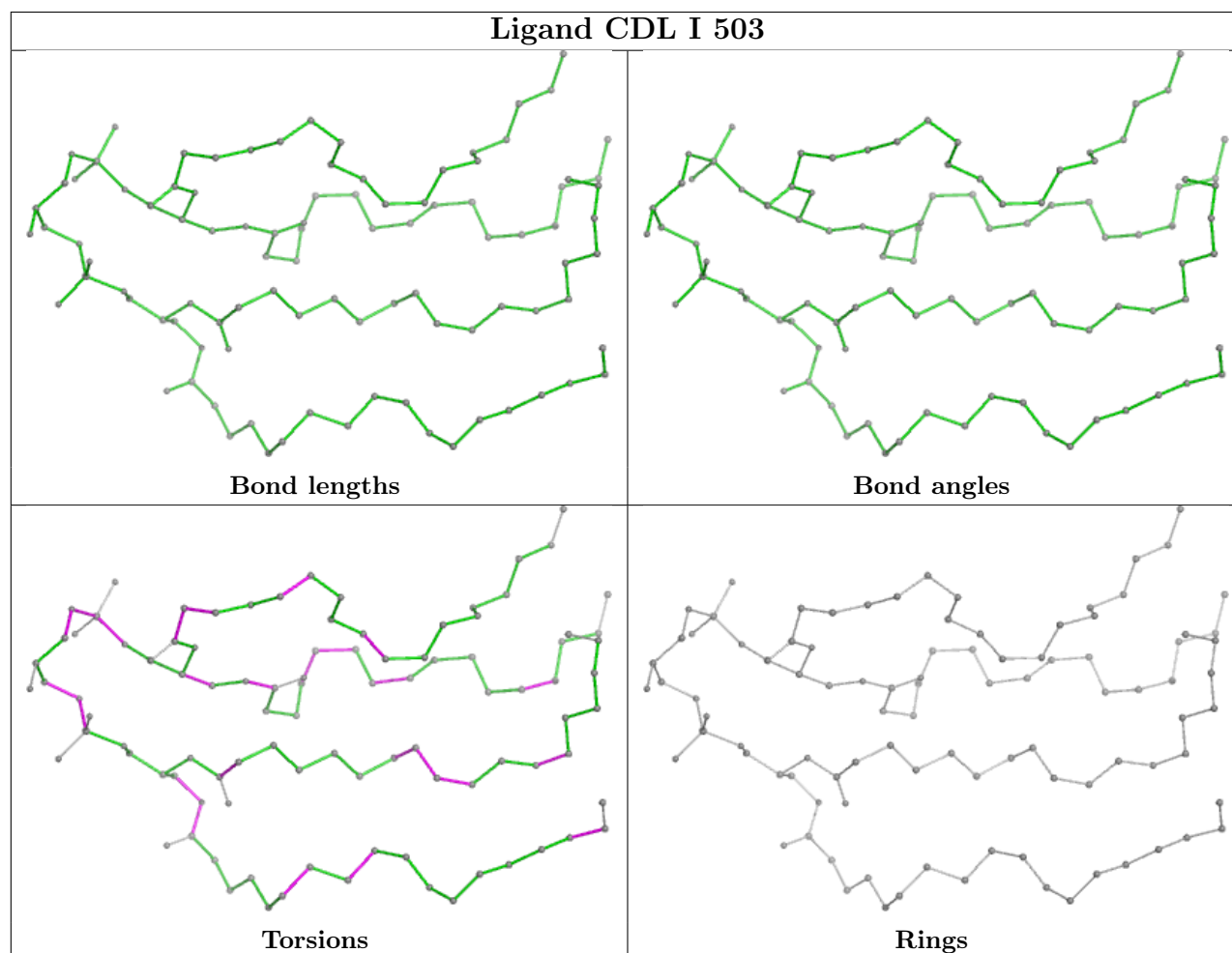
Mol	Chain	Res	Type	Atoms
50	H	502	PEV	C14-C15-C16-C17
48	J	401	CDL	C31-CA7-OA8-CA6
48	J	401	CDL	C24-C25-C26-C27
50	H	502	PEV	C4-O4P-P-O3P
48	J	401	CDL	C52-C53-C54-C55
48	I	502	CDL	C78-C79-C80-C81
48	I	503	CDL	C44-C45-C46-C47
48	I	502	CDL	C20-C21-C22-C23
48	I	503	CDL	C15-C16-C17-C18
52	T	501	NDP	O4D-C4D-C5D-O5D
48	I	502	CDL	C51-CB5-OB6-CB4
48	I	502	CDL	C32-C33-C34-C35
48	I	502	CDL	C73-C74-C75-C76
48	J	401	CDL	C32-C31-CA7-OA8
47	p	301	T7X	C32-C33-C34-C35
47	p	301	T7X	C1-O1-P1-O13
49	H	501	U10	C16-C17-C18-C19
47	I	501	T7X	C31-C11-O18-C9
48	I	502	CDL	OB7-CB5-OB6-CB4
47	I	501	T7X	C38-C39-C40-C41
48	I	503	CDL	CB2-OB2-PB2-OB3
48	I	503	CDL	CB3-OB5-PB2-OB3
48	I	502	CDL	C51-C52-C53-C54
49	H	501	U10	C33-C34-C36-C37
50	H	502	PEV	C1-C2-O2-C31
47	I	501	T7X	O18-C11-C31-C32
49	H	501	U10	C27-C28-C29-C30
47	p	301	T7X	C34-C35-C36-C37
48	I	502	CDL	C36-C37-C38-C39
48	I	503	CDL	C52-C51-CB5-OB6
48	I	503	CDL	C12-C11-CA5-OA7
48	I	503	CDL	C12-C11-CA5-OA6
48	J	401	CDL	C32-C31-CA7-OA9
50	H	502	PEV	C12-C13-C14-C15
47	I	501	T7X	O19-C11-C31-C32
50	H	502	PEV	C37-C38-C39-C40
47	p	301	T7X	C42-C43-C44-C45
50	H	502	PEV	O2-C31-C32-C33

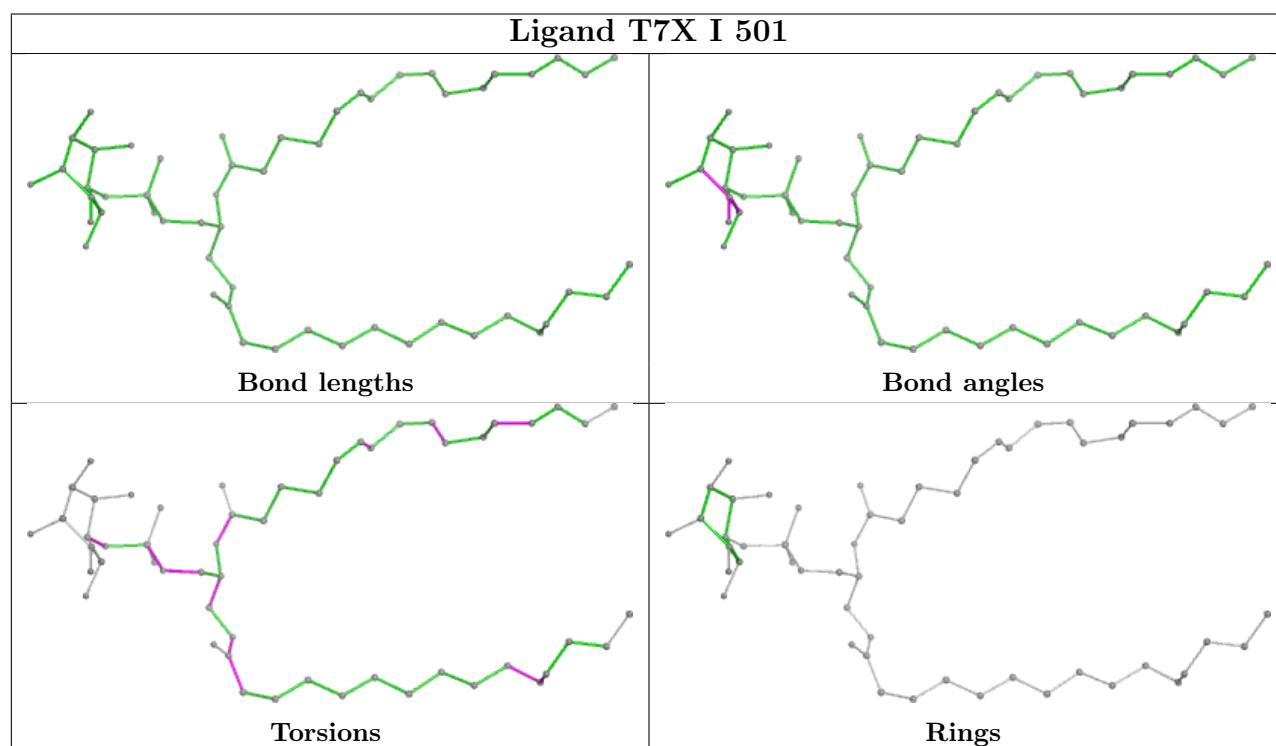
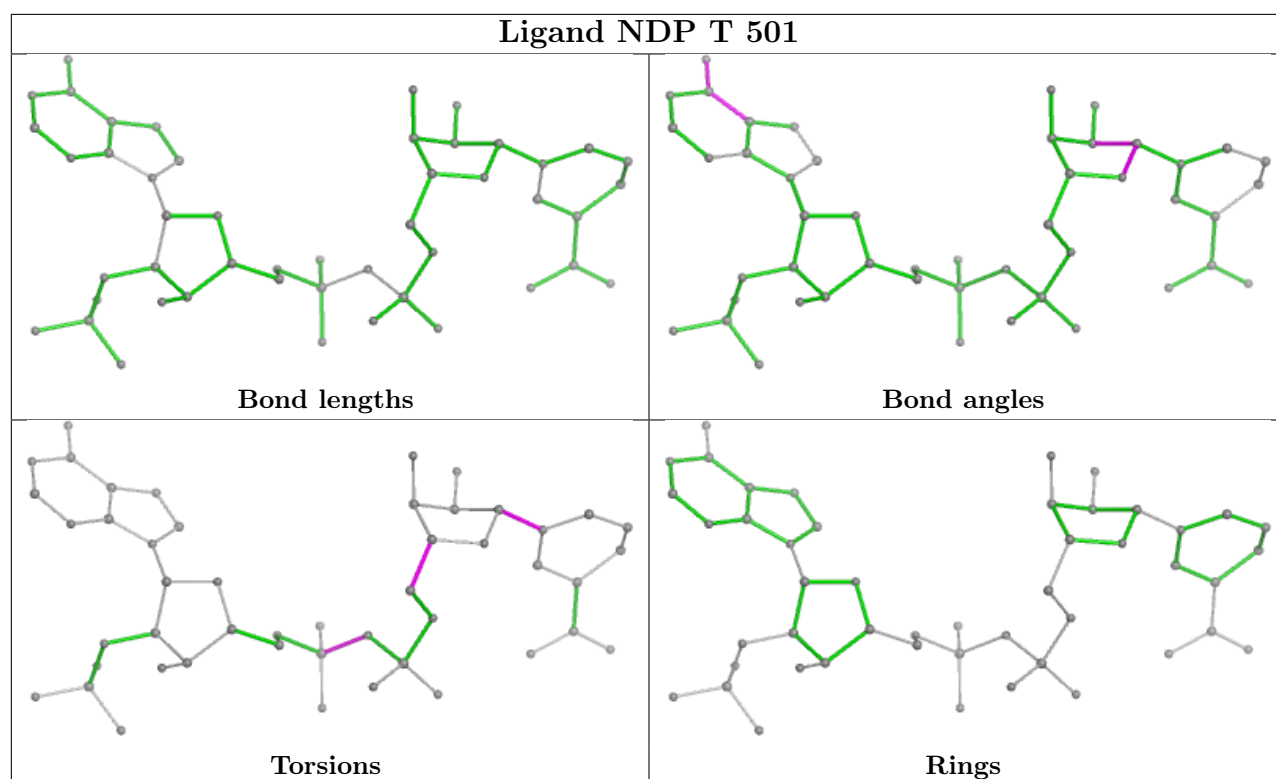
There are no ring outliers.

No monomer is involved in short contacts.

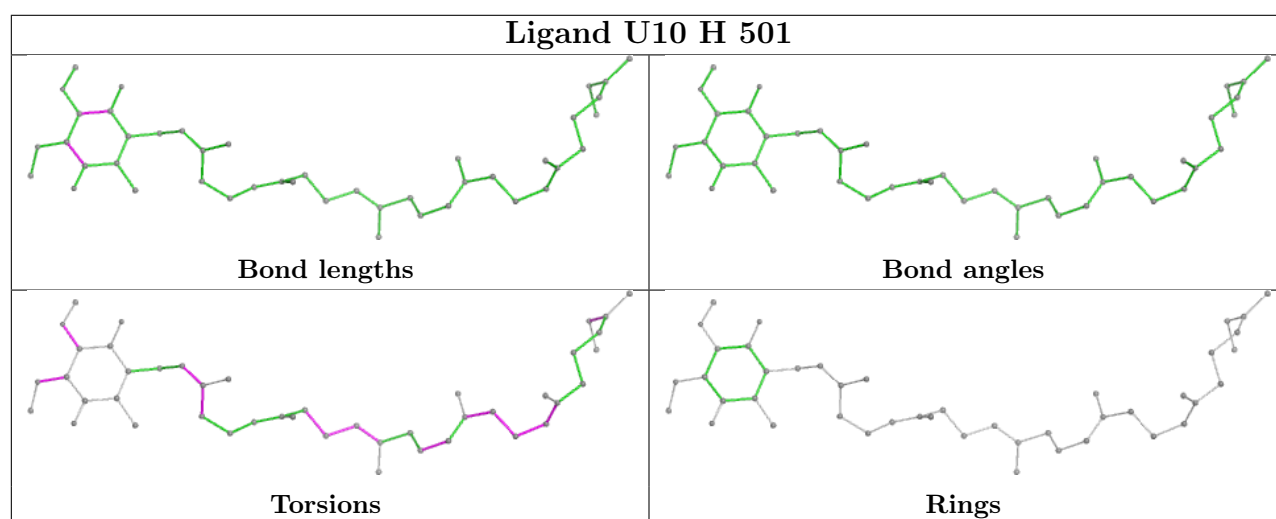
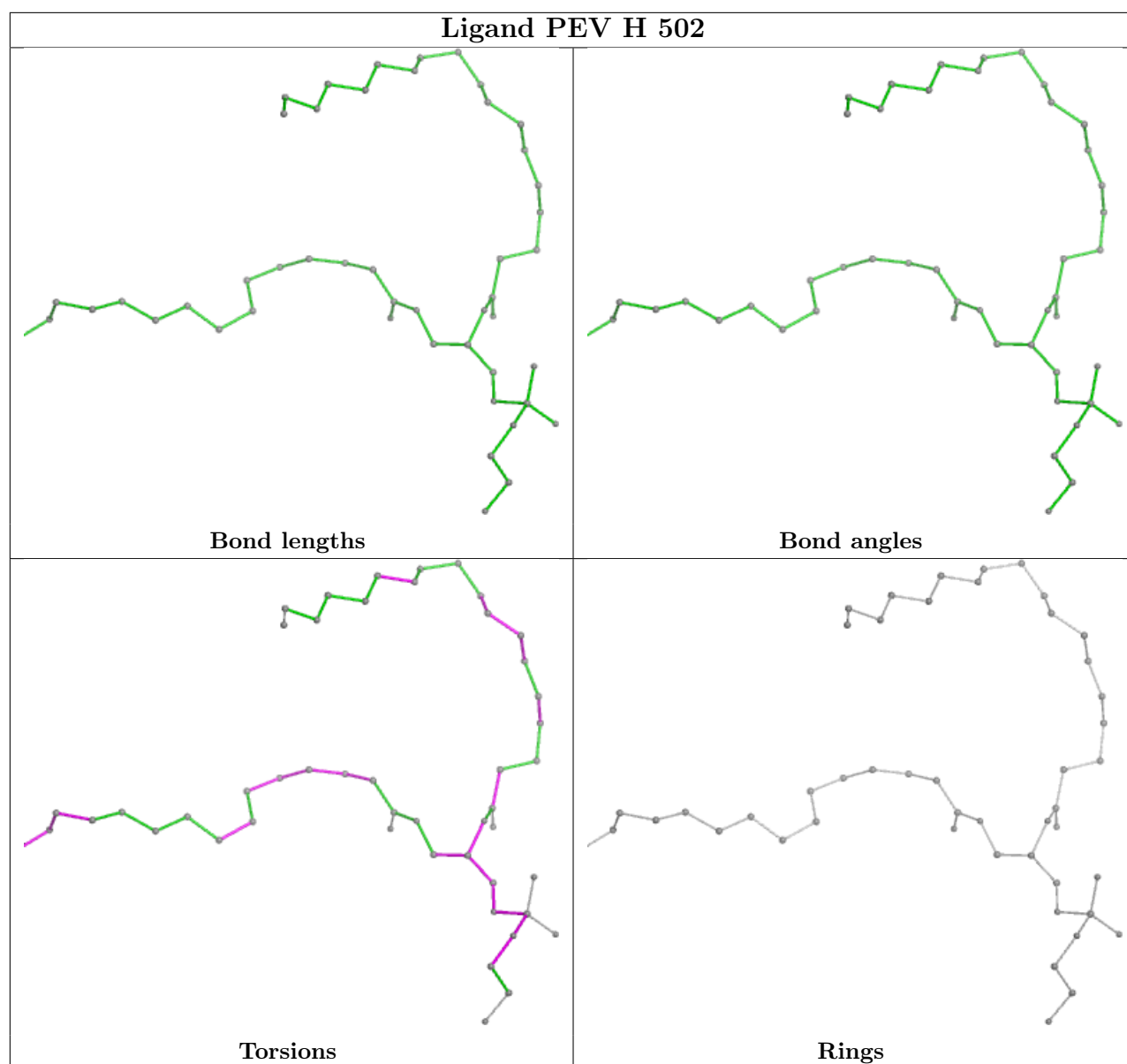
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

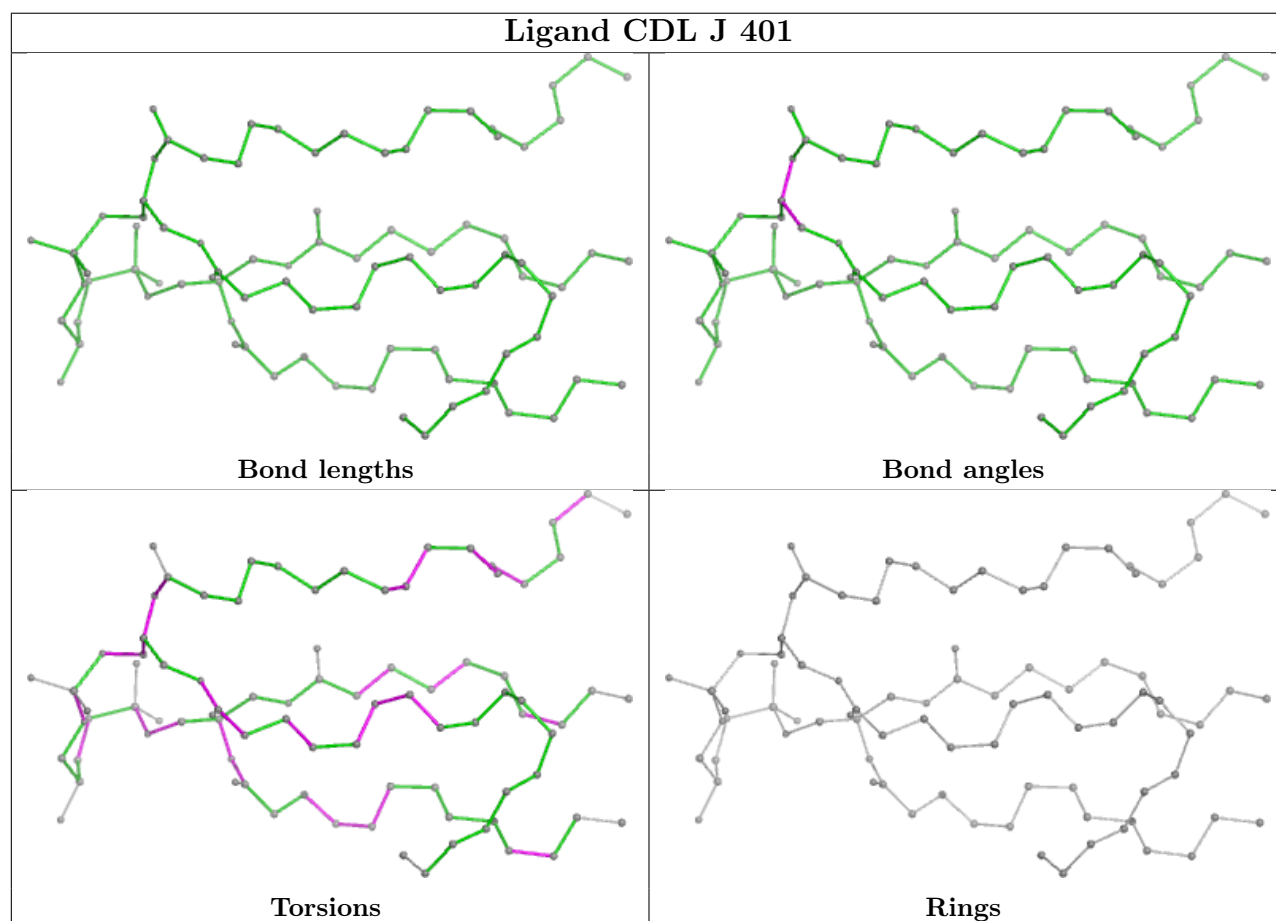
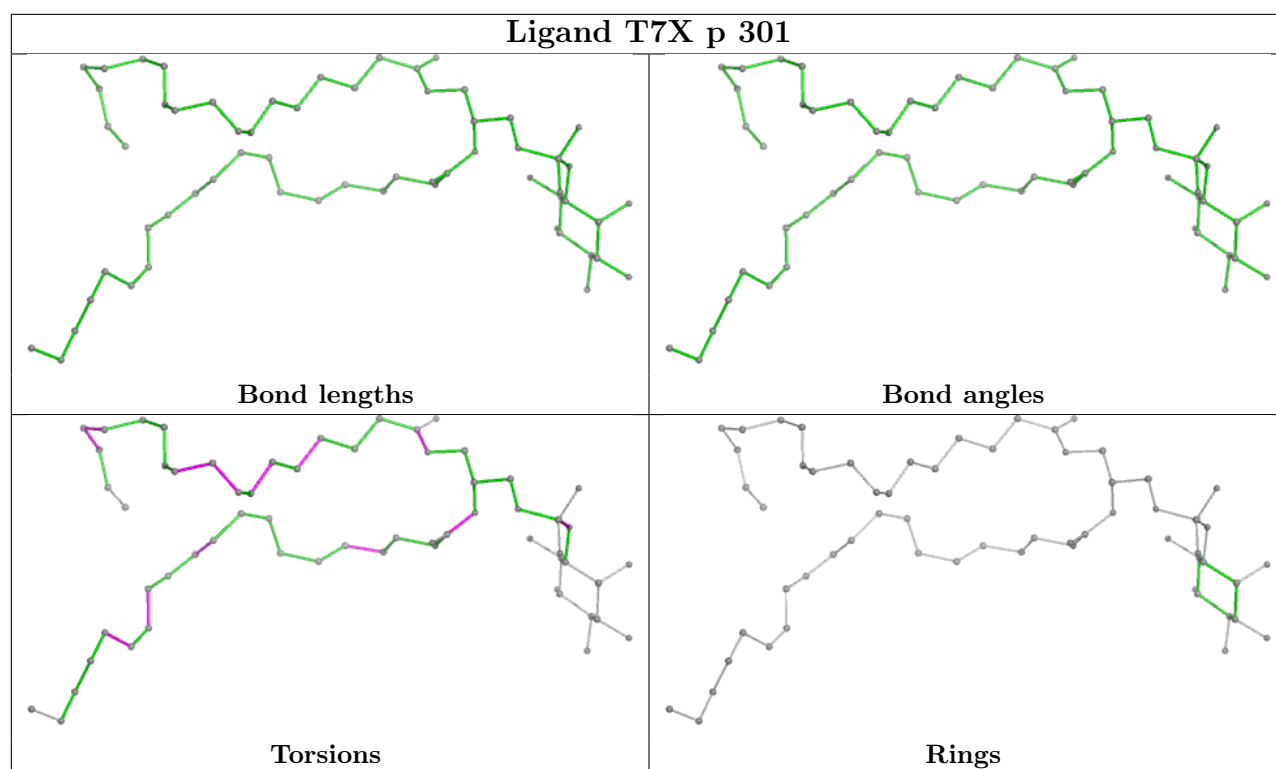
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

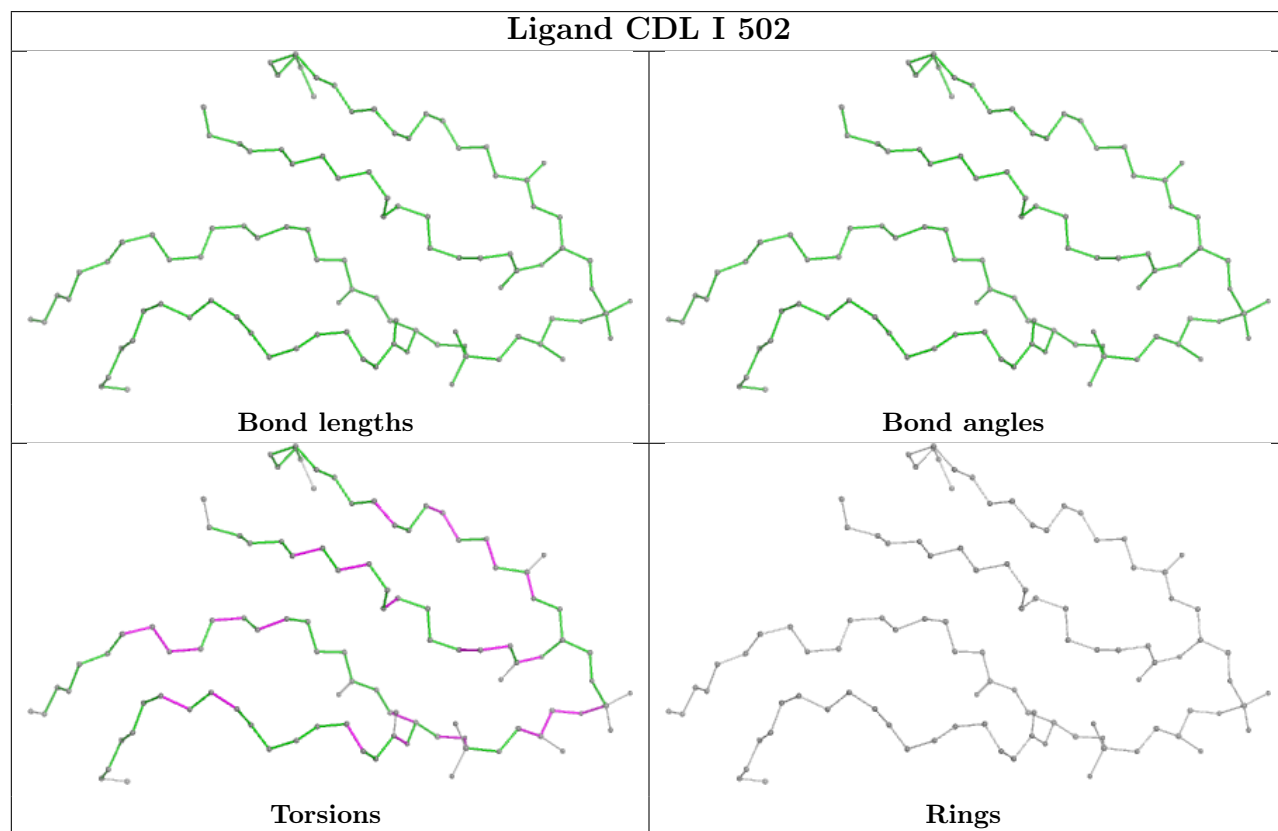
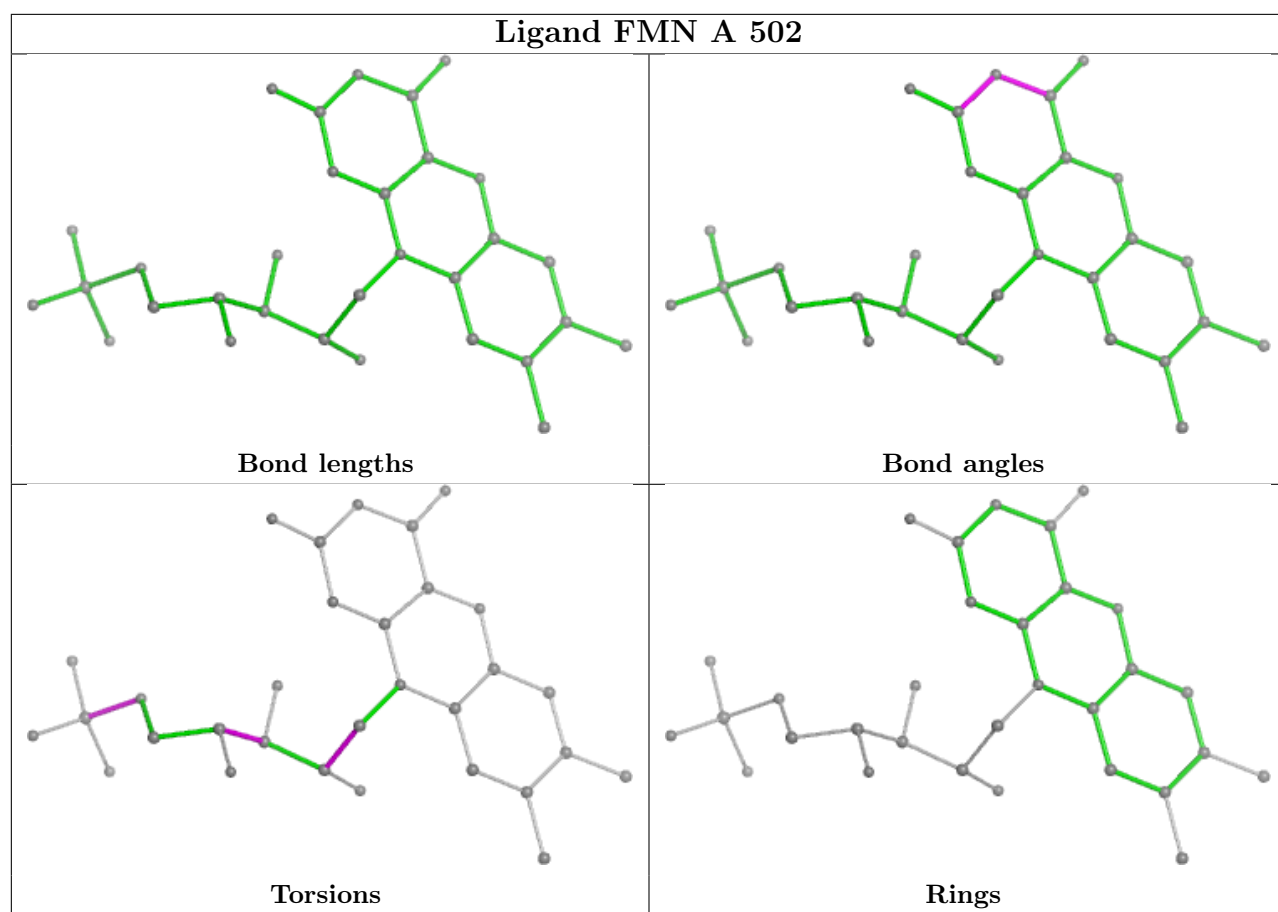












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

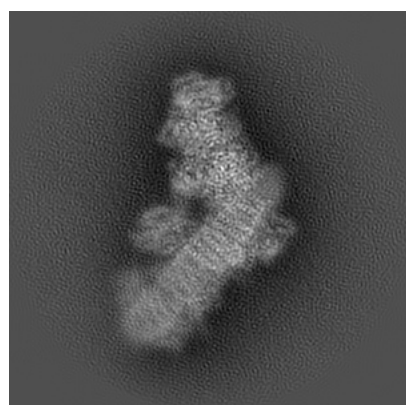
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11614. These allow visual inspection of the internal detail of the map and identification of artifacts.

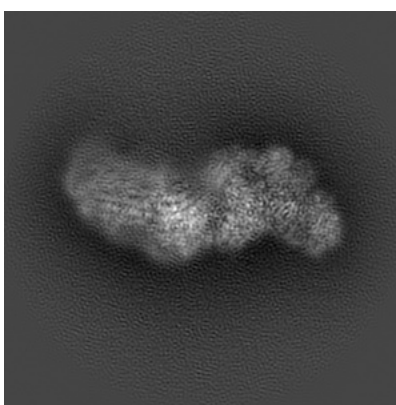
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

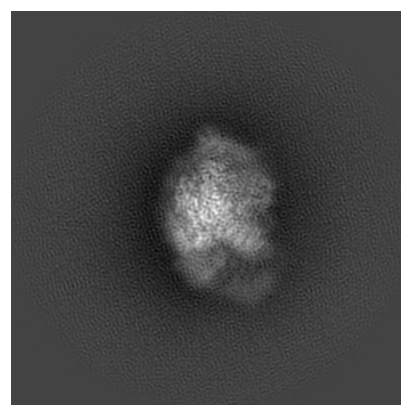
#### 6.1.1 Primary map



X



Y

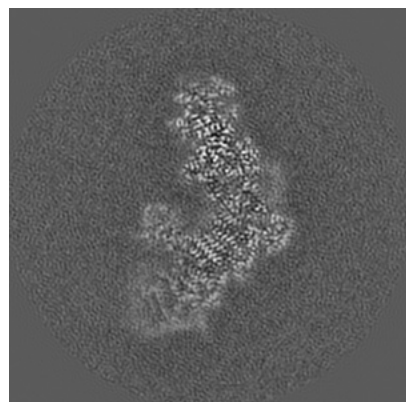


Z

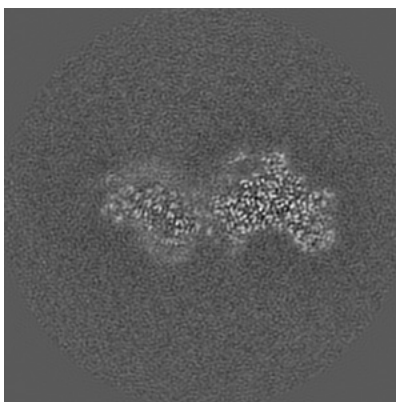
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

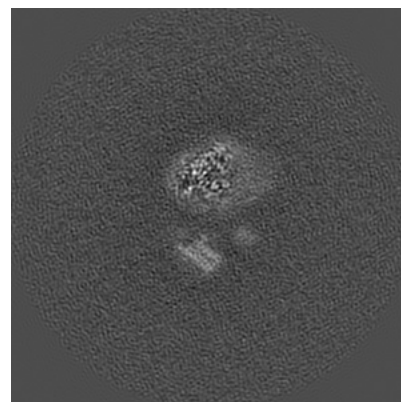
#### 6.2.1 Primary map



X Index: 180



Y Index: 180

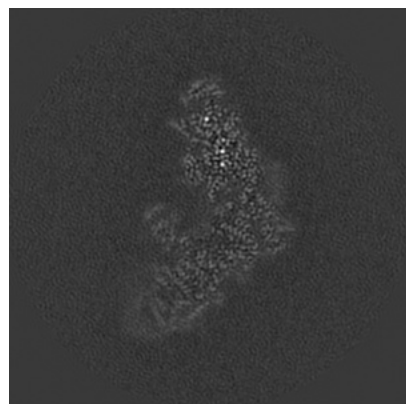


Z Index: 180

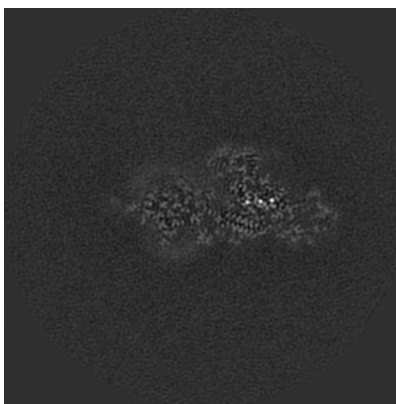
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

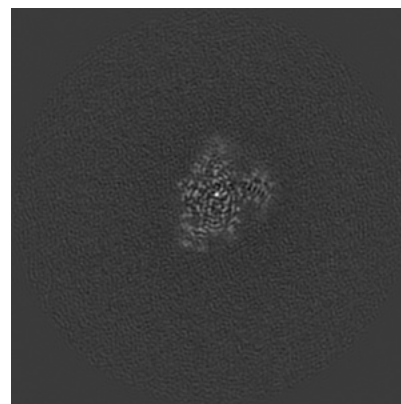
### 6.3.1 Primary map



X Index: 185



Y Index: 192

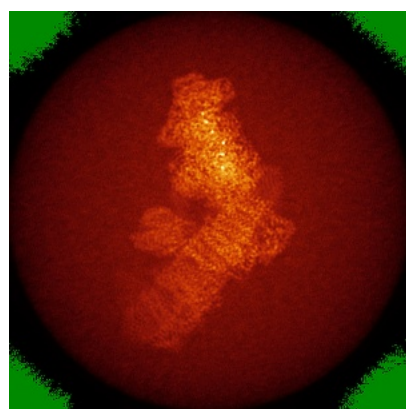


Z Index: 218

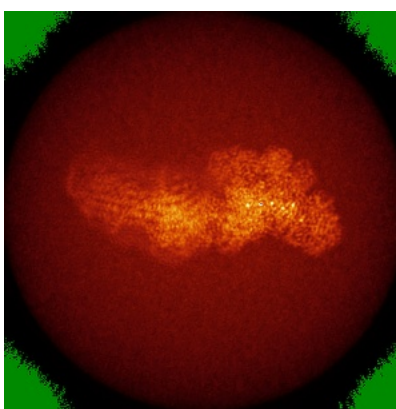
The images above show the largest variance slices of the map in three orthogonal directions.

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

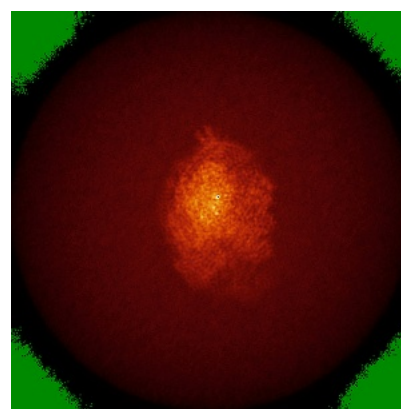
### 6.4.1 Primary map



X



Y

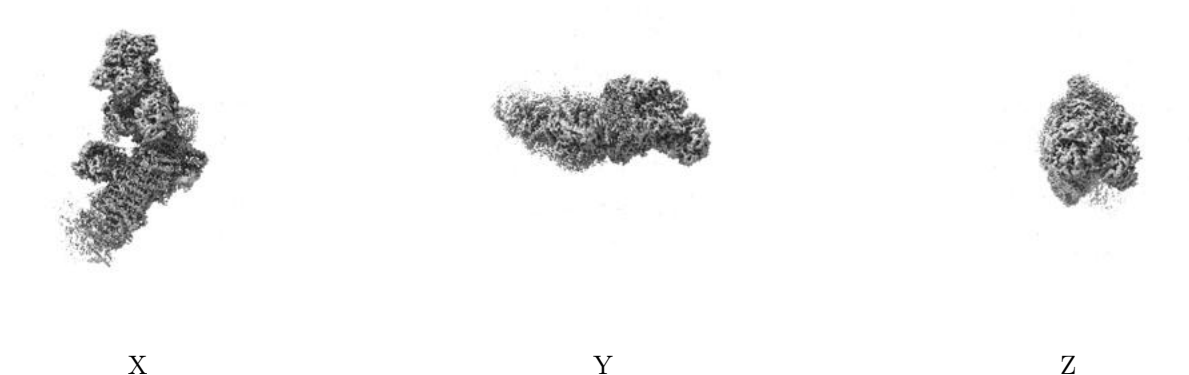


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0235. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

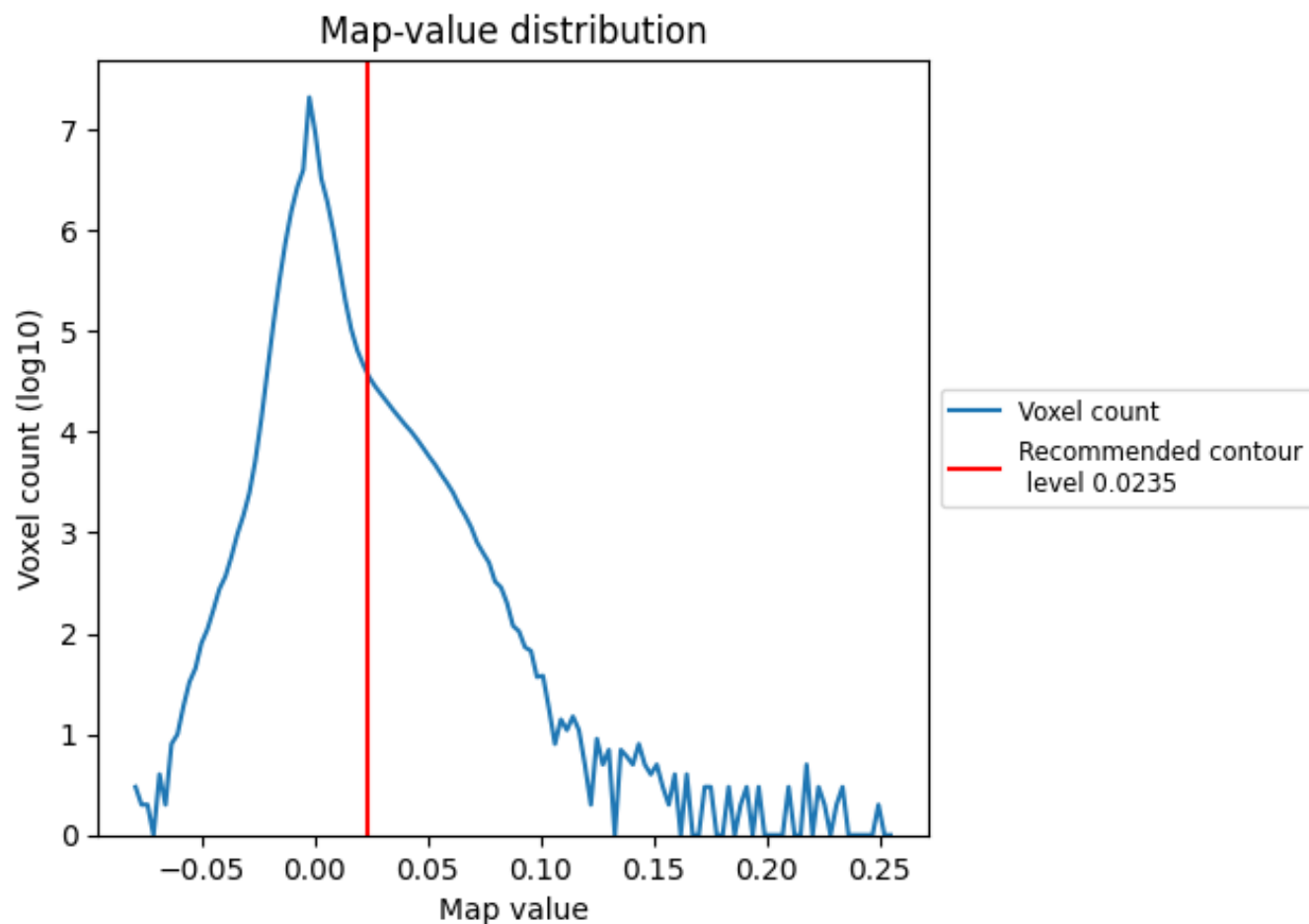
## 6.6 Mask visualisation [i](#)

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.

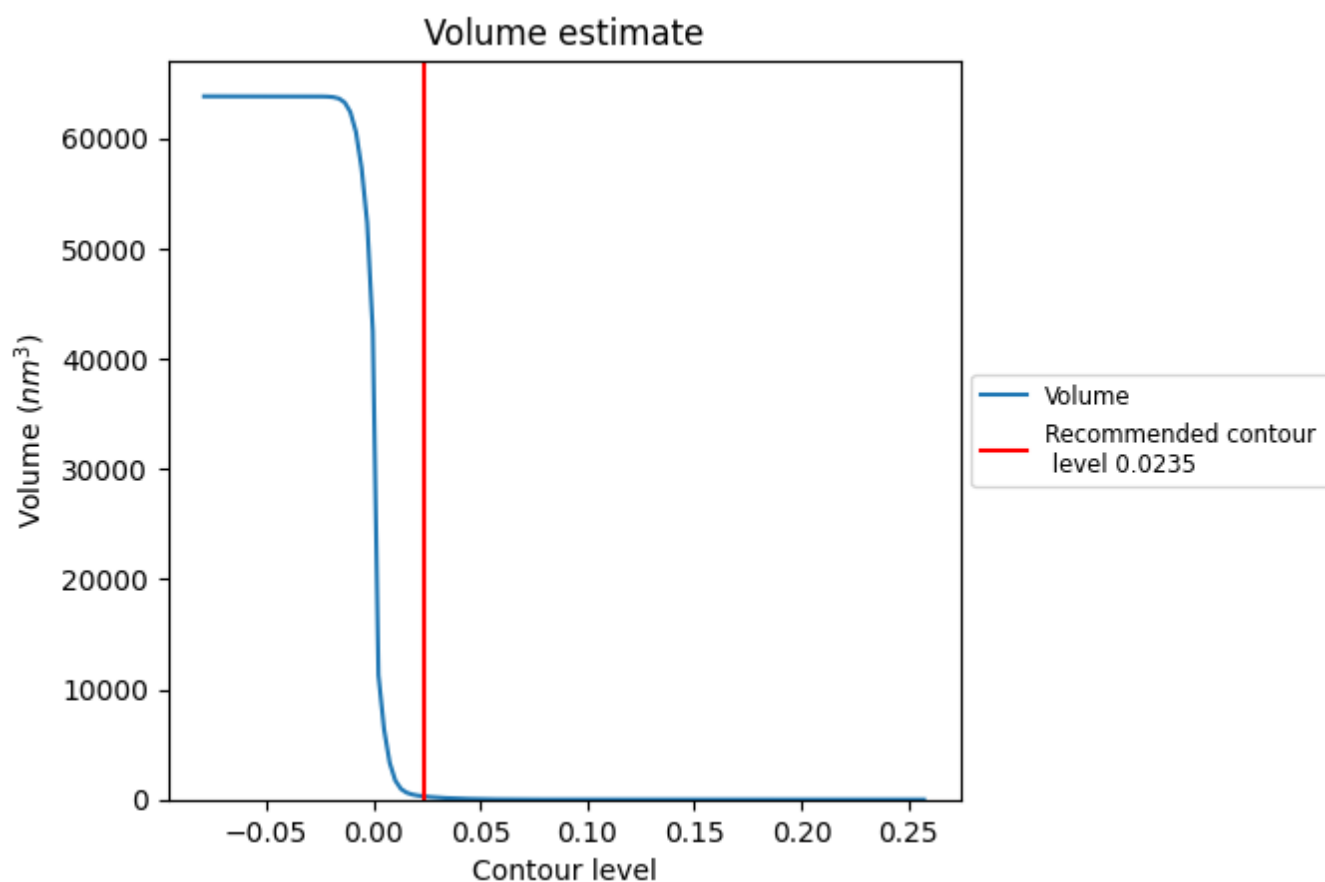
### 7.1 Map-value distribution [i](#)



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.



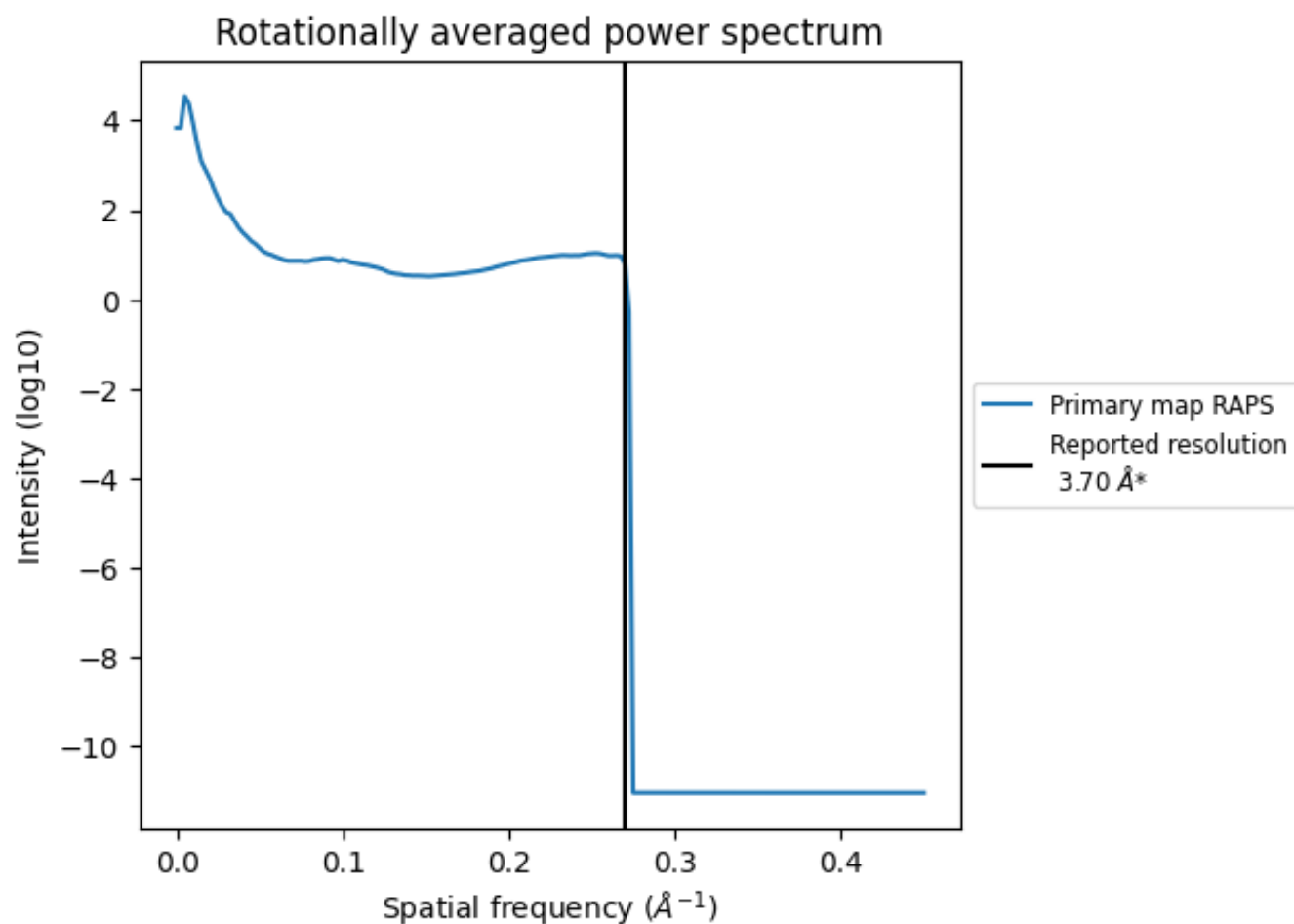
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 289  $\text{nm}^3$ ; this corresponds to an approximate mass of 261 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 0.270 Å<sup>-1</sup>

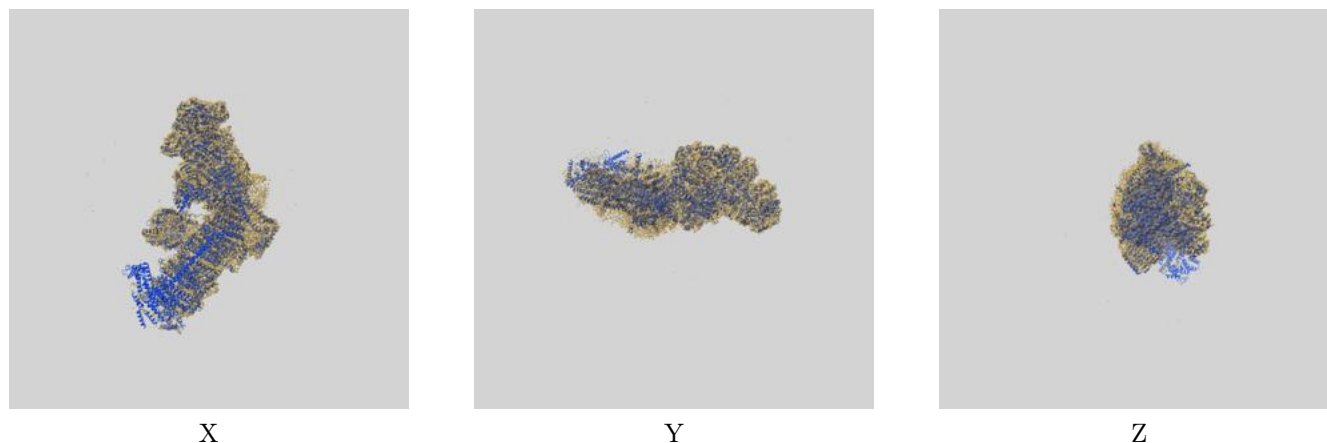
## 8 Fourier-Shell correlation ⓘ

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

## 9 Map-model fit [i](#)

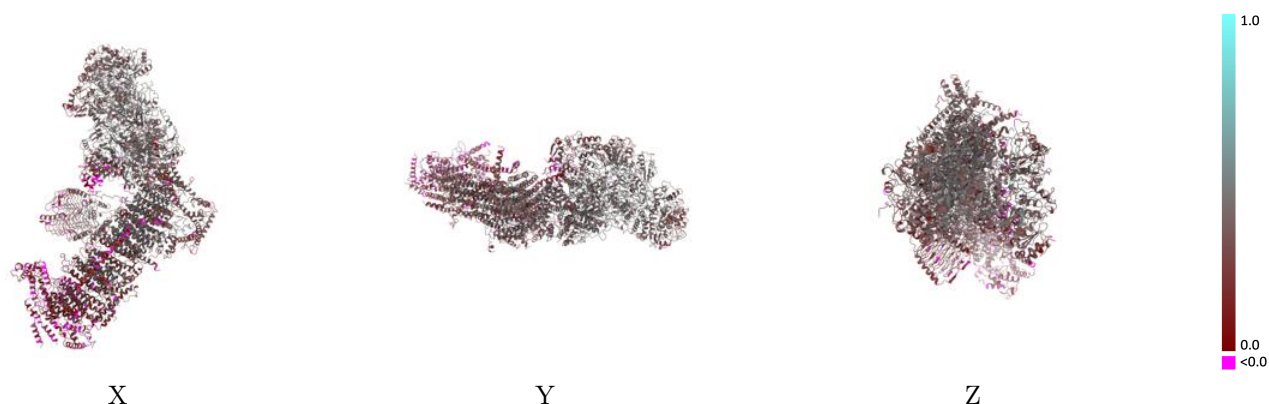
This section contains information regarding the fit between EMDB map EMD-11614 and PDB model 7A23. Per-residue inclusion information can be found in [section 3](#) on [page 18](#).

### 9.1 Map-model overlay [i](#)



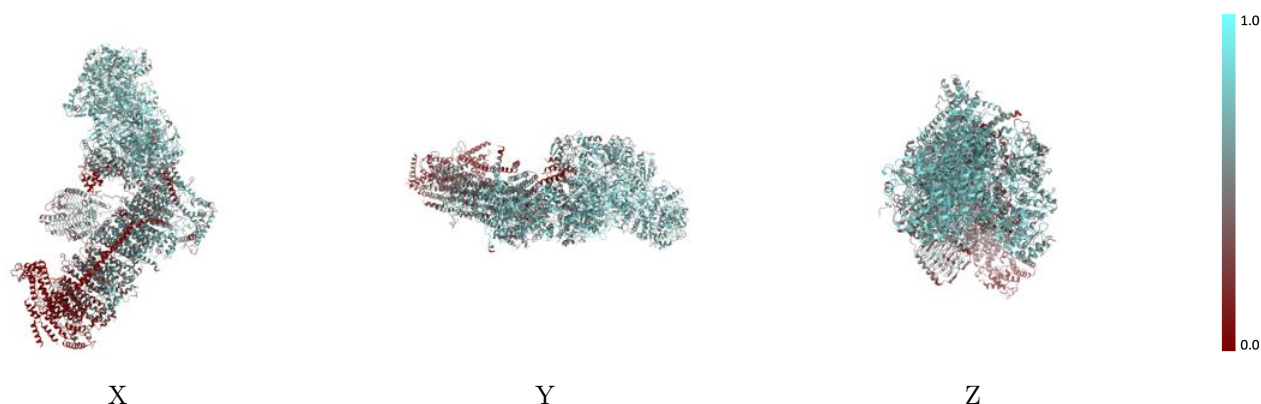
The images above show the 3D surface view of the map at the recommended contour level 0.0235 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



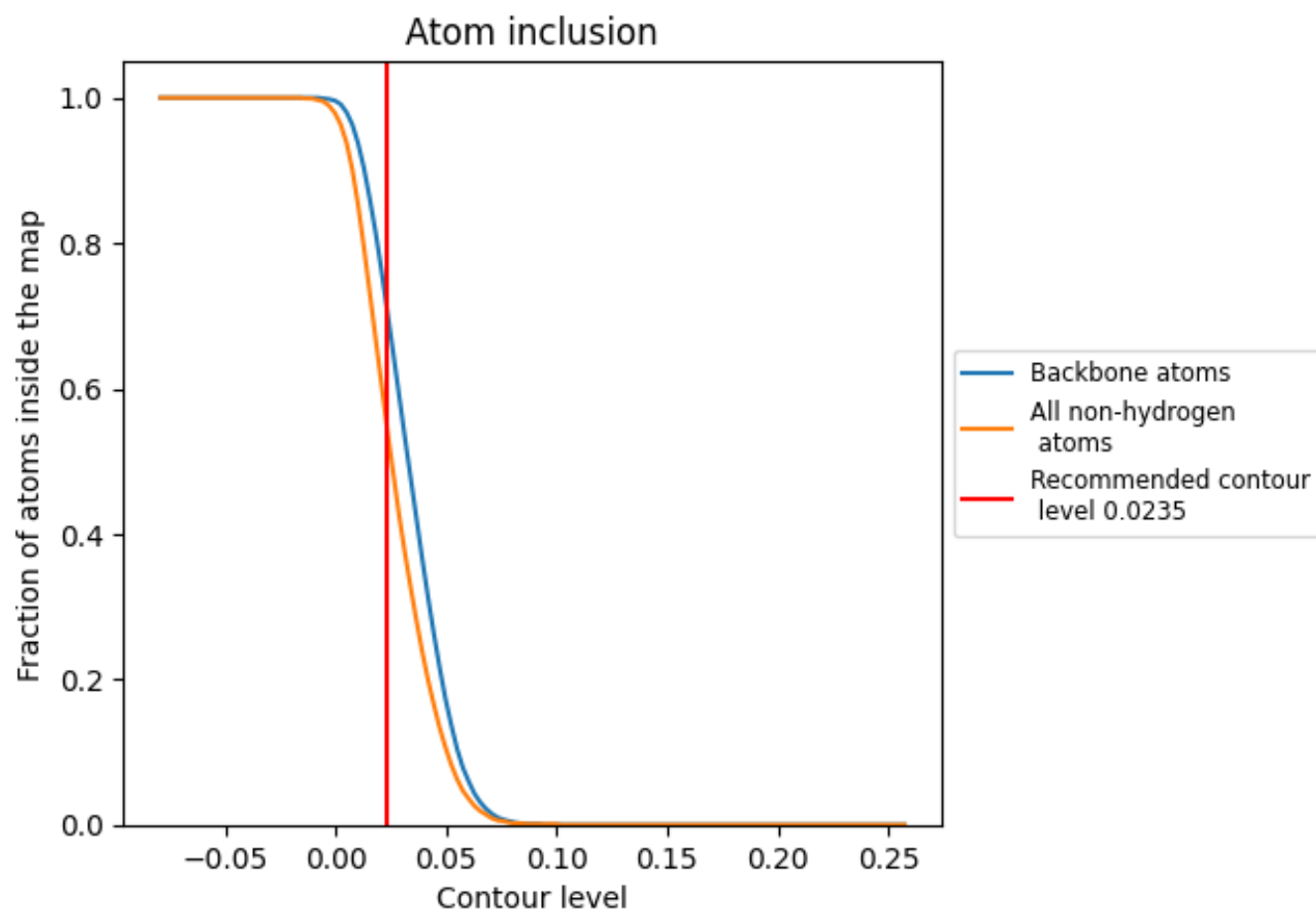
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0235).







































































## 9.4 Atom inclusion ⓘ



At the recommended contour level, 70% of all backbone atoms, 54% 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 (0.0235) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5400	 0.3380
A	 0.6630	 0.3770
B	 0.6470	 0.3780
C	 0.6700	 0.4080
D	 0.7190	 0.4150
E	 0.7260	 0.4370
F	 0.7080	 0.4270
G	 0.7300	 0.4520
H	 0.5850	 0.3950
I	 0.5690	 0.3810
J	 0.4370	 0.3530
K	 0.5780	 0.3770
M	 0.4620	 0.3120
N	 0.4910	 0.3570
O	 0.7180	 0.4410
P	 0.7020	 0.4350
Q	 0.6090	 0.3270
R	 0.6310	 0.3710
S	 0.6060	 0.3930
T	 0.6050	 0.3630
U	 0.6830	 0.4150
V	 0.6490	 0.3530
W	 0.6540	 0.4230
X	 0.4210	 0.2880
Y	 0.5930	 0.3280
Z	 0.6220	 0.3560
a	 0.1390	 0.1650
b	 0.1360	 0.1300
c	 0.6500	 0.4030
d	 0.0090	 0.0930
e	 0.0020	 0.1210
f	 0.4360	 0.2460
g	 0.3580	 0.2190
h	 0.0660	 0.1130
i	 0.6290	 0.3360



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
j	 0.5940	 0.3200
k	 0.1080	 0.1130
l	 0.5980	 0.2820
m	 0.6050	 0.2770
n	 0.5100	 0.3030
o	 0.5260	 0.3010
p	 0.4400	 0.2200
q	 0.4600	 0.2210
r	 0.6500	 0.4050
s	 0.3200	 0.2040
t	 0.0090	 0.0990