



wwPDB EM Validation Summary Report ⓘ

Sep 22, 2025 – 01:54 PM EDT

PDB ID : 9ED4 / pdb_00009ed4
EMDB ID : EMD-47932
Title : A composite map of mTORC1-Rag-Ragulator-4EBP1 on membrane
Authors : Cui, Z.; Hurley, J.
Deposited on : 2024-11-15
Resolution : 3.23 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:

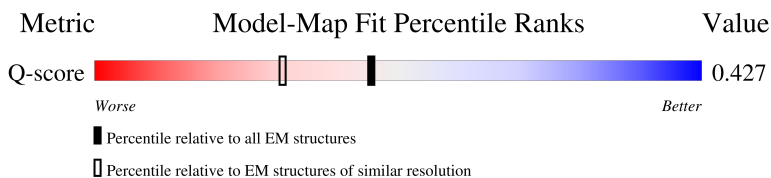
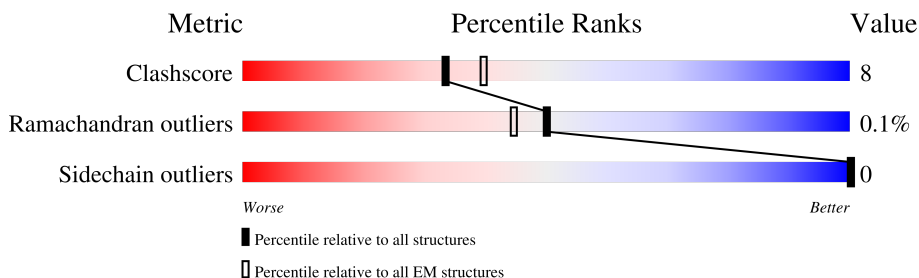
EMDB validation analysis : 0.0.1.dev129
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive 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) : 2.46

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 3.23 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.





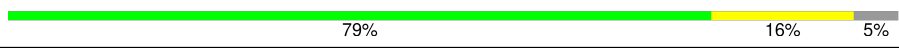



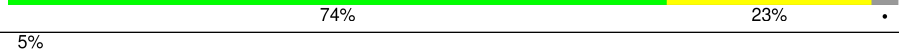
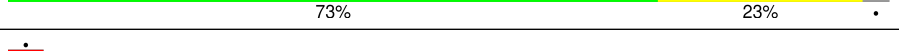
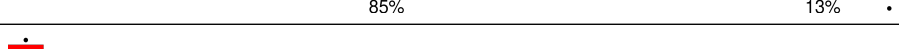
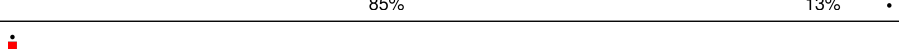
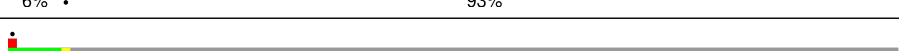
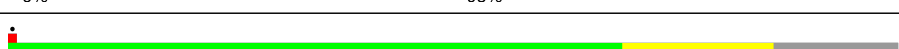


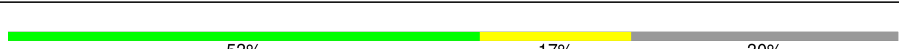





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	14612 (2.73 - 3.73)

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	B	326	
1	M	326	
2	L	184	
2	N	184	

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Mol	Chain	Length	Quality of chain
3	A	2549	
3	O	2549	
4	D	313	
4	P	313	
5	G	125	
5	Q	125	
6	H	124	
6	R	124	
7	J	91	
7	S	91	
8	K	118	
8	T	118	
9	C	1335	
9	U	1335	
10	E	399	
10	V	399	
11	F	161	
11	W	161	
12	I	99	
12	X	99	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 161433 atoms, of which 80663 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 Target of rapamycin complex subunit LST8.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	B	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		
1	M	317	Total	C	H	N	O	S	0	0
			4797	1526	2341	436	476	18		

- Molecule 2 is a protein called GTP-binding protein Rheb.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	L	170	Total	C	H	N	O	S	0	0
			2698	860	1355	219	260	4		
2	N	170	Total	C	H	N	O	S	0	0
			2698	860	1355	219	260	4		

- Molecule 3 is a protein called Serine/threonine-protein kinase mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	A	2305	Total	C	H	N	O	S	0	0
			37222	11782	18711	3247	3357	125		
3	O	2305	Total	C	H	N	O	S	0	0
			37222	11782	18711	3247	3357	125		

- Molecule 4 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	298	Total	C	H	N	O	S	0	0
			4882	1553	2438	427	447	17		
4	P	298	Total	C	H	N	O	S	0	0
			4882	1553	2438	427	447	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	66	LEU	GLN	conflict	UNP Q7L523

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Chain	Residue	Modelled	Actual	Comment	Reference
P	66	LEU	GLN	conflict	UNP Q7L523

- Molecule 5 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	G	124	Total	C	H	N	O	S	0	0
			1888	590	950	161	180	7		
5	Q	124	Total	C	H	N	O	S	0	0
			1888	590	950	161	180	7		

- Molecule 6 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	120	Total	C	H	N	O	S	0	0
			1892	601	958	157	175	1		
6	R	120	Total	C	H	N	O	S	0	0
			1892	601	958	157	175	1		

- Molecule 7 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	J	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		
7	S	89	Total	C	H	N	O	S	0	0
			1311	400	656	113	135	7		

- Molecule 8 is a protein called Eukaryotic translation initiation factor 4E-binding protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	K	8	Total	C	H	N	O	S	0	0
			126	42	57	9	17	1		
8	T	8	Total	C	H	N	O	S	0	0
			126	42	57	9	17	1		

- Molecule 9 is a protein called Regulatory-associated protein of mTOR.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	C	1142	Total	C	H	N	O	S	0	0
			18164	5804	9067	1581	1651	61		
9	U	1142	Total	C	H	N	O	S	0	0
			18165	5804	9068	1581	1651	61		

- Molecule 10 is a protein called Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	E	281	Total	C	H	N	O	S	0	0
			4523	1459	2258	370	424	12		
10	V	281	Total	C	H	N	O	S	0	0
			4523	1459	2258	370	424	12		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	75	ASN	SER	engineered mutation	UNP Q9HB90
V	75	ASN	SER	engineered mutation	UNP Q9HB90

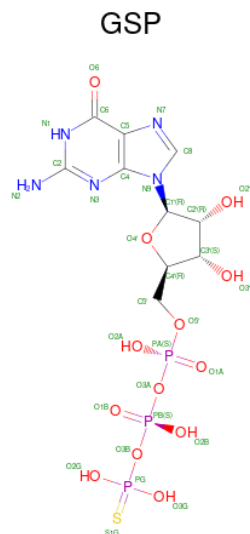
- Molecule 11 is a protein called Ragulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	F	111	Total	C	H	N	O	S	0	0
			1738	547	870	150	170	1		
11	W	111	Total	C	H	N	O	S	0	0
			1738	547	870	150	170	1		

- Molecule 12 is a protein called Ragulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	I	84	Total	C	H	N	O	S	0	0
			1294	404	652	115	122	1		
12	X	84	Total	C	H	N	O	S	0	0
			1294	404	652	115	122	1		

- Molecule 13 is 5'-GUANOSINE-DIPHOSPHATE-MONOTHIOPHOSPHATE (CCD ID: GSP) (formula: C₁₀H₁₆N₅O₁₃P₃S).

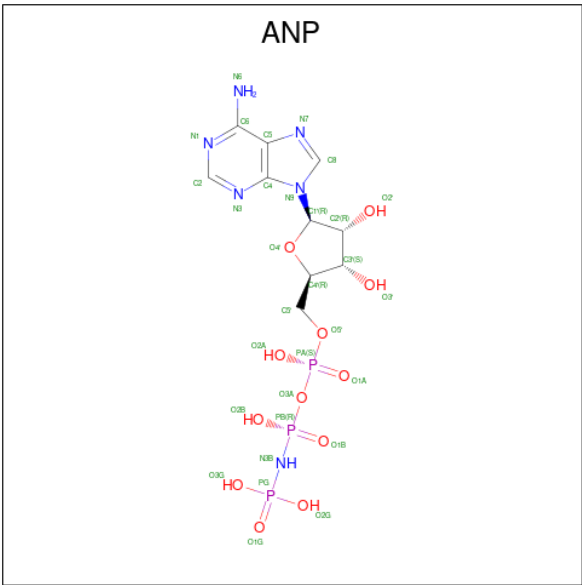


Mol	Chain	Residues	Atoms					AltConf	
13	L	1	Total 32	C 10	N 5	O 13	P 3	S 1	0
13	N	1	Total 32	C 10	N 5	O 13	P 3	S 1	0

- Molecule 14 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

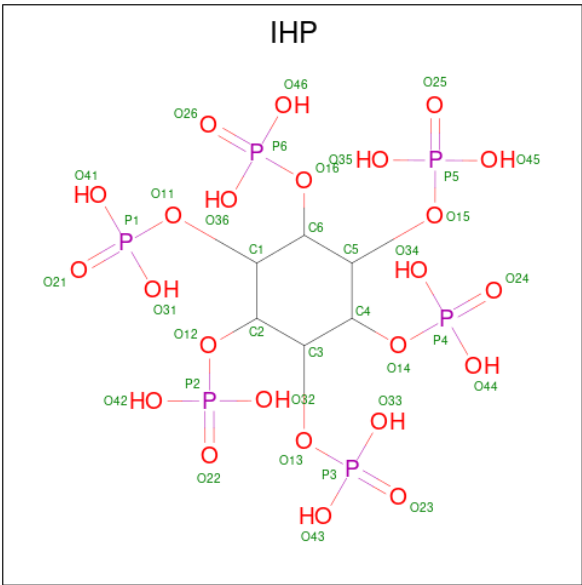
Mol	Chain	Residues	Atoms	AltConf
14	L	1	Total Mg 1 1	0
14	A	2	Total Mg 2 2	0
14	D	1	Total Mg 1 1	0
14	N	1	Total Mg 1 1	0
14	O	2	Total Mg 2 2	0
14	P	1	Total Mg 1 1	0

- Molecule 15 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).



Mol	Chain	Residues	Atoms						AltConf
15	A	1	Total	C	H	N	O	P	0
			43	10	12	6	12	3	
15	O	1	Total	C	H	N	O	P	0
			43	10	12	6	12	3	

- Molecule 16 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



Mol	Chain	Residues	Atoms					AltConf
16	A	1	Total	C	H	O	P	0
			42	6	6	24	6	
16	O	1	Total	C	H	O	P	0
			42	6	6	24	6	

-
- The image displays the chemical structure of Guanosine Triphosphate (GTP). It consists of a guanine base (a purine ring system with an amino group at C2 and a carbonyl group at C6) linked to a ribose sugar via a glycosidic bond. The ribose sugar is further linked to three phosphate groups (labeled 1, 2, and 3) via phosphodiester bonds. The structure is shown in a 3D representation with stereochemistry indicated by wedges and dashes. The atoms are labeled with their respective element symbols and indices (e.g., N1, C2, O3, P1, O1A, etc.).

Mol	Chain	Residues	Atoms					AltConf
17	D	1	Total 32	C 10	N 5	O 14	P 3	0
17	P	1	Total 32	C 10	N 5	O 14	P 3	0

-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including the amino group at the 2-position. The ribose sugar is a five-membered ring with hydroxyl groups at the 2' and 3' positions. The two phosphate groups are connected by a pyrophosphate linkage, with the second phosphate group being a diphosphate (P₂O₇) moiety. The structure is labeled with various atoms and bonds, including the guanine base (N1, N2, N3, N7, C2, C4, C6, C8), the ribose sugar (C1', C2', C3', C4', C5'), and the phosphate groups (P1, P2, O1A, O1B, O2A, O2B, O3A, O3B, O4A, O4B, O5A, O5B).

Mol	Chain	Residues	Atoms					AltConf
18	E	1	Total	C	N	O	P	0
			28	10	5	11	2	

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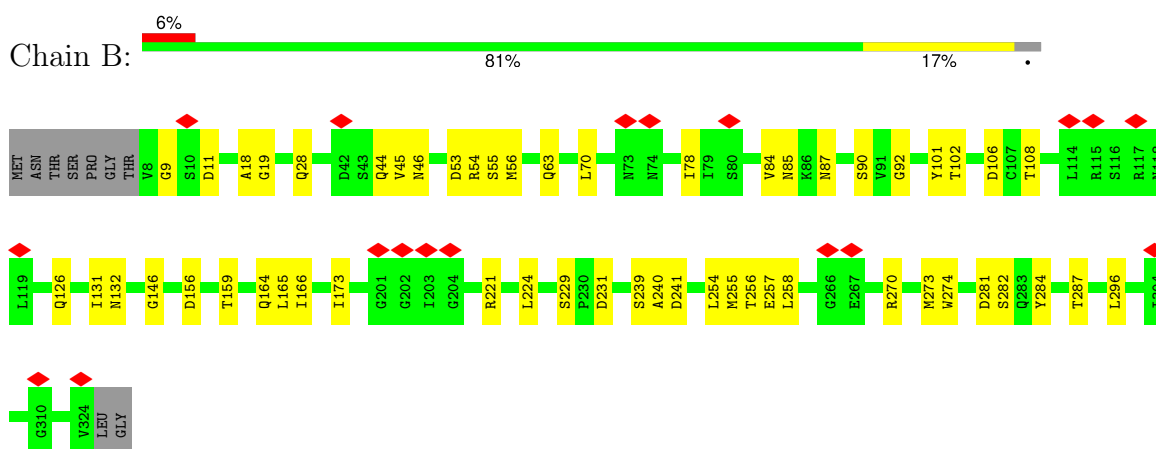
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
18	V	1	28	10	5	11	2	0

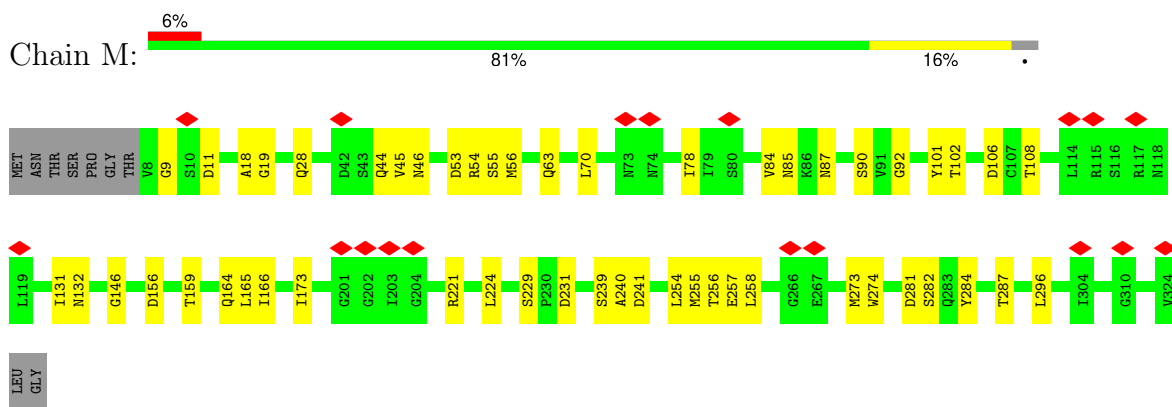
3 Residue-property plots

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.

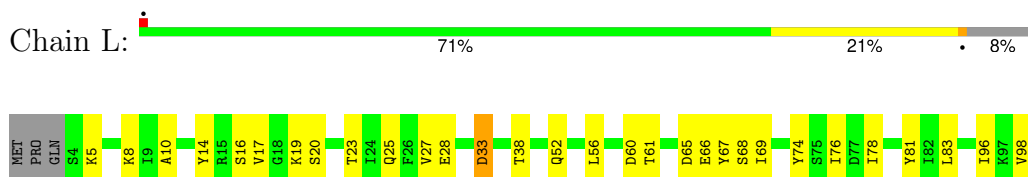
- Molecule 1: Target of rapamycin complex subunit LST8



- Molecule 1: Target of rapamycin complex subunit LST8



- Molecule 2: GTP-binding protein Rheb

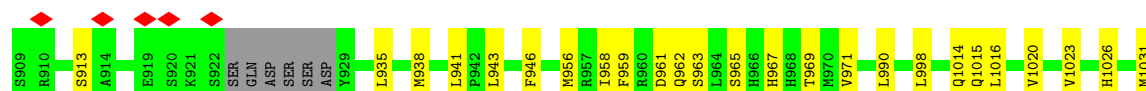
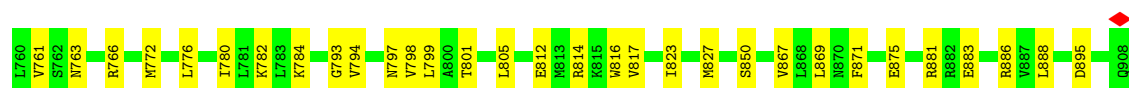
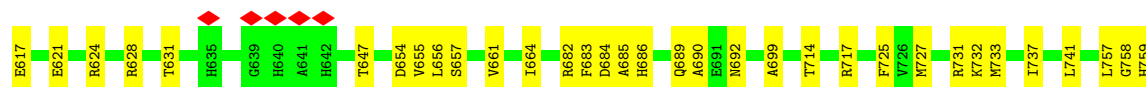
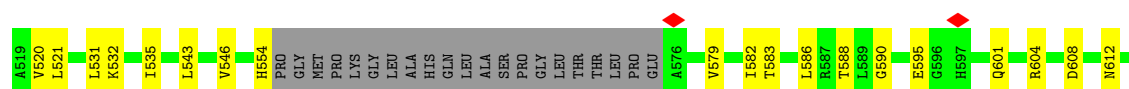
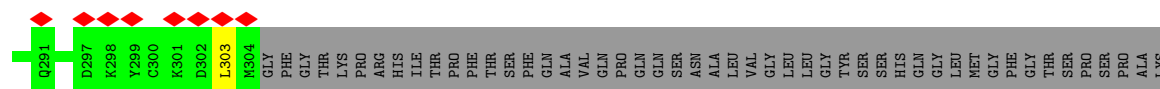
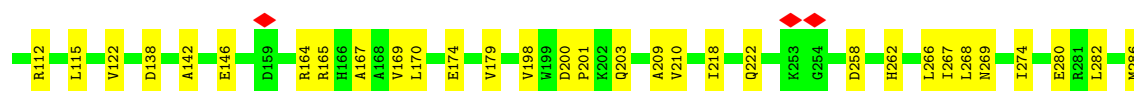


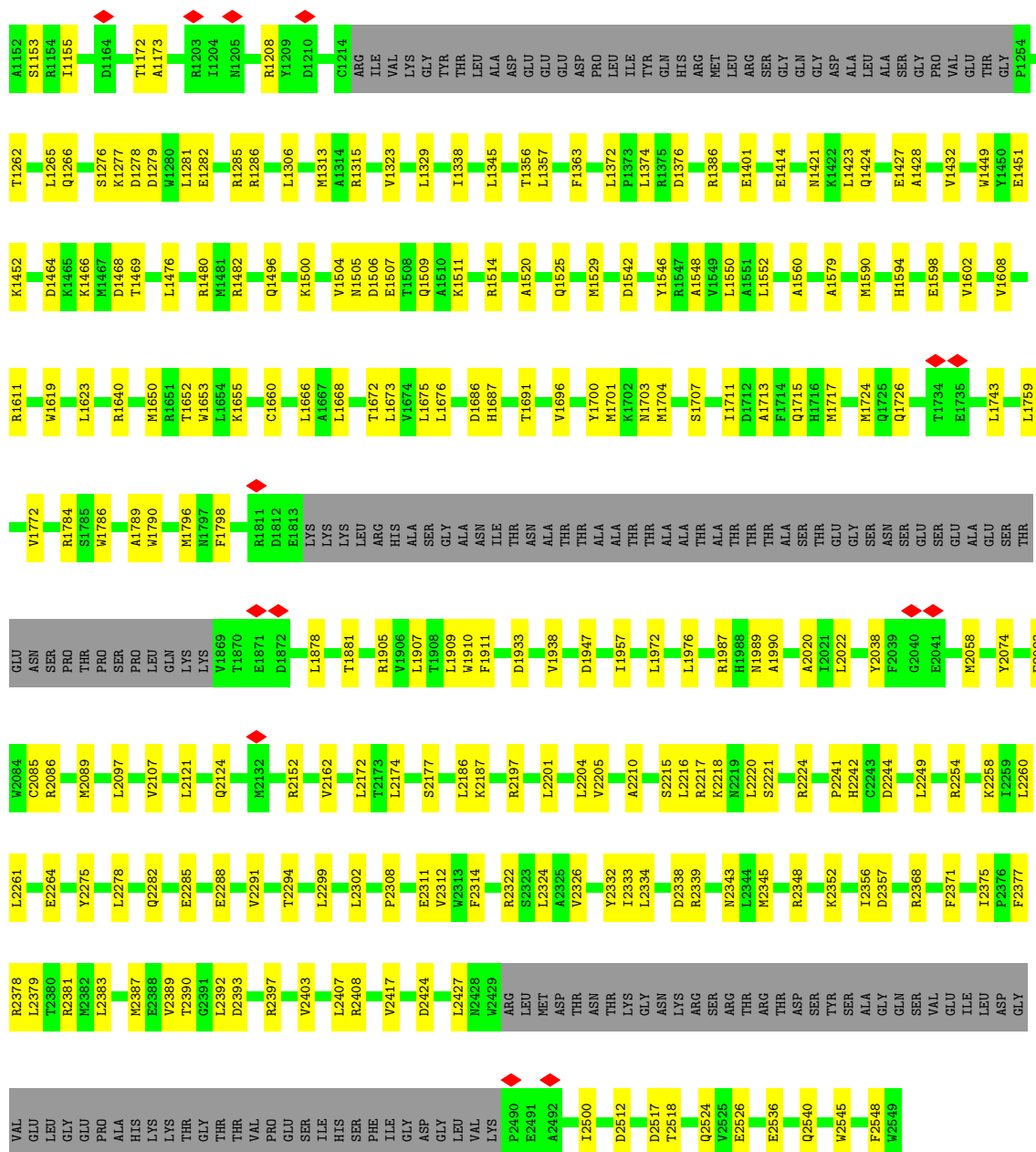


• Molecule 2: GTP-binding protein Rheb



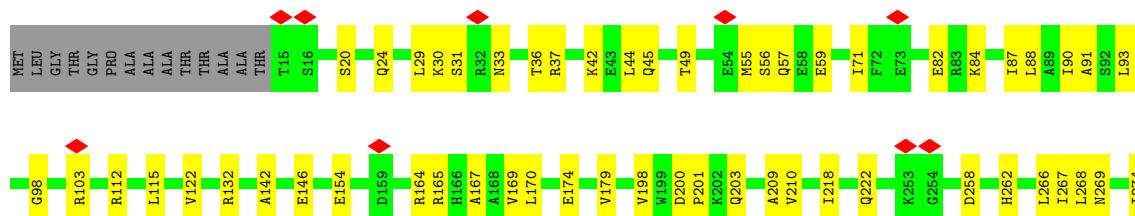
• Molecule 3: Serine/threonine-protein kinase mTOR



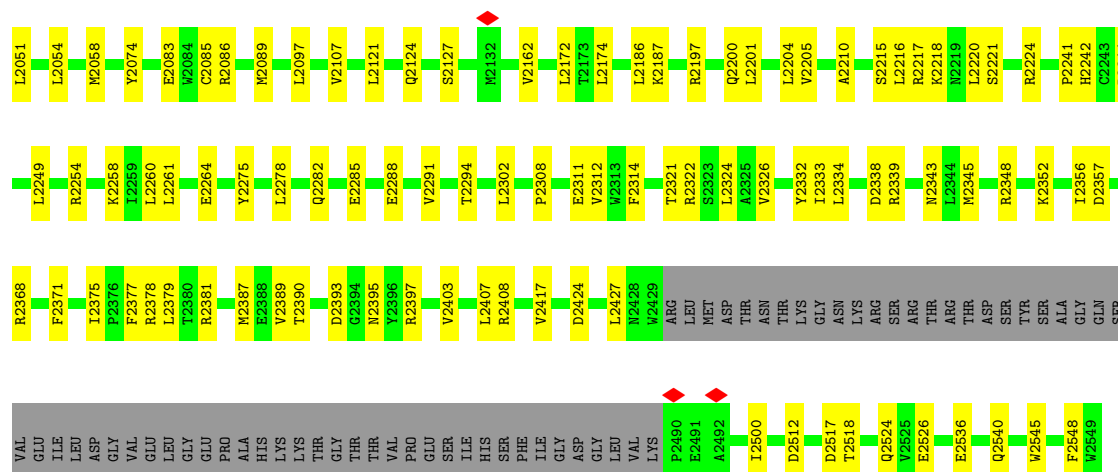


• Molecule 3: Serine/threonine-protein kinase mTOR

Chain O: 72% 18% 10%

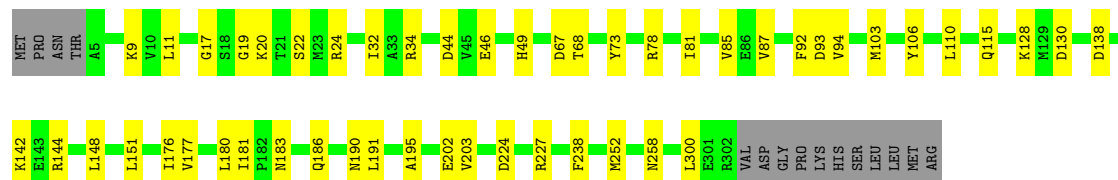






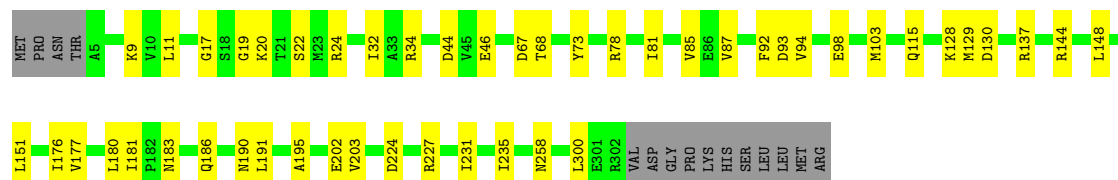
• Molecule 4: Ras-related GTP-binding protein A

Chain D: 79% 16% 5%



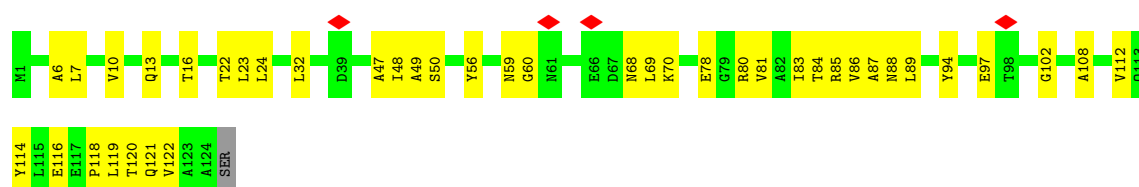
• Molecule 4: Ras-related GTP-binding protein A

Chain P: 80% 15% 5%



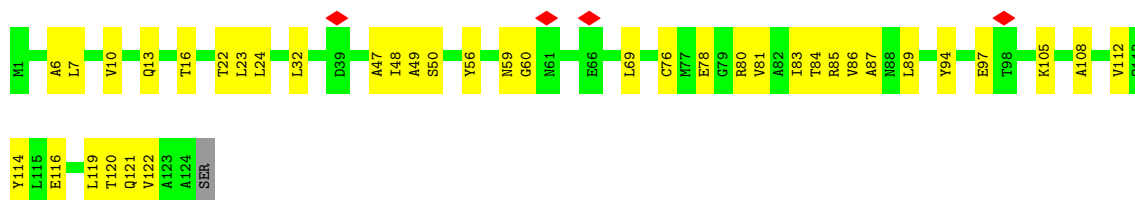
• Molecule 5: Regulator complex protein LAMTOR2

Chain G: 66% 33%

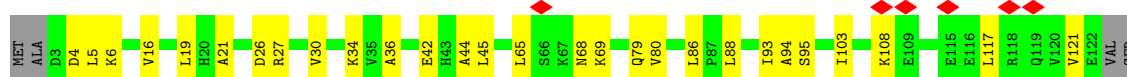
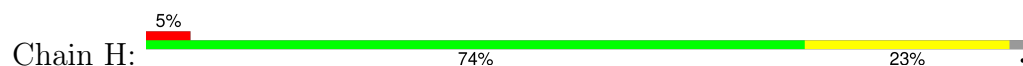


• Molecule 5: Regulator complex protein LAMTOR2

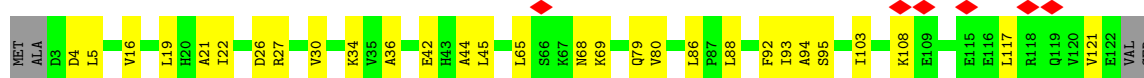
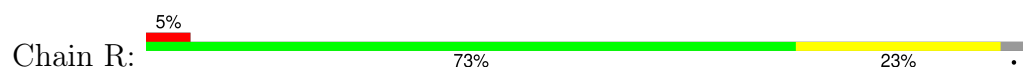
Chain Q: 69% 30%



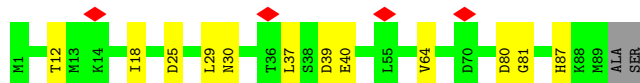
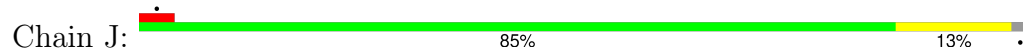
- Molecule 6: Regulator complex protein LAMTOR3



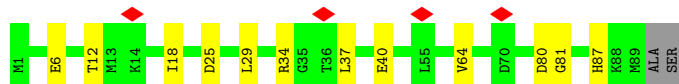
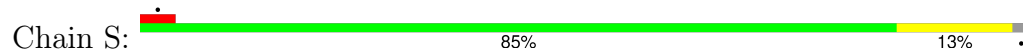
- Molecule 6: Regulator complex protein LAMTOR3



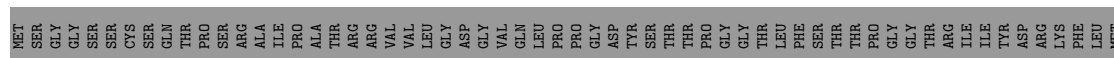
- Molecule 7: Regulator complex protein LAMTOR5



- Molecule 7: Regulator complex protein LAMTOR5

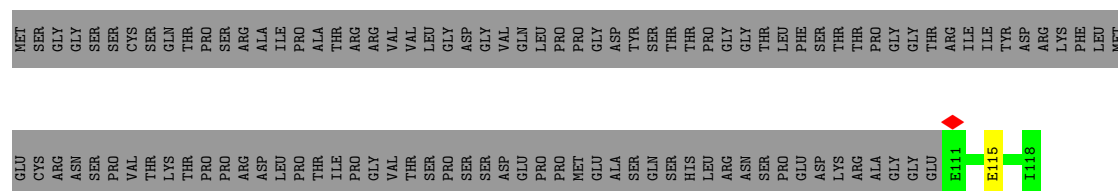


- Molecule 8: Eukaryotic translation initiation factor 4E-binding protein 1



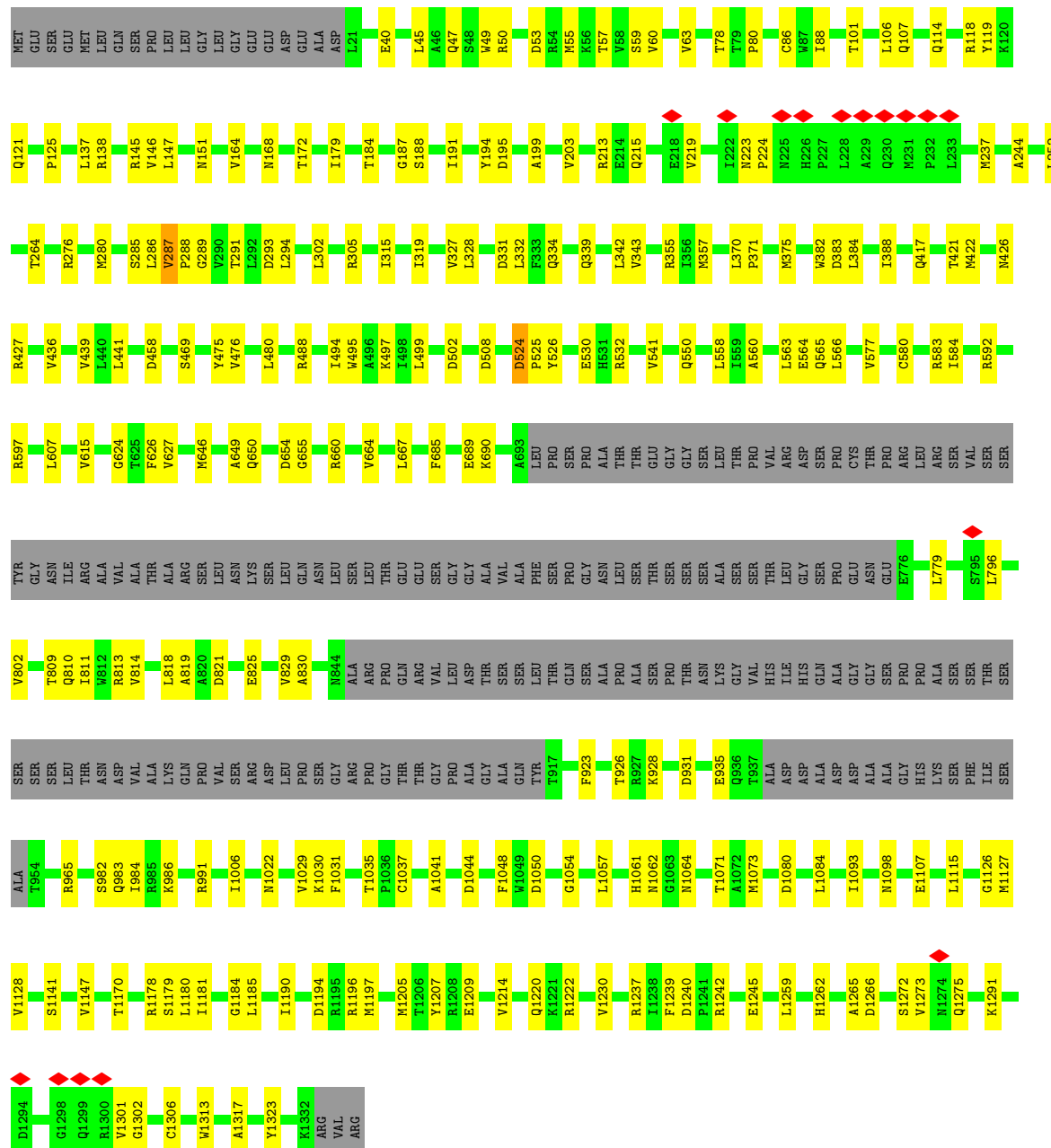
- Molecule 8: Eukaryotic translation initiation factor 4E-binding protein 1





• Molecule 9: Regulatory-associated protein of mTOR

Chain C:



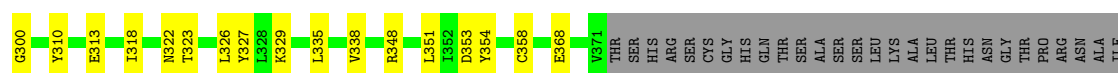
• Molecule 9: Regulatory-associated protein of mTOR

Chain U:

68%

17%

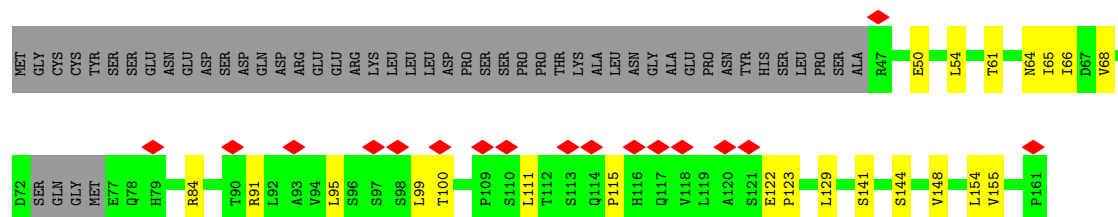
14%



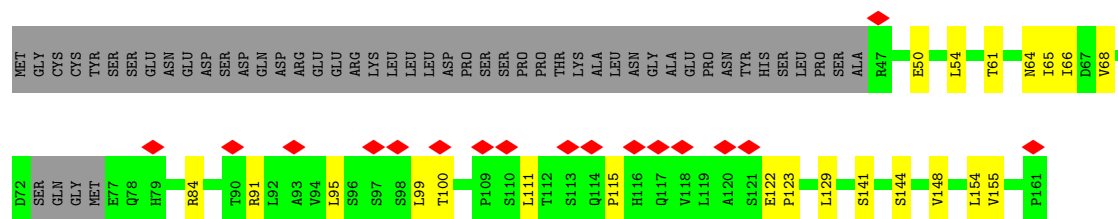
• Molecule 10: Ras-related GTP-binding protein C



• Molecule 11: Regulator complex protein LAMTOR1

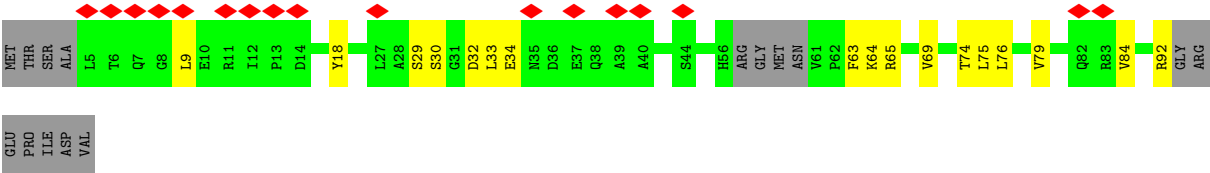


• Molecule 11: Regulator complex protein LAMTOR1

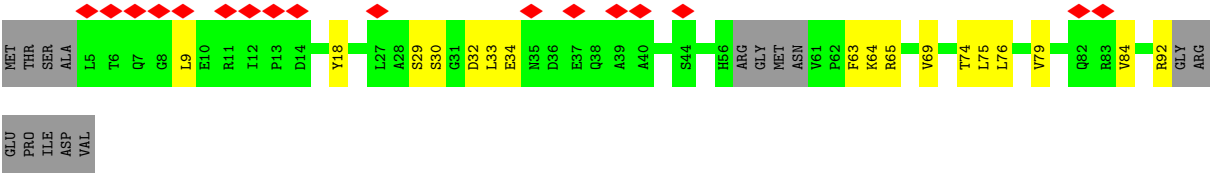


• Molecule 12: Regulator complex protein LAMTOR4





● Molecule 12: Regulator complex protein LAMTOR4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	359012	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.123	Depositor
Minimum map value	-0.073	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.023	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	465.91998, 465.91998, 465.91998	wwPDB
Map dimensions	448, 448, 448	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	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: GDP, IHP, GSP, GTP, ANP, MG

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	B	0.16	0/2514	0.39	0/3426
1	M	0.16	0/2514	0.38	0/3426
2	L	0.22	0/1365	0.42	0/1842
2	N	0.22	0/1365	0.42	0/1842
3	A	0.19	0/18892	0.39	0/25566
3	O	0.19	0/18892	0.39	0/25566
4	D	0.22	0/2489	0.40	0/3350
4	P	0.22	0/2489	0.40	0/3350
5	G	0.18	0/949	0.44	0/1285
5	Q	0.17	0/949	0.43	0/1285
6	H	0.17	0/951	0.38	0/1290
6	R	0.17	0/951	0.39	0/1290
7	J	0.15	0/661	0.38	0/896
7	S	0.14	0/661	0.38	0/896
8	K	0.13	0/69	0.23	0/89
8	T	0.13	0/69	0.22	0/89
9	C	0.21	0/9319	0.40	0/12677
9	U	0.22	0/9319	0.40	0/12677
10	E	0.21	0/2309	0.45	0/3114
10	V	0.22	0/2309	0.45	0/3114
11	F	0.16	0/884	0.37	0/1201
11	W	0.16	0/884	0.37	0/1201
12	I	0.13	0/649	0.34	0/876
12	X	0.13	0/649	0.34	0/876
All	All	0.20	0/82102	0.40	0/111224

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	1
2	N	0	1
9	C	0	3
9	U	0	3
10	E	0	1
10	V	0	1
All	All	0	10

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	C	223	ASN	Peptide
9	C	287	VAL	Peptide
9	C	524	ASP	Peptide
10	E	168	ASN	Peptide
2	L	33	ASP	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2456	2341	2341	37	0
1	M	2456	2341	2341	35	0
2	L	1343	1355	1355	33	0
2	N	1343	1355	1356	36	0
3	A	18511	18711	18711	294	0
3	O	18511	18711	18711	299	0
4	D	2444	2438	2438	38	0
4	P	2444	2438	2438	36	0
5	G	938	950	950	29	0
5	Q	938	950	950	27	0
6	H	934	958	958	21	0
6	R	934	958	958	24	0
7	J	655	656	656	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	S	655	656	656	11	0
8	K	69	57	57	1	0
8	T	69	57	57	1	0
9	C	9097	9067	9068	146	0
9	U	9097	9068	9068	143	0
10	E	2265	2258	2258	52	0
10	V	2265	2258	2258	54	0
11	F	868	870	870	18	0
11	W	868	870	870	18	0
12	I	642	652	652	13	0
12	X	642	652	652	14	0
13	L	32	0	12	5	0
13	N	32	0	12	5	0
14	A	2	0	0	0	0
14	D	1	0	0	0	0
14	L	1	0	0	0	0
14	N	1	0	0	0	0
14	O	2	0	0	0	0
14	P	1	0	0	0	0
15	A	31	12	13	1	0
15	O	31	12	13	1	0
16	A	36	6	6	1	0
16	O	36	6	6	1	0
17	D	32	0	12	5	0
17	P	32	0	12	5	0
18	E	28	0	12	3	0
18	V	28	0	12	3	0
All	All	80770	80663	80739	1306	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 8.

The worst 5 of 1306 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)
3:O:518:THR:HG21	3:O:588:THR:HG21	1.45	0.97
3:A:518:THR:HG21	3:A:588:THR:HG21	1.45	0.95
9:C:558:LEU:HD23	9:C:584:ILE:HD12	1.54	0.90
9:U:558:LEU:HD23	9:U:584:ILE:HD12	1.54	0.90
2:L:56:LEU:HD21	2:L:164:ILE:HD11	1.52	0.89

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	B	315/326 (97%)	293 (93%)	22 (7%)	0	100	100
1	M	315/326 (97%)	294 (93%)	21 (7%)	0	100	100
2	L	168/184 (91%)	155 (92%)	13 (8%)	0	100	100
2	N	168/184 (91%)	155 (92%)	13 (8%)	0	100	100
3	A	2291/2549 (90%)	2219 (97%)	72 (3%)	0	100	100
3	O	2291/2549 (90%)	2218 (97%)	73 (3%)	0	100	100
4	D	296/313 (95%)	280 (95%)	16 (5%)	0	100	100
4	P	296/313 (95%)	280 (95%)	16 (5%)	0	100	100
5	G	122/125 (98%)	108 (88%)	14 (12%)	0	100	100
5	Q	122/125 (98%)	110 (90%)	12 (10%)	0	100	100
6	H	118/124 (95%)	108 (92%)	10 (8%)	0	100	100
6	R	118/124 (95%)	108 (92%)	10 (8%)	0	100	100
7	J	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
7	S	87/91 (96%)	83 (95%)	4 (5%)	0	100	100
8	K	6/118 (5%)	6 (100%)	0	0	100	100
8	T	6/118 (5%)	6 (100%)	0	0	100	100
9	C	1134/1335 (85%)	1056 (93%)	74 (6%)	4 (0%)	30	62
9	U	1134/1335 (85%)	1052 (93%)	78 (7%)	4 (0%)	30	62
10	E	275/399 (69%)	255 (93%)	19 (7%)	1 (0%)	30	62
10	V	275/399 (69%)	255 (93%)	19 (7%)	1 (0%)	30	62
11	F	107/161 (66%)	103 (96%)	3 (3%)	1 (1%)	14	46
11	W	107/161 (66%)	103 (96%)	3 (3%)	1 (1%)	14	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	I	80/99 (81%)	73 (91%)	7 (9%)	0	100	100
12	X	80/99 (81%)	72 (90%)	8 (10%)	0	100	100
All	All	9998/11648 (86%)	9473 (95%)	513 (5%)	12 (0%)	50	78

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	C	224	PRO
9	C	288	PRO
9	C	525	PRO
9	C	983	GLN
10	E	169	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	B	269/276 (98%)	269 (100%)	0	100	100
1	M	269/276 (98%)	269 (100%)	0	100	100
2	L	149/161 (92%)	149 (100%)	0	100	100
2	N	149/161 (92%)	149 (100%)	0	100	100
3	A	2027/2220 (91%)	2027 (100%)	0	100	100
3	O	2027/2220 (91%)	2027 (100%)	0	100	100
4	D	271/287 (94%)	271 (100%)	0	100	100
4	P	271/287 (94%)	271 (100%)	0	100	100
5	G	97/98 (99%)	97 (100%)	0	100	100
5	Q	97/98 (99%)	97 (100%)	0	100	100
6	H	105/108 (97%)	105 (100%)	0	100	100
6	R	105/108 (97%)	105 (100%)	0	100	100
7	J	76/77 (99%)	76 (100%)	0	100	100
7	S	76/77 (99%)	76 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	K	8/102 (8%)	8 (100%)	0	100	100
8	T	8/102 (8%)	8 (100%)	0	100	100
9	C	1007/1163 (87%)	1007 (100%)	0	100	100
9	U	1007/1163 (87%)	1007 (100%)	0	100	100
10	E	255/340 (75%)	255 (100%)	0	100	100
10	V	255/340 (75%)	255 (100%)	0	100	100
11	F	97/141 (69%)	97 (100%)	0	100	100
11	W	97/141 (69%)	97 (100%)	0	100	100
12	I	71/83 (86%)	71 (100%)	0	100	100
12	X	71/83 (86%)	71 (100%)	0	100	100
All	All	8864/10112 (88%)	8864 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
9	U	303	ASN
9	U	557	ASN
10	V	234	GLN
9	C	428	ASN
9	C	380	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	IHP	O	3003	-	36,36,36	2.08	6 (16%)	60,60,60	1.23	6 (10%)
15	ANP	O	3000	14	29,33,33	4.02	17 (58%)	31,52,52	3.86	5 (16%)
13	GSP	L	201	14	29,34,34	2.17	3 (10%)	32,54,54	1.59	5 (15%)
17	GTP	D	401	14	29,34,34	1.23	2 (6%)	35,54,54	1.41	5 (14%)
17	GTP	P	401	14	29,34,34	1.23	2 (6%)	35,54,54	1.42	5 (14%)
18	GDP	V	401	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
18	GDP	E	401	-	25,30,30	0.97	1 (4%)	30,47,47	1.07	2 (6%)
13	GSP	N	201	14	29,34,34	2.17	3 (10%)	32,54,54	1.58	5 (15%)
16	IHP	A	3003	-	36,36,36	2.07	6 (16%)	60,60,60	1.23	5 (8%)
15	ANP	A	3000	14	29,33,33	4.03	17 (58%)	31,52,52	3.86	5 (16%)

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
16	IHP	O	3003	-	-	7/30/54/54	0/1/1/1
15	ANP	O	3000	14	-	1/14/38/38	0/3/3/3
13	GSP	L	201	14	-	3/17/38/38	0/3/3/3
17	GTP	D	401	14	-	6/18/38/38	0/3/3/3
17	GTP	P	401	14	-	6/18/38/38	0/3/3/3
18	GDP	V	401	-	-	2/12/32/32	0/3/3/3
18	GDP	E	401	-	-	3/12/32/32	0/3/3/3
13	GSP	N	201	14	-	2/17/38/38	0/3/3/3
16	IHP	A	3003	-	-	7/30/54/54	0/1/1/1
15	ANP	A	3000	14	-	1/14/38/38	0/3/3/3

The worst 5 of 58 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	O	3000	ANP	C2'-C3'	-10.87	1.23	1.53
15	A	3000	ANP	C2'-C3'	-10.86	1.23	1.53
13	L	201	GSP	PG-S1G	-9.56	1.69	1.90
13	N	201	GSP	PG-S1G	-9.55	1.69	1.90
15	A	3000	ANP	O4'-C1'	7.90	1.51	1.40

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	O	3000	ANP	C5-C6-N6	14.67	142.65	120.31
15	A	3000	ANP	C5-C6-N6	14.66	142.65	120.31
15	O	3000	ANP	N6-C6-N1	-9.99	96.99	118.33
15	A	3000	ANP	N6-C6-N1	-9.98	97.00	118.33
15	A	3000	ANP	C1'-N9-C4	-8.28	112.08	126.64

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	L	201	GSP	PB-O3B-PG-O2G
13	L	201	GSP	PB-O3B-PG-O3G
13	N	201	GSP	PB-O3B-PG-O2G
13	N	201	GSP	PB-O3B-PG-O3G
15	A	3000	ANP	PB-N3B-PG-O1G

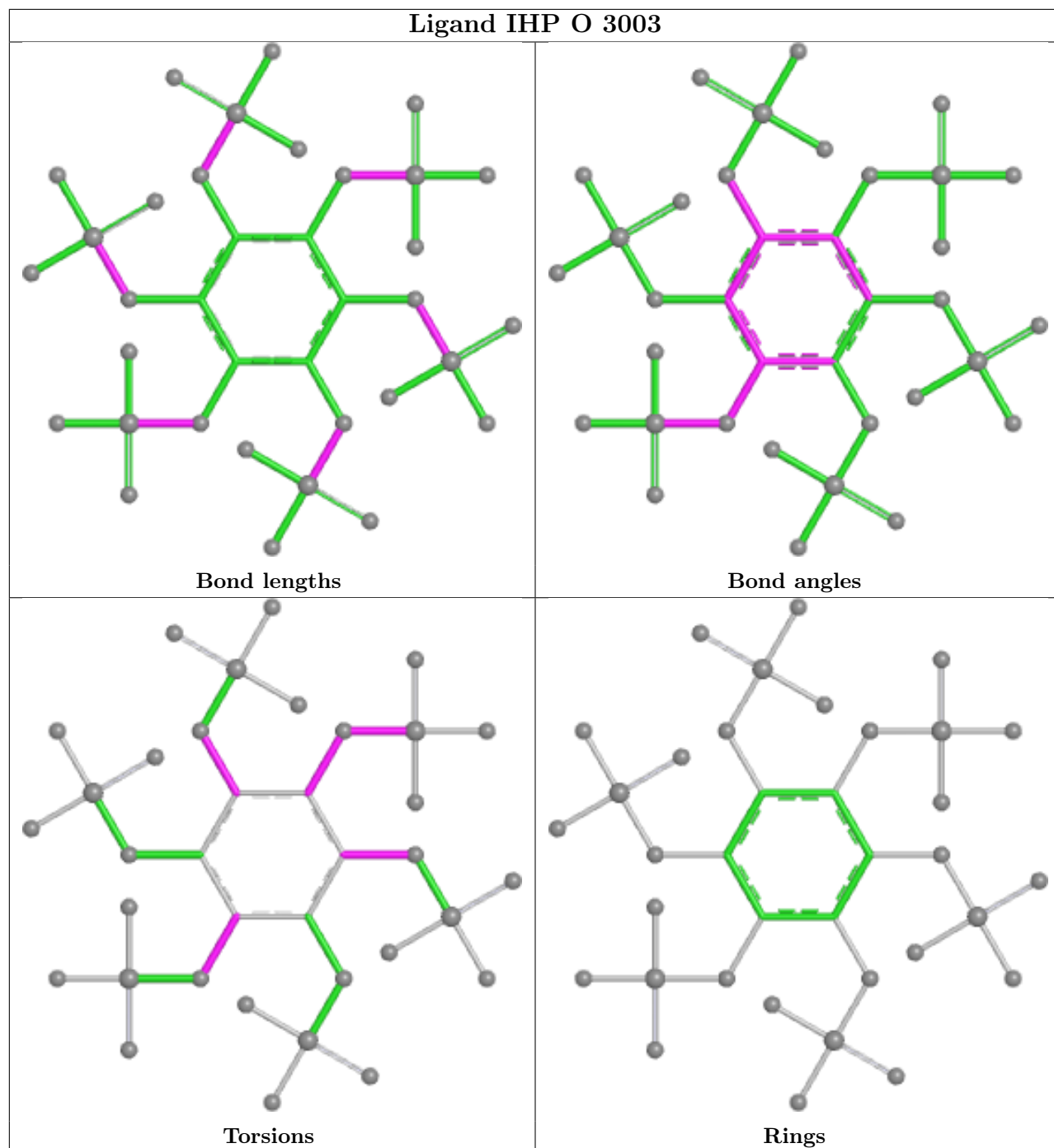
There are no ring outliers.

10 monomers are involved in 30 short contacts:

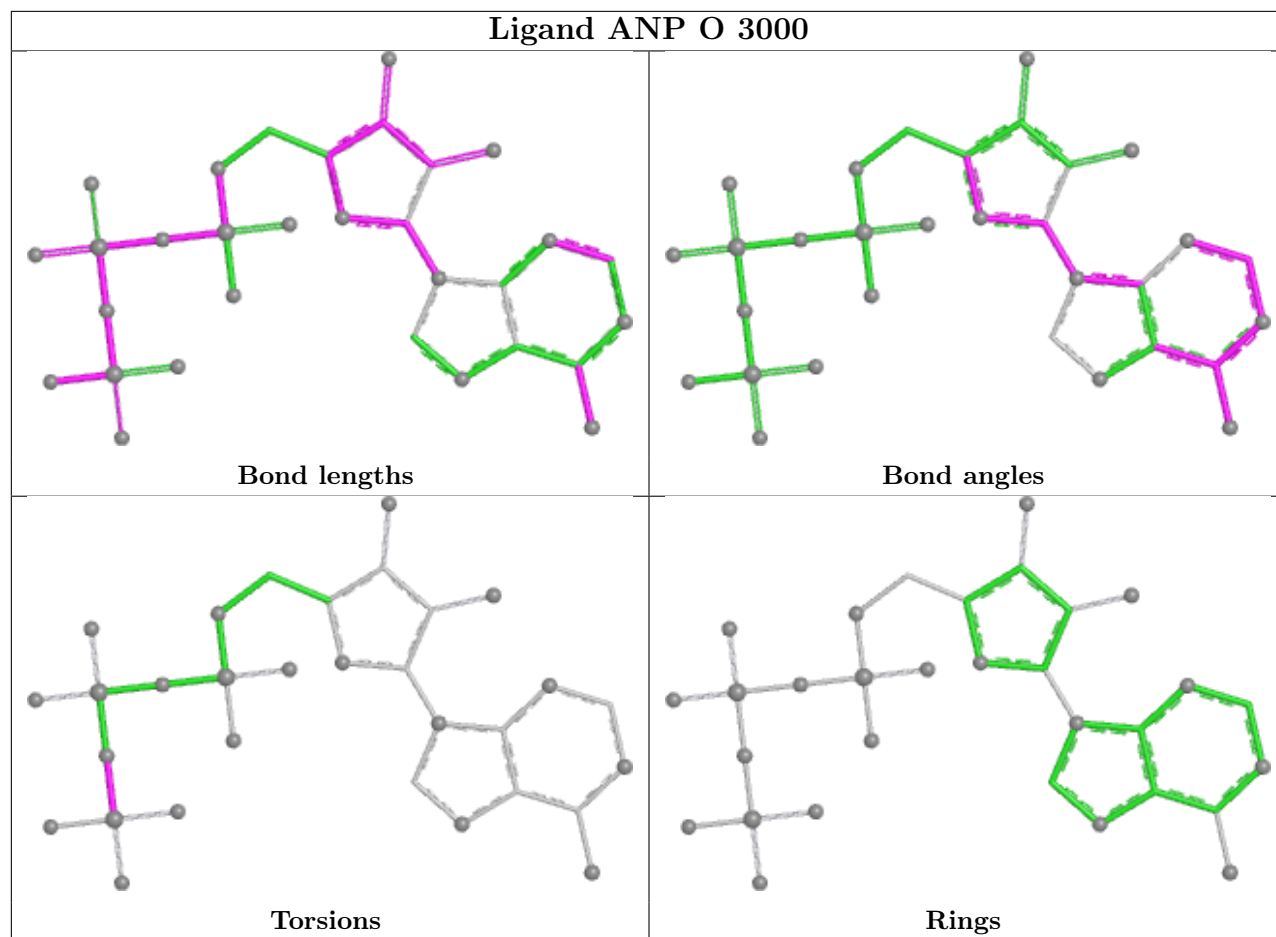
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	O	3003	IHP	1	0
15	O	3000	ANP	1	0
13	L	201	GSP	5	0
17	D	401	GTP	5	0
17	P	401	GTP	5	0
18	V	401	GDP	3	0
18	E	401	GDP	3	0
13	N	201	GSP	5	0
16	A	3003	IHP	1	0
15	A	3000	ANP	1	0

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

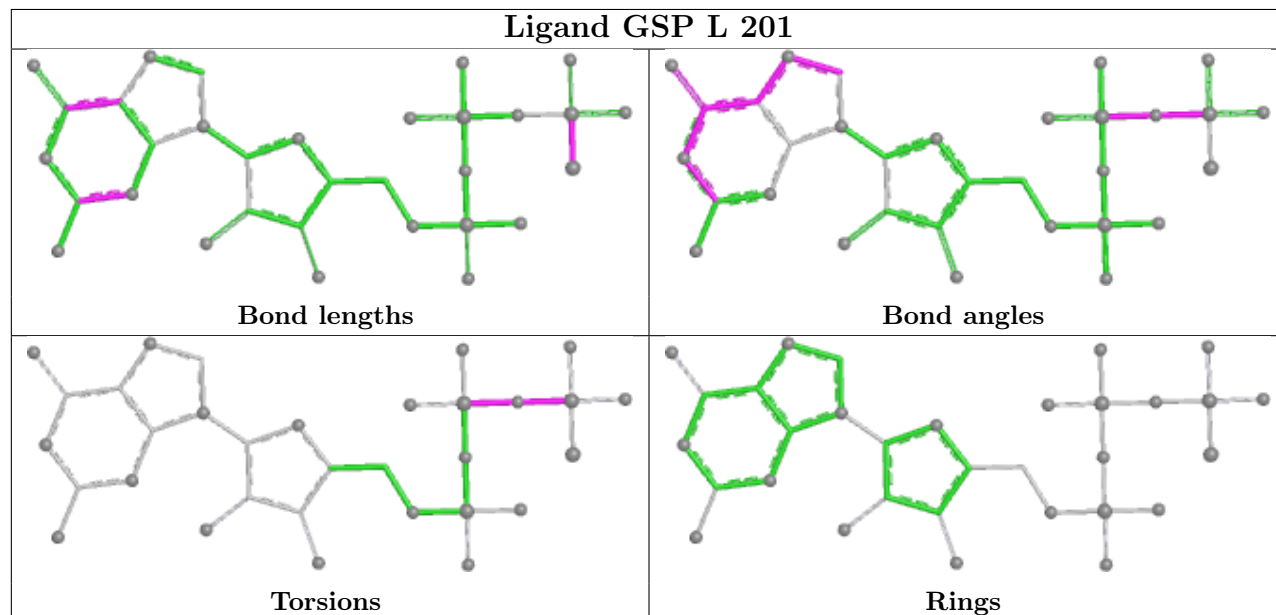
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

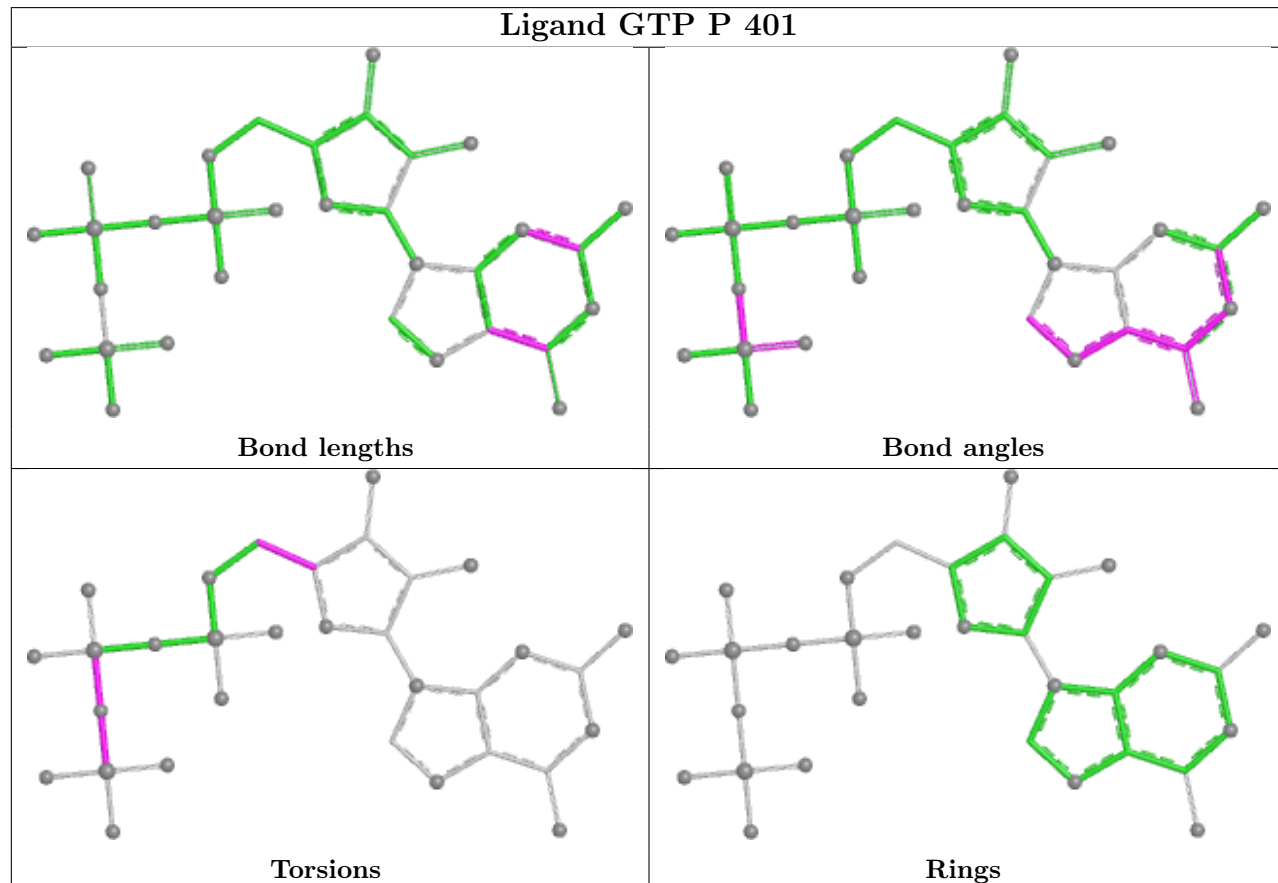
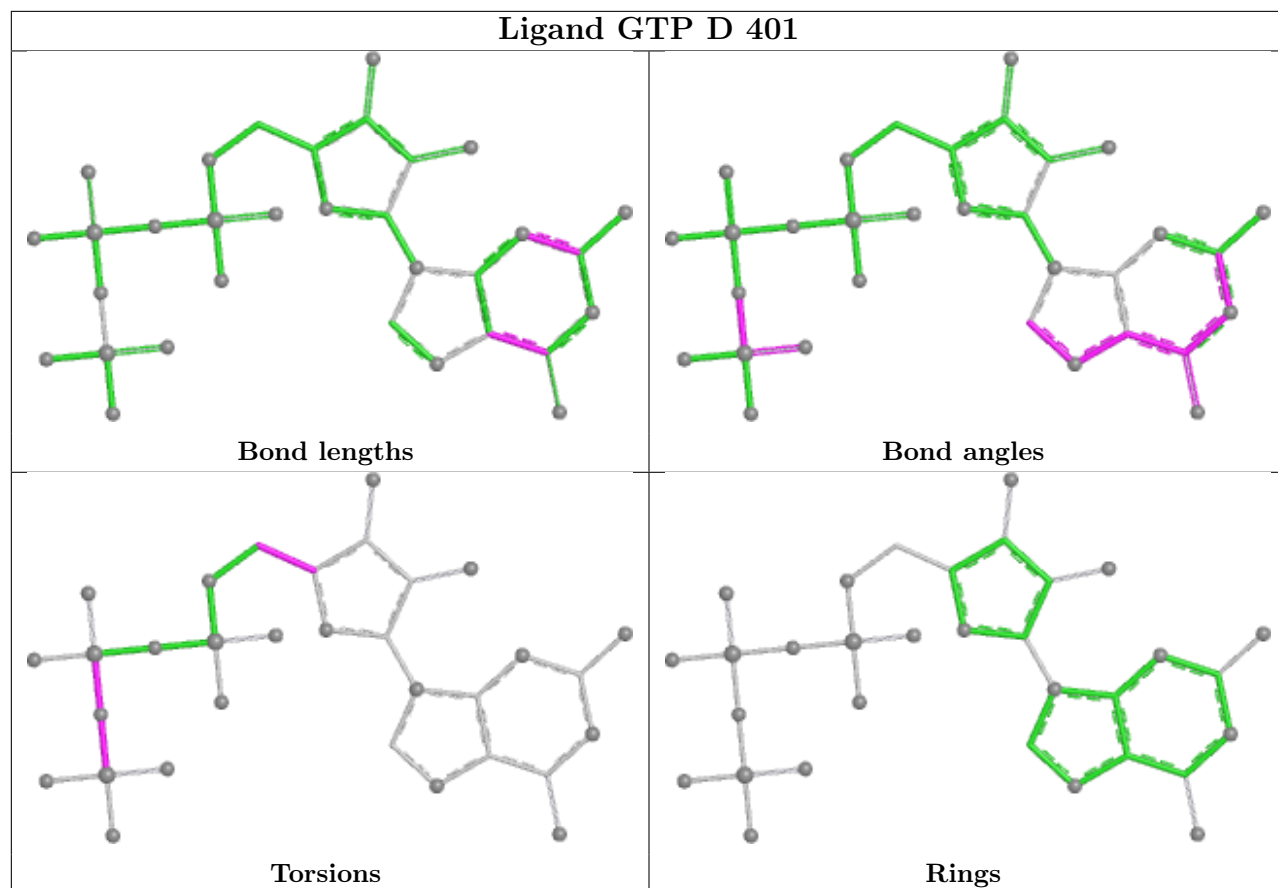


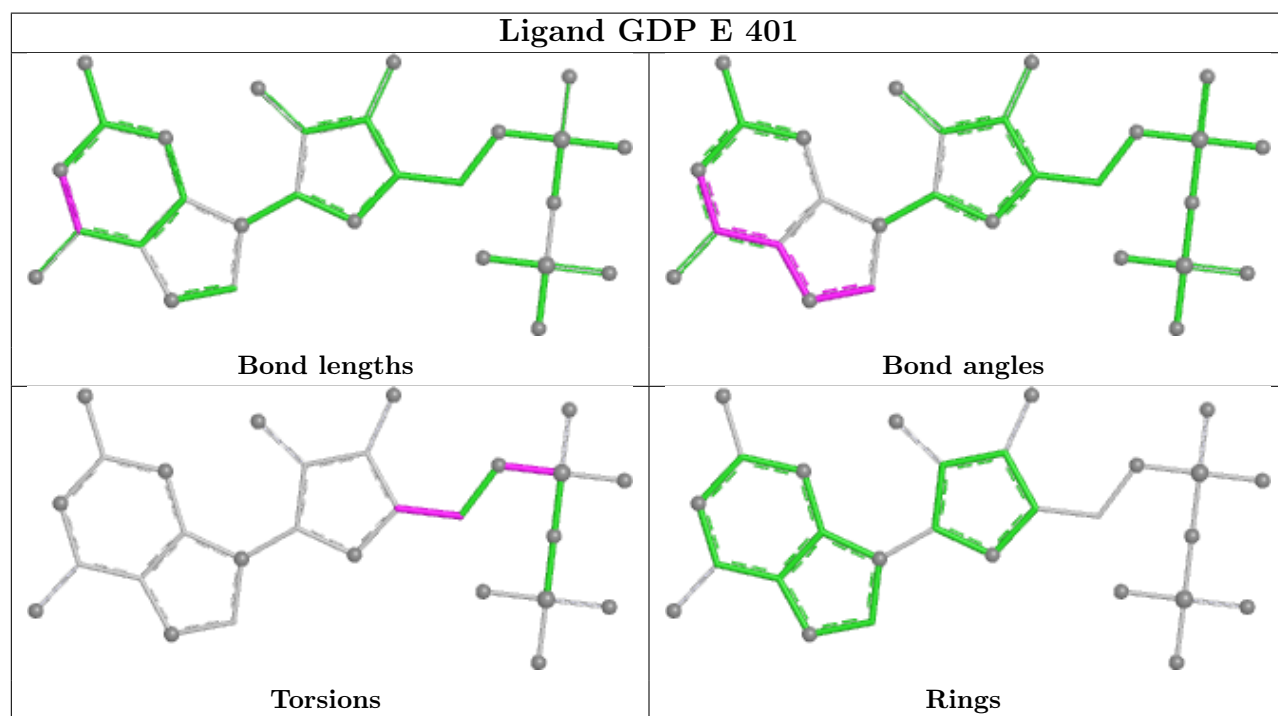
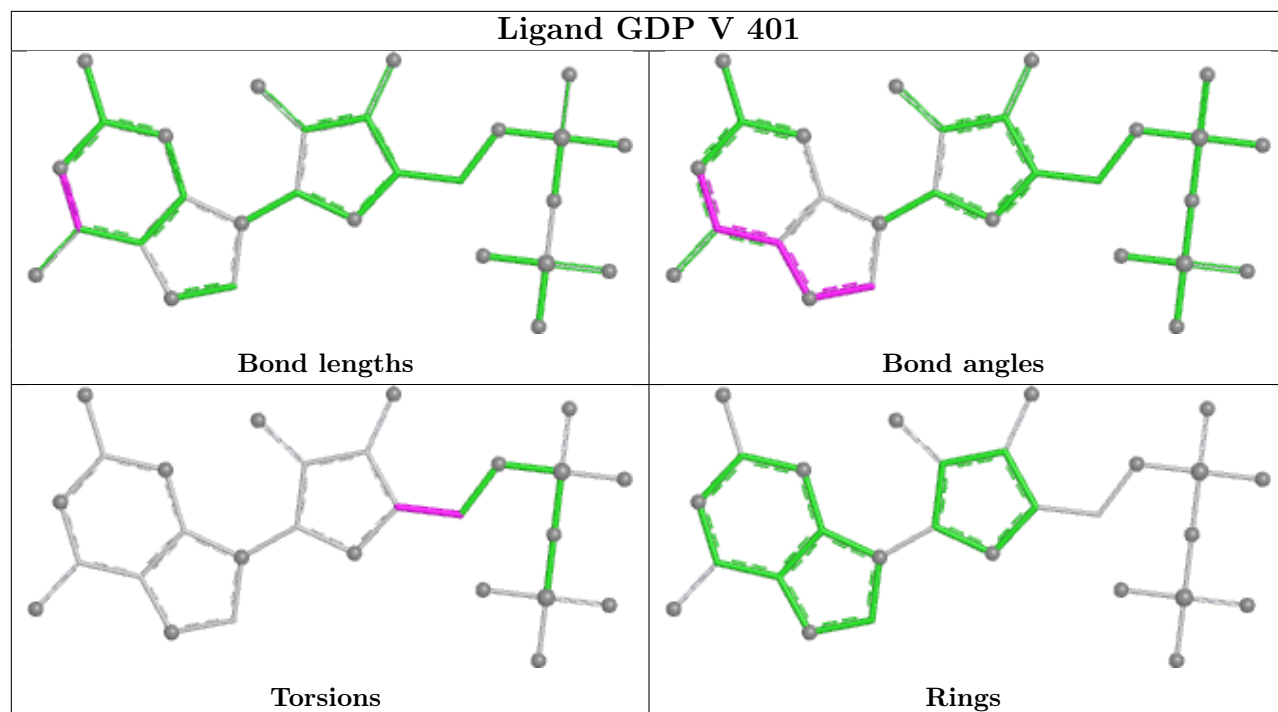
Ligand ANP O 3000

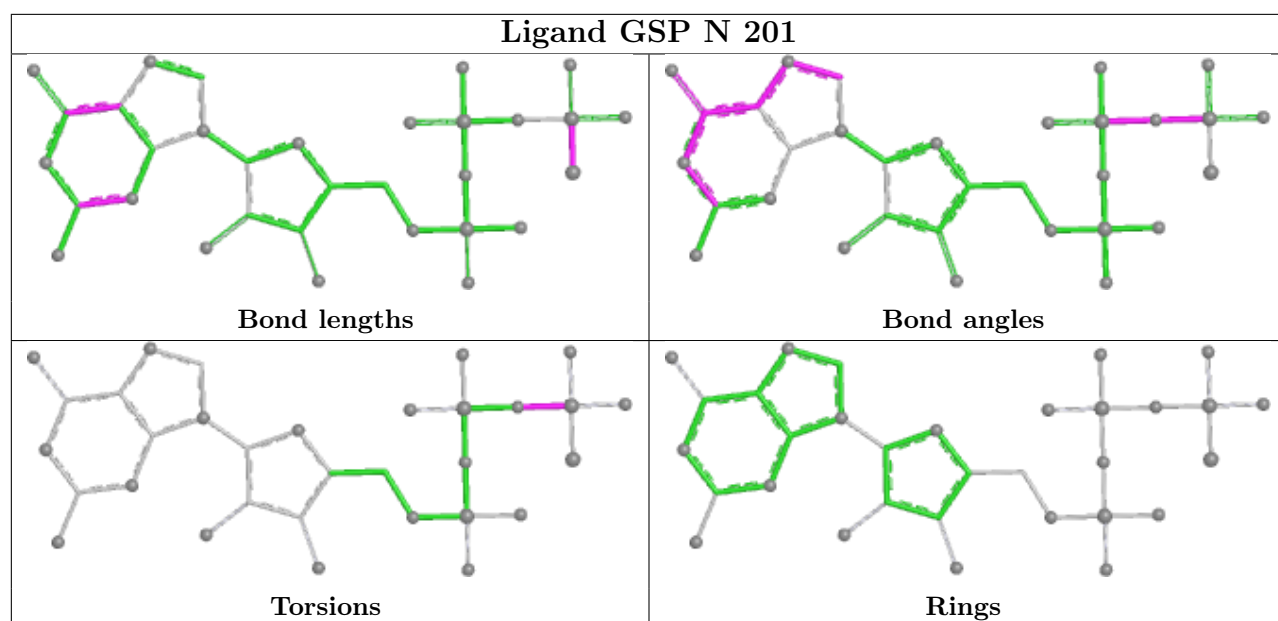


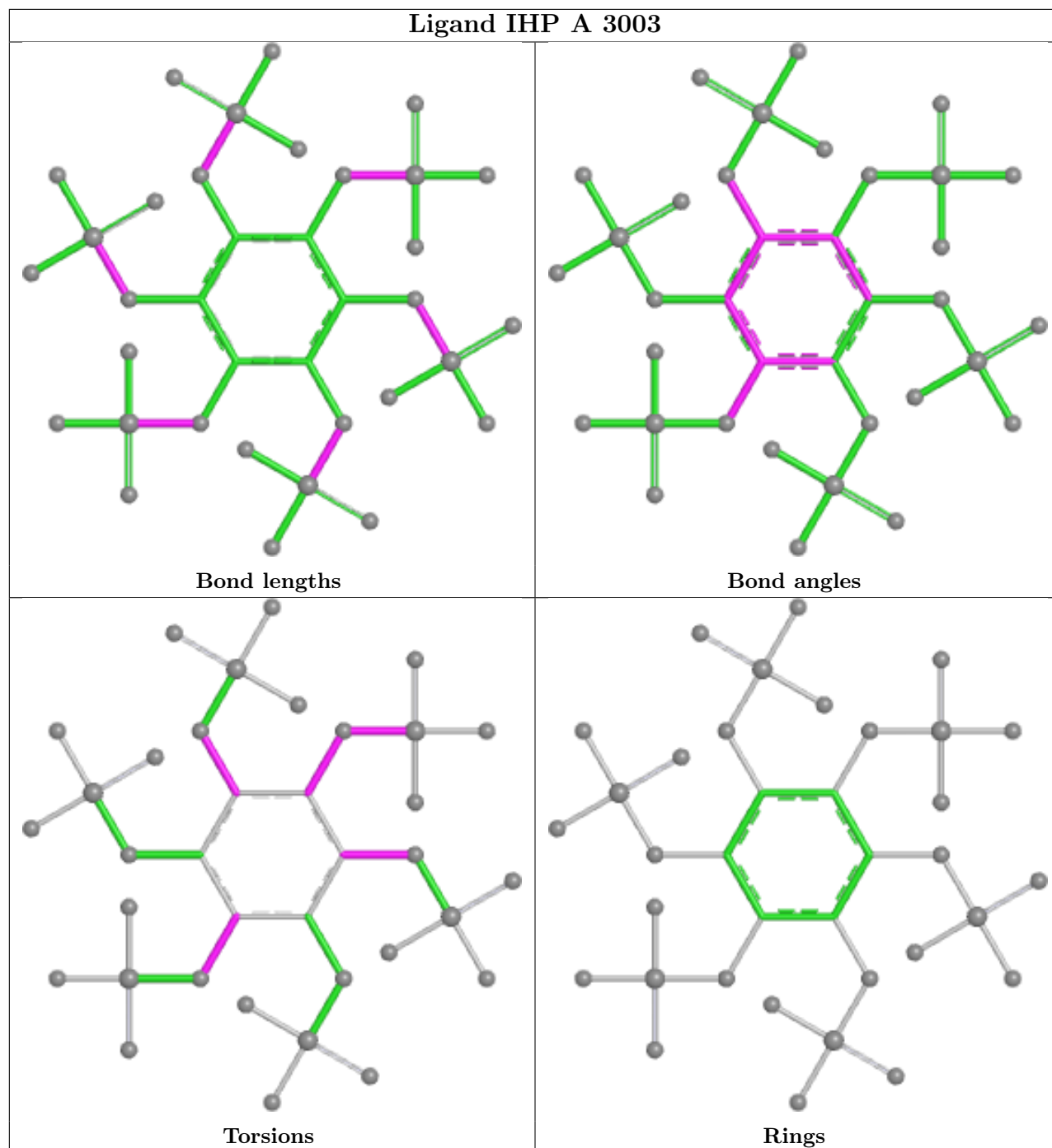
Ligand GSP L 201

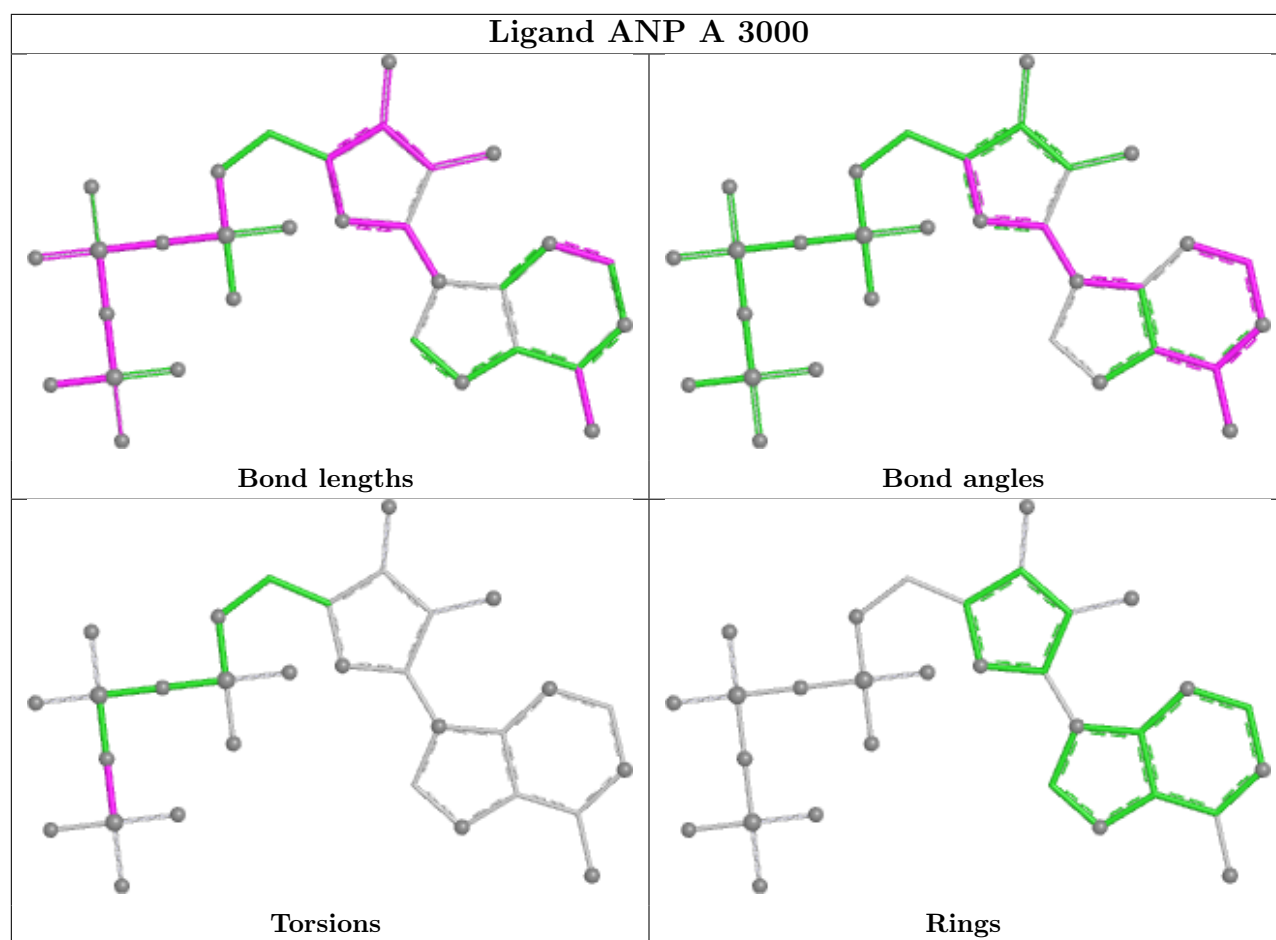












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

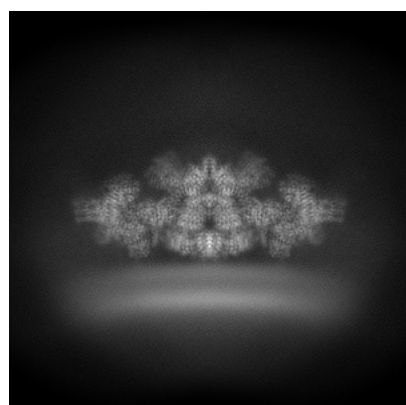
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47932. These allow visual inspection of the internal detail of the map and identification of artifacts.

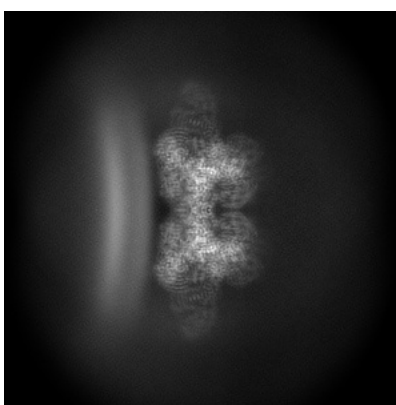
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

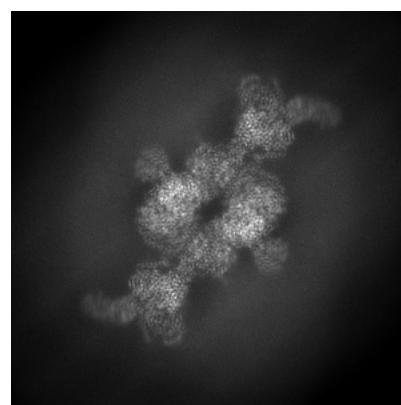
6.1.1 Primary map



X



Y

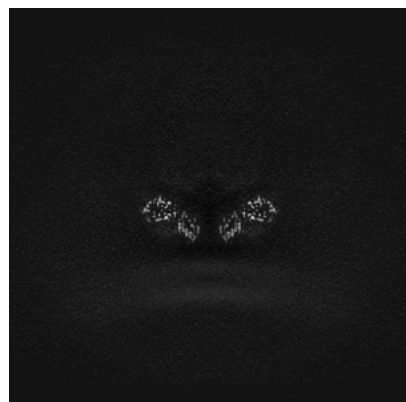


Z

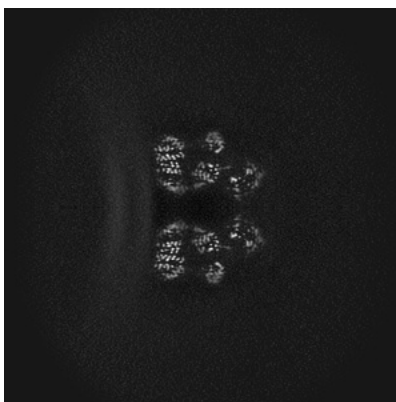
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

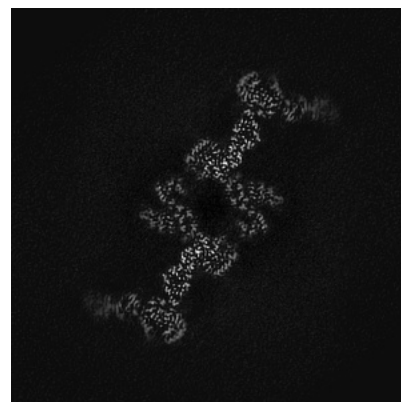
6.2.1 Primary map



X Index: 224



Y Index: 224



Z Index: 224

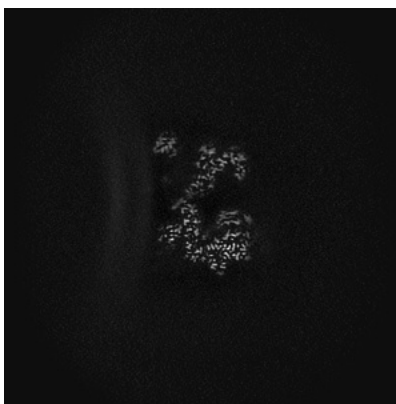
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

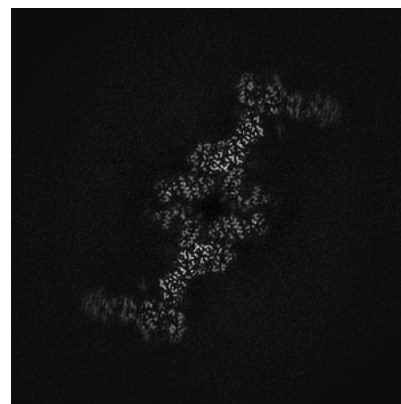
6.3.1 Primary map



X Index: 178



Y Index: 241

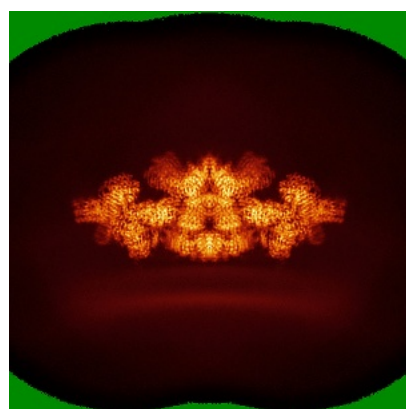


Z Index: 216

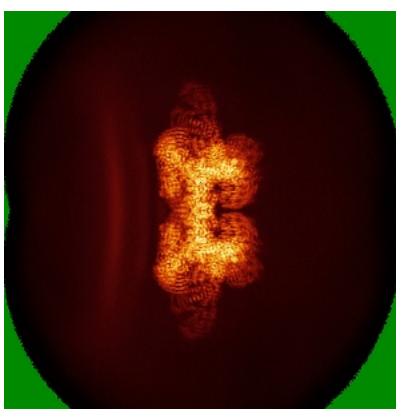
The images above show the largest variance slices of the map in three orthogonal directions.

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

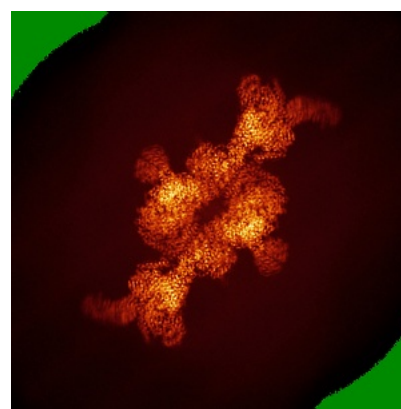
6.4.1 Primary map



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

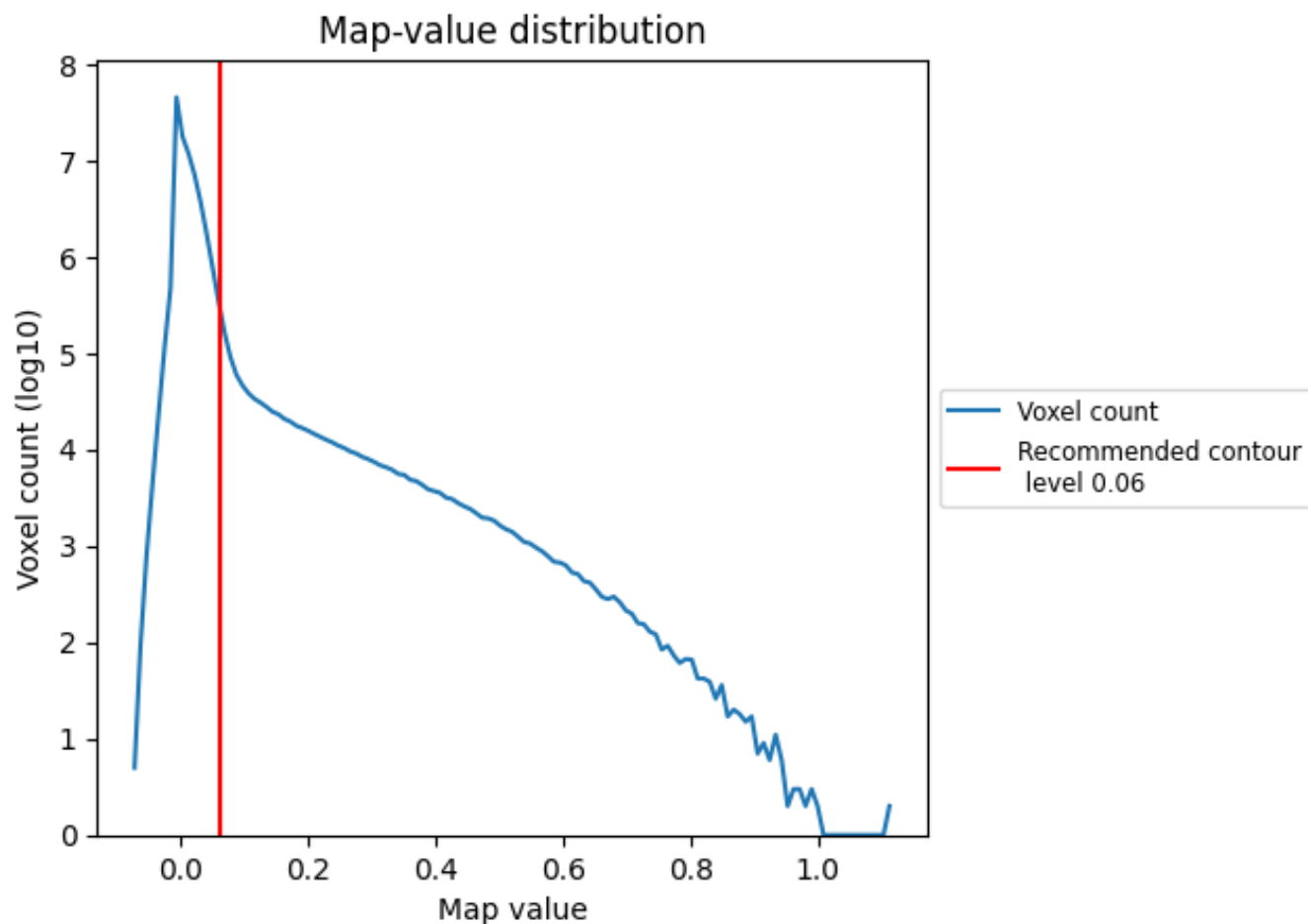
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

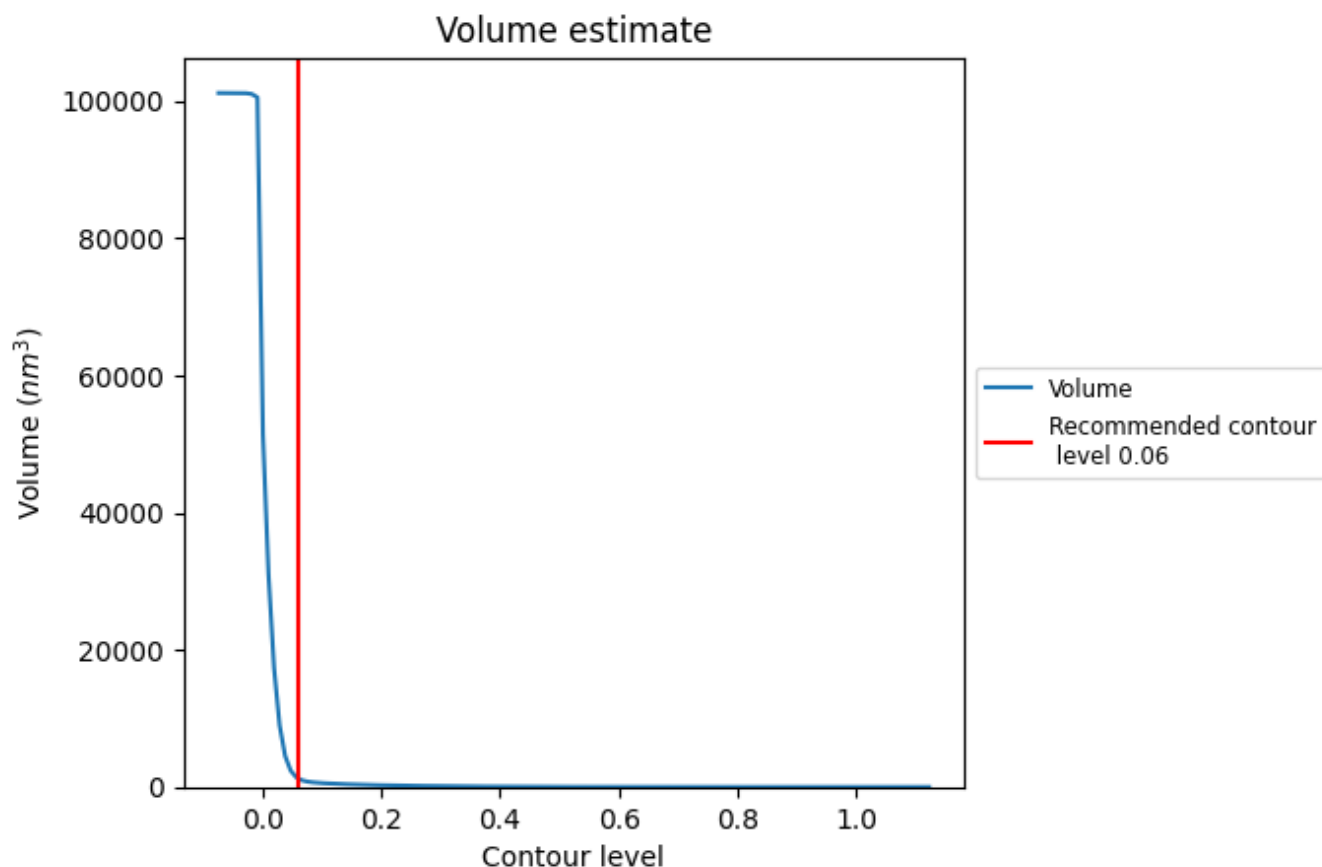
This section contains the results of statistical analysis of the map.

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.

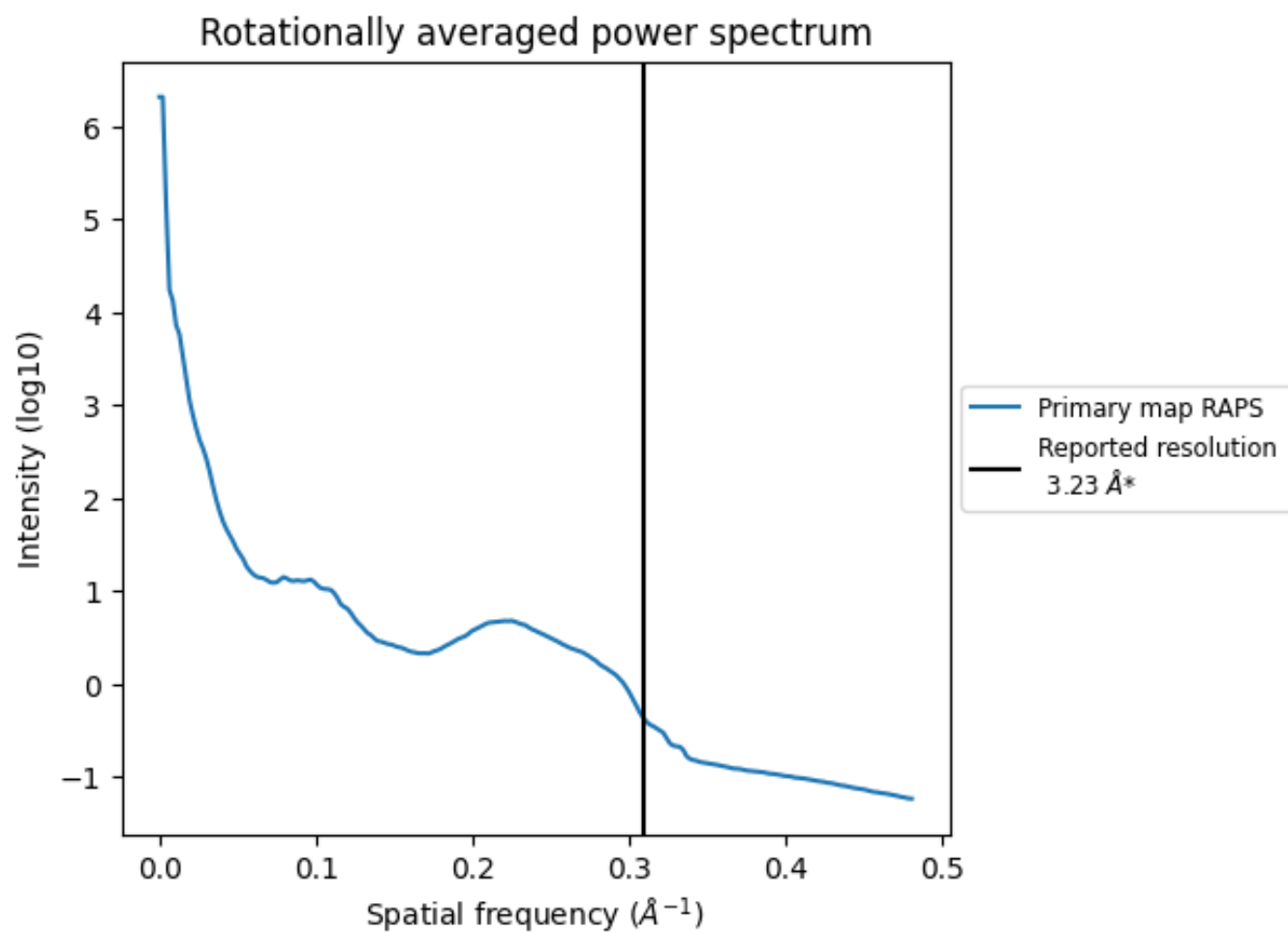
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1293 nm^3 ; this corresponds to an approximate mass of 1168 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 0.310 Å⁻¹

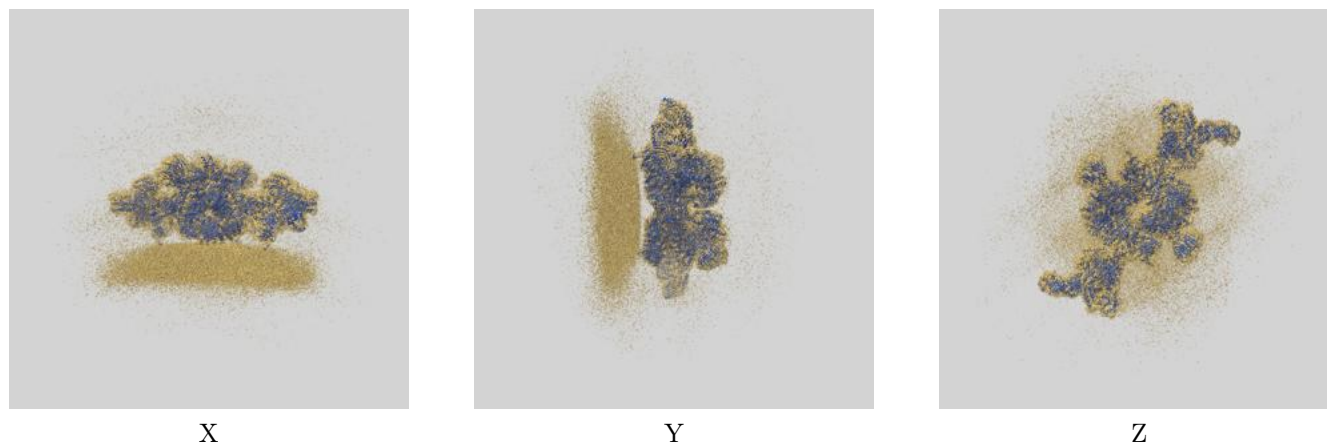
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

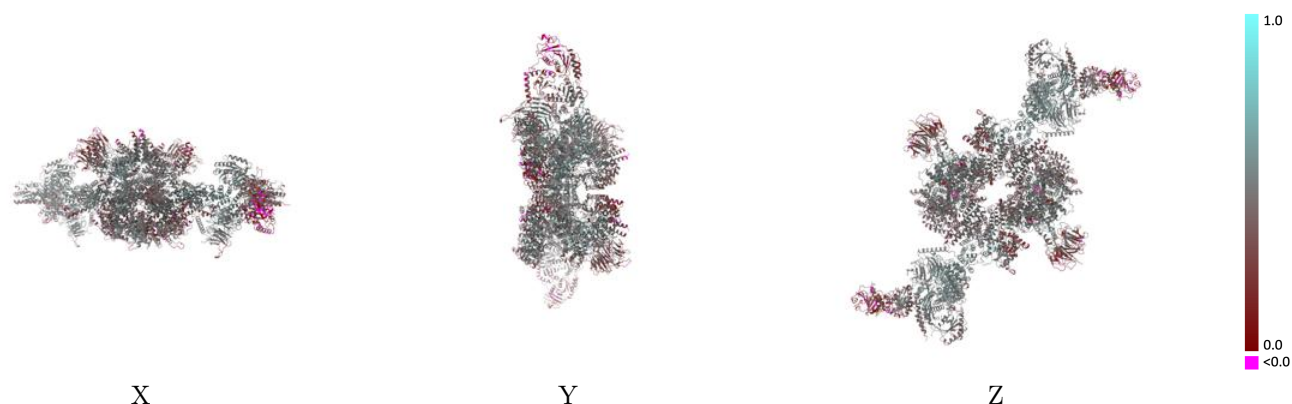
This section contains information regarding the fit between EMDB map EMD-47932 and PDB model 9ED4. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



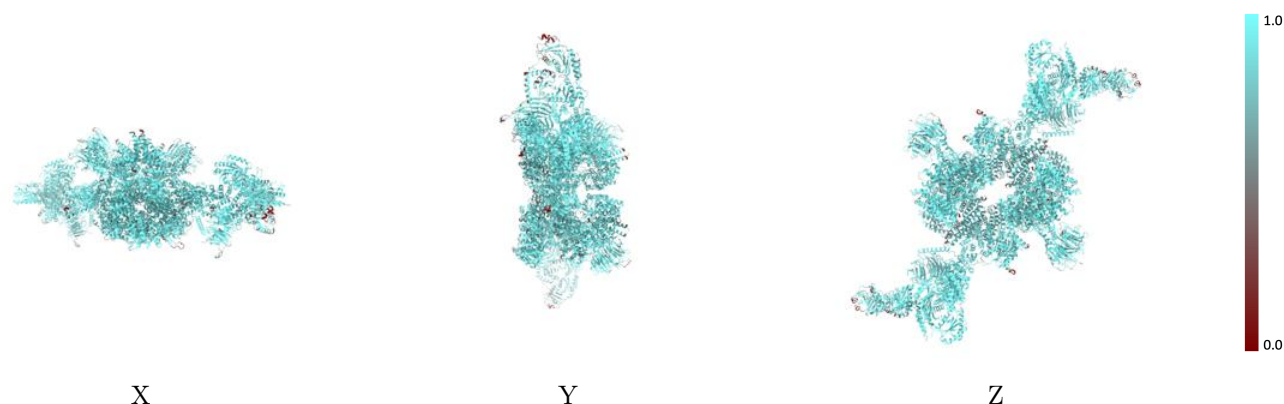
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



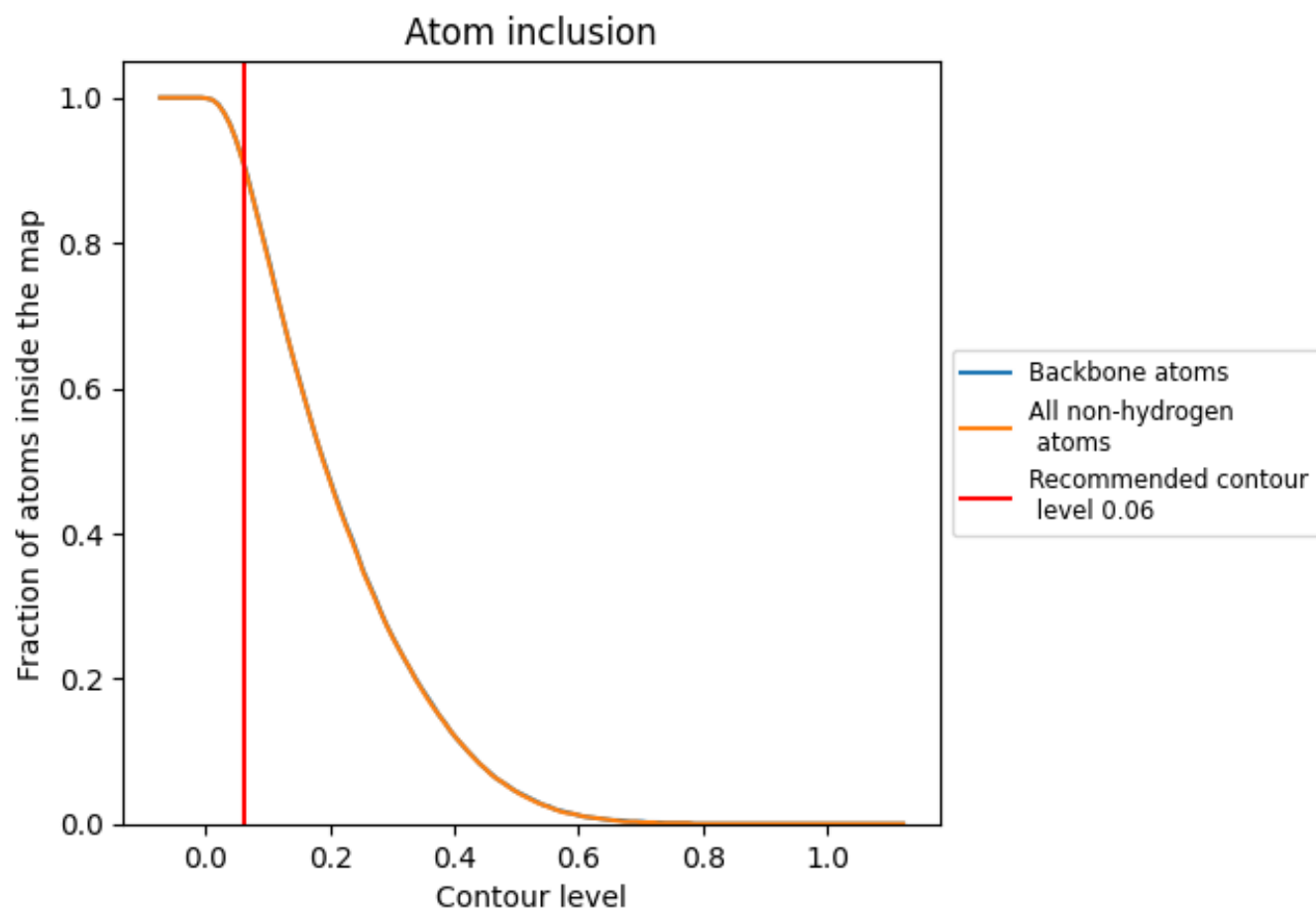
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 91% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9110	 0.4270
A	 0.9120	 0.4250
B	 0.8730	 0.3160
C	 0.9490	 0.4890
D	 0.9670	 0.5040
E	 0.9480	 0.4580
F	 0.7390	 0.2440
G	 0.9150	 0.3910
H	 0.8290	 0.2810
I	 0.6790	 0.1580
J	 0.8160	 0.2490
K	 0.7830	 0.4120
L	 0.9400	 0.4870
M	 0.8730	 0.3170
N	 0.9400	 0.4850
O	 0.9120	 0.4240
P	 0.9670	 0.5030
Q	 0.9140	 0.3950
R	 0.8290	 0.2840
S	 0.8180	 0.2540
T	 0.7830	 0.4070
U	 0.9500	 0.4910
V	 0.9480	 0.4570
W	 0.7360	 0.2470
X	 0.6800	 0.1600

