



wwPDB EM Validation Summary Report ⓘ

Nov 3, 2024 – 04:22 PM EST

PDB ID : 7K58
EMDB ID : EMD-22677
Title : Structure of outer-arm dyneins bound to microtubule with microtubule binding state 1(MTBS-1)
Authors : Qinhui, R.; Kai, Z.
Deposited on : 2020-09-16
Resolution : 4.00 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

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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 : 2022.3.0, CSD as543be (2022)
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

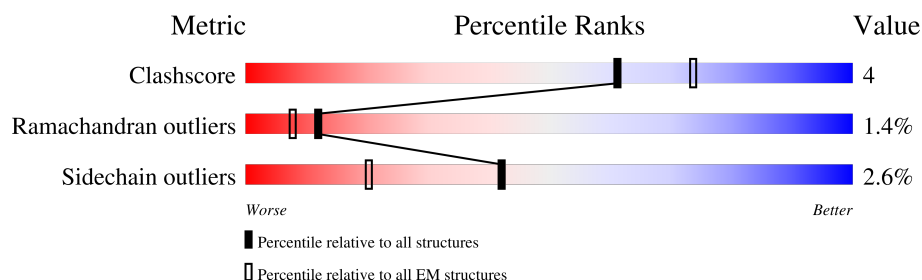
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
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 ≥ 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	4615	<div> <div>19%</div> <div>86%</div> <div>9%</div> <div>•</div> </div>
2	C	3943	<div> <div>22%</div> <div>90%</div> <div>10%</div> <div>•</div> </div>
3	Q	192	<div> <div>12%</div> <div>95%</div> <div>5%</div> <div></div> </div>
4	B	4588	<div> <div>17%</div> <div>85%</div> <div>12%</div> <div>••</div> </div>
5	I	106	<div> <div>26%</div> <div>79%</div> <div>18%</div> <div>•</div> </div>
6	H	91	<div> <div>30%</div> <div>90%</div> <div>9%</div> <div>•</div> </div>
7	G	96	<div> <div>31%</div> <div>86%</div> <div>14%</div> <div></div> </div>
8	F	110	<div> <div>25%</div> <div>82%</div> <div>17%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
9	N	114	
10	O	120	
11	E	557	
12	D	595	
13	P	112	
14	L	98	
15	K	90	
16	J	95	
17	M	87	

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 117936 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 Dynein heavy chain, outer arm protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4443	Total	C	N	O	S	0	0
			33894	21519	5788	6429	158		

- Molecule 2 is a protein called gamma heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	3943	Total	C	N	O	S	0	0
			30436	19390	5162	5735	149		

- Molecule 3 is a protein called Dynein light chain 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	Q	192	Total	C	N	O	2	0
			1002	607	202	193		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Q	2	ALA	SER	conflict	UNP Q1HGH9

- Molecule 4 is a protein called Outer arm dynein beta heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	4516	Total	C	N	O	S	0	0
			34604	21978	5928	6547	151		

- Molecule 5 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	106	Total	C	N	O	S	0	0
			827	526	134	161	6		

- Molecule 6 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	91	Total	C	N	O	S	0	0
			750	483	124	139	4		

- Molecule 7 is a protein called Dynein light chain roadblock.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	96	Total	C	N	O	S	0	0
			749	471	129	148	1		

- Molecule 8 is a protein called Dynein light chain roadblock-type 2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	F	110	Total	C	N	O	S	0	0
			863	544	152	165	2		

- Molecule 9 is a protein called Dynein light chain tctex-type 1 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	114	Total	C	N	O	S	0	0
			855	543	143	166	3		

- Molecule 10 is a protein called Dynein light chain 2A.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	120	Total	C	N	O	S	0	0
			986	634	172	177	3		

- Molecule 11 is a protein called Flagellar outer dynein arm intermediate protein, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	E	555	Total	C	N	O	S	0	0
			4423	2786	759	856	22		

- Molecule 12 is a protein called Dynein intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	579	Total	C	N	O	S	0	0
			4664	2964	787	883	30		

- Molecule 13 is a protein called Thioredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace
13	P	109	Total	C	N	O	0	0
			541	323	109	109		

- Molecule 14 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	98	Total	C	N	O	S	0	0
			783	511	132	137	3		

- Molecule 15 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	90	Total	C	N	O	S	0	0
			754	489	124	137	4		

- Molecule 16 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	J	95	Total	C	N	O	S	0	0
			806	527	135	140	4		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	32	ALA	CYS	conflict	UNP Q22R86

- Molecule 17 is a protein called Dynein light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	M	87	Total	C	N	O	S	0	0
			735	477	123	130	5		

- Molecule 18 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
18	A	1	Total 27	C 10	N 5	O 10	P 2	0
18	A	1	Total 27	C 10	N 5	O 10	P 2	0
18	C	1	Total 27	C 10	N 5	O 10	P 2	0
18	C	1	Total 27	C 10	N 5	O 10	P 2	0
18	B	1	Total 27	C 10	N 5	O 10	P 2	0
18	B	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 19 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 31	C 10	N 5	O 13	P 3	0
19	C	1	Total 31	C 10	N 5	O 13	P 3	0
19	B	1	Total 31	C 10	N 5	O 13	P 3	0

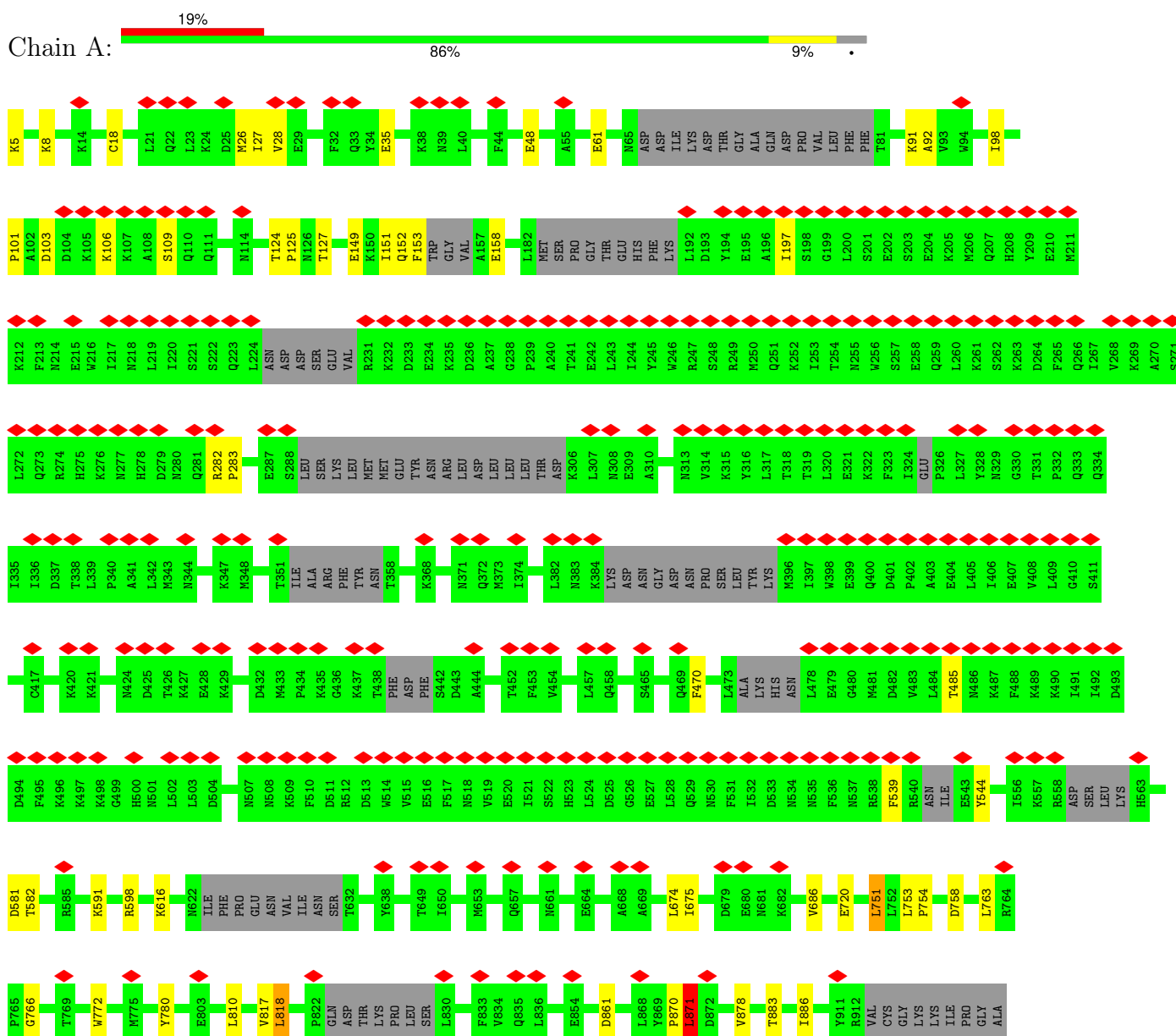
- Molecule 20 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

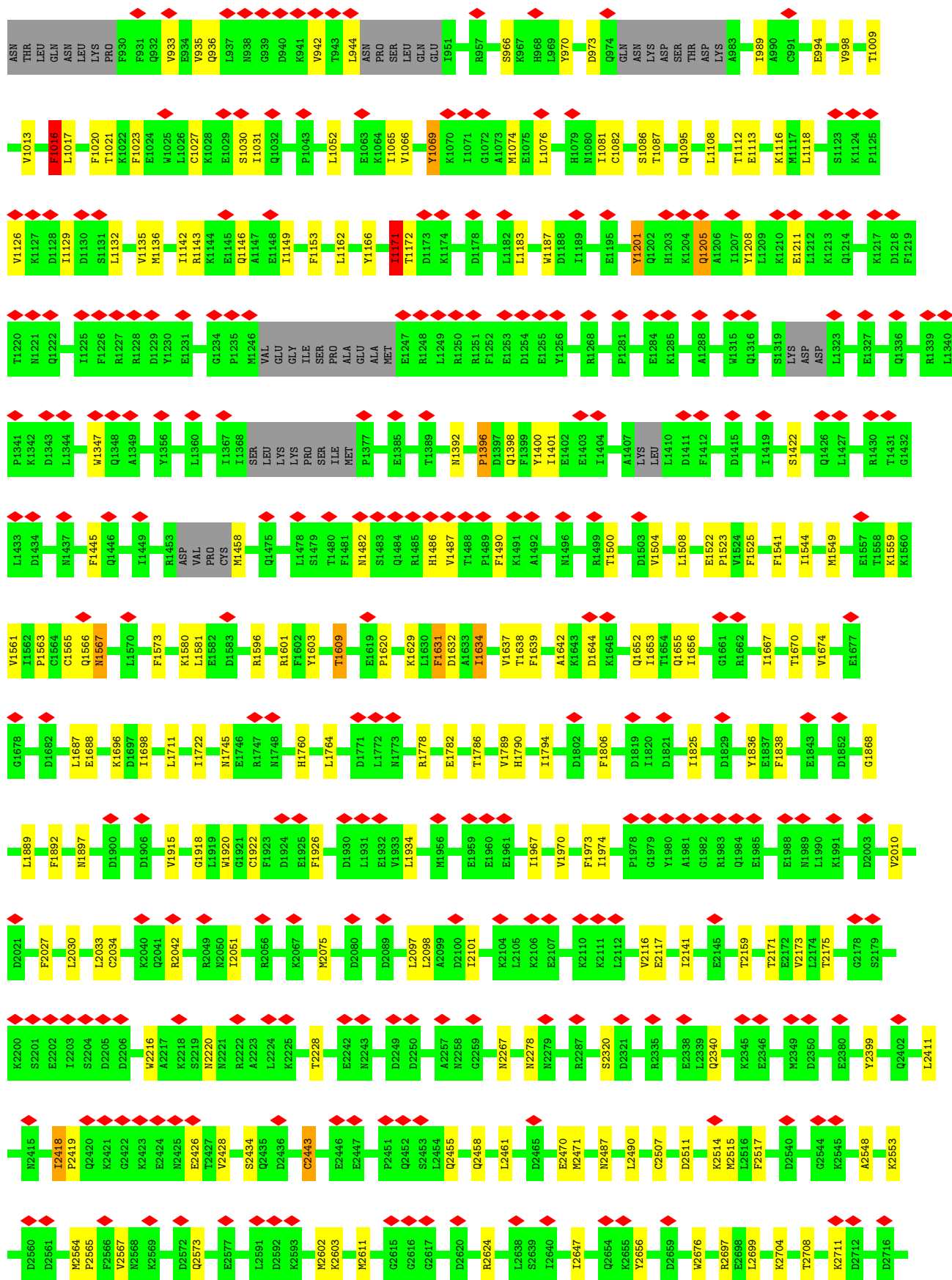
Mol	Chain	Residues	Atoms	AltConf
20	A	3	Total Mg 3 3	0
20	C	3	Total Mg 3 3	0
20	B	3	Total Mg 3 3	0

3 Residue-property plots

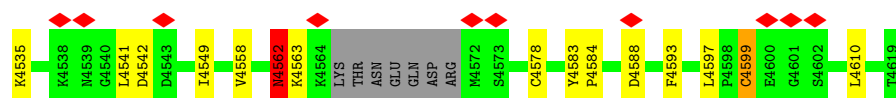
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Dynein heavy chain, outer arm protein

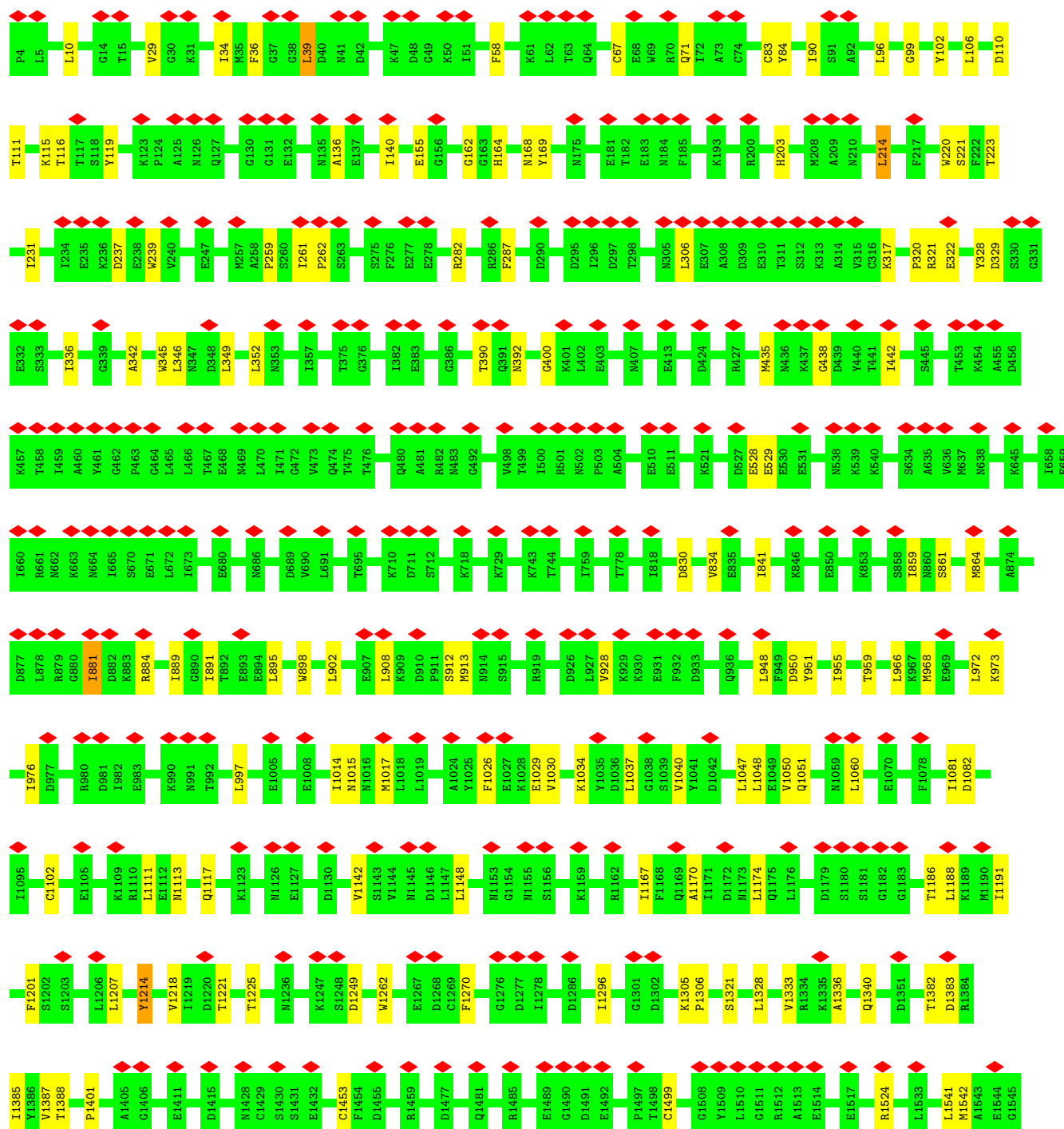
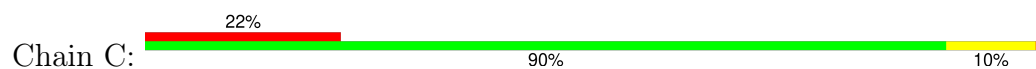


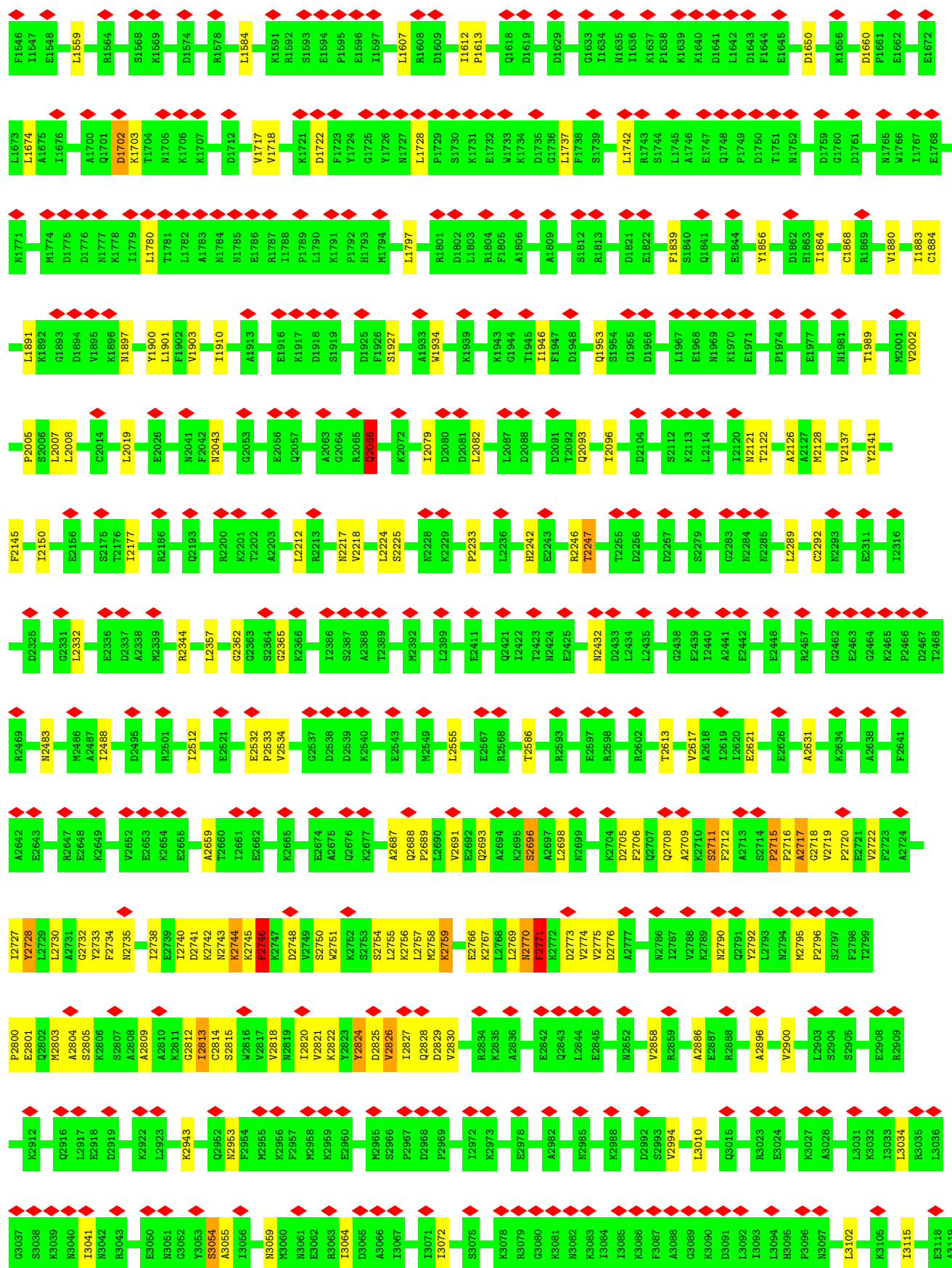






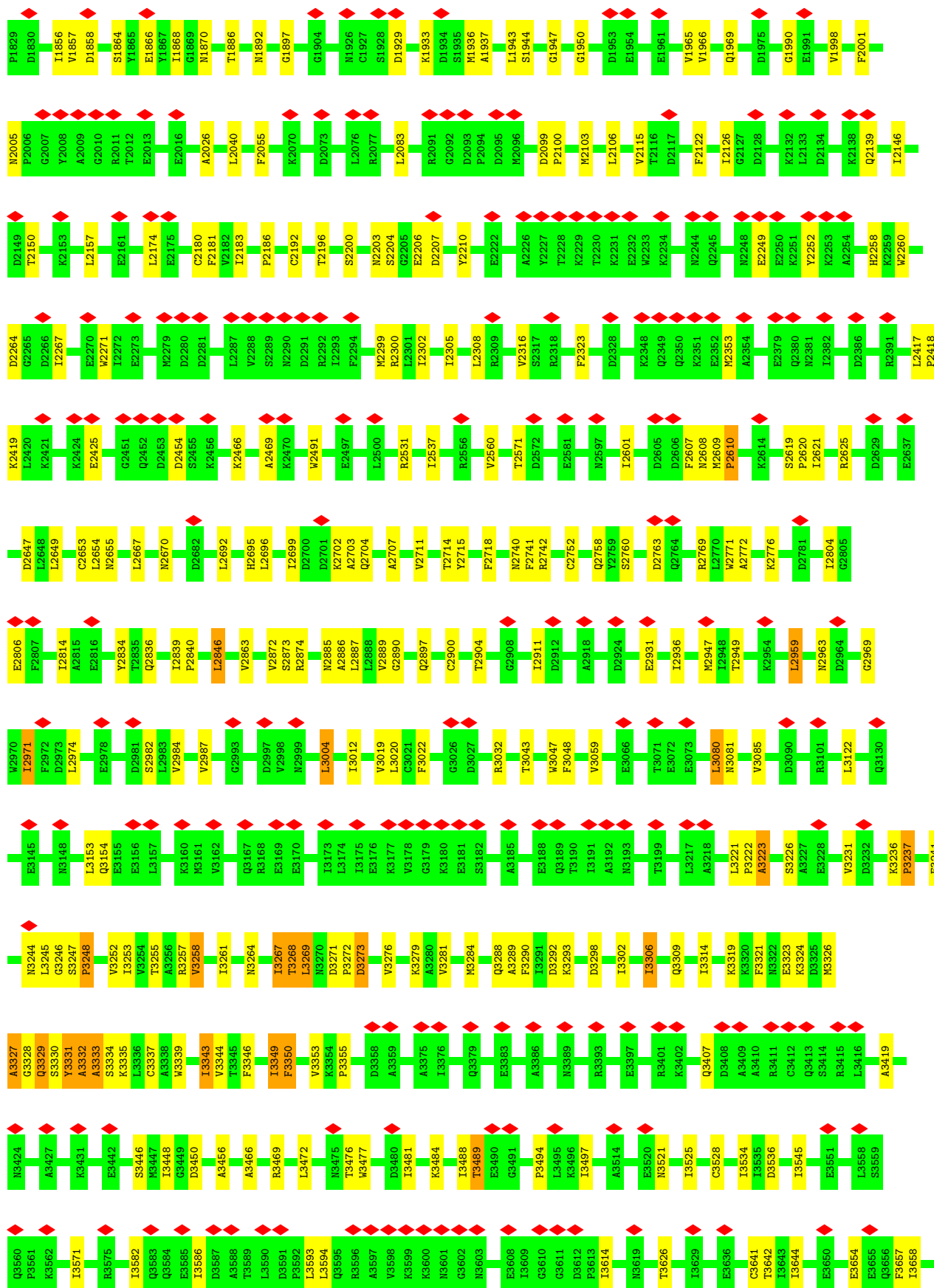
• Molecule 2: gamma heavy chain

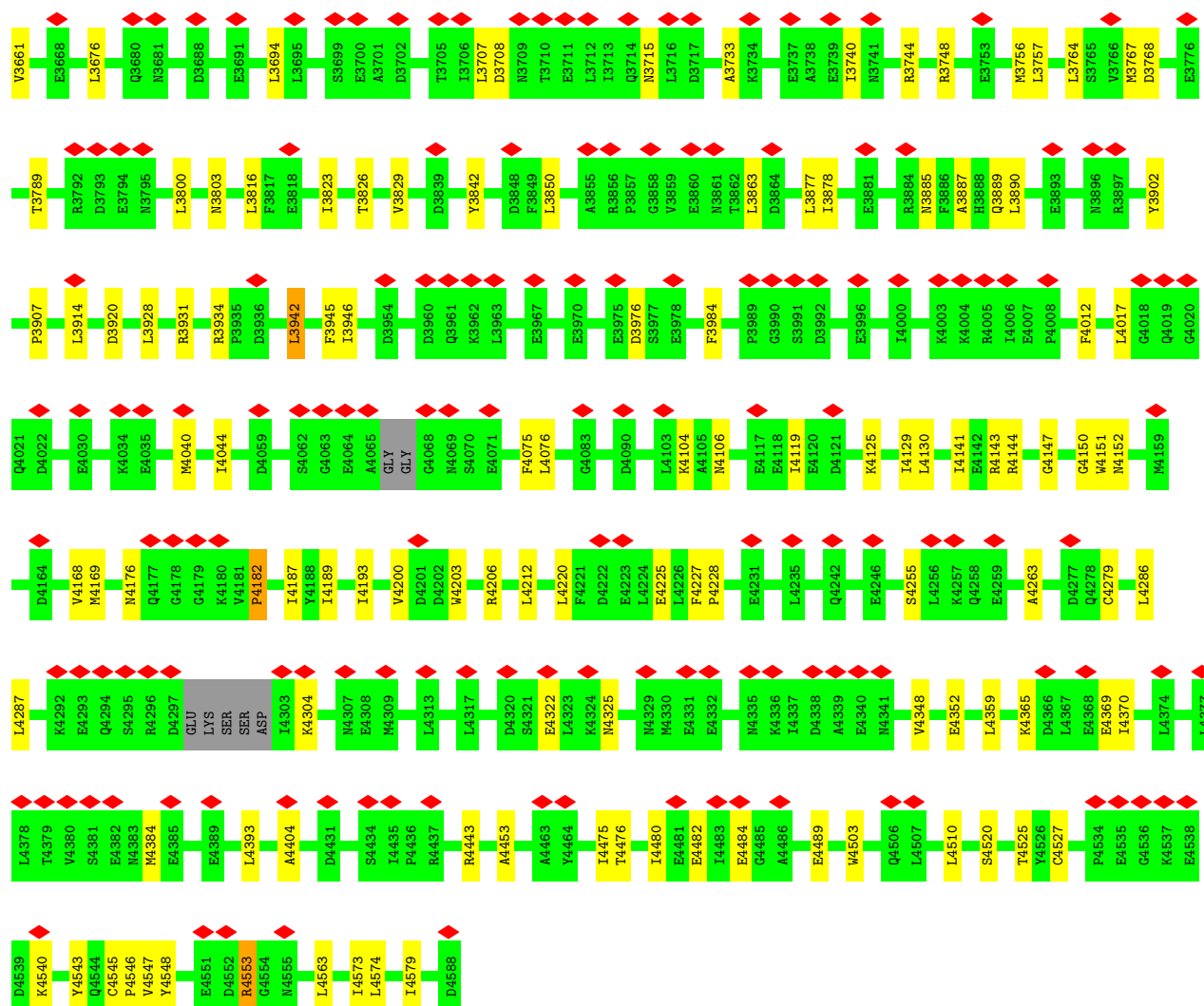




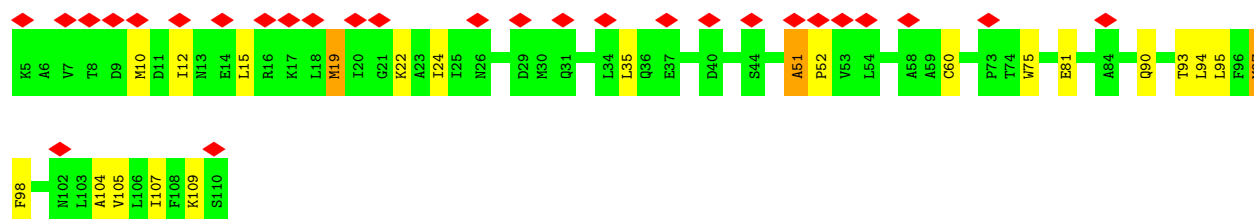
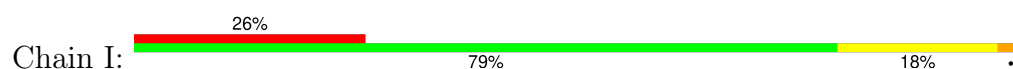




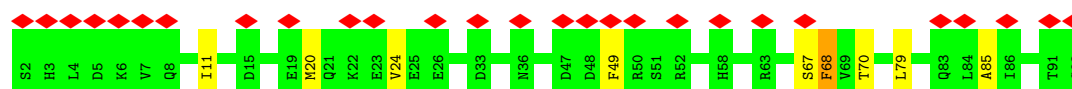
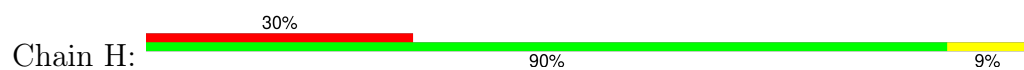




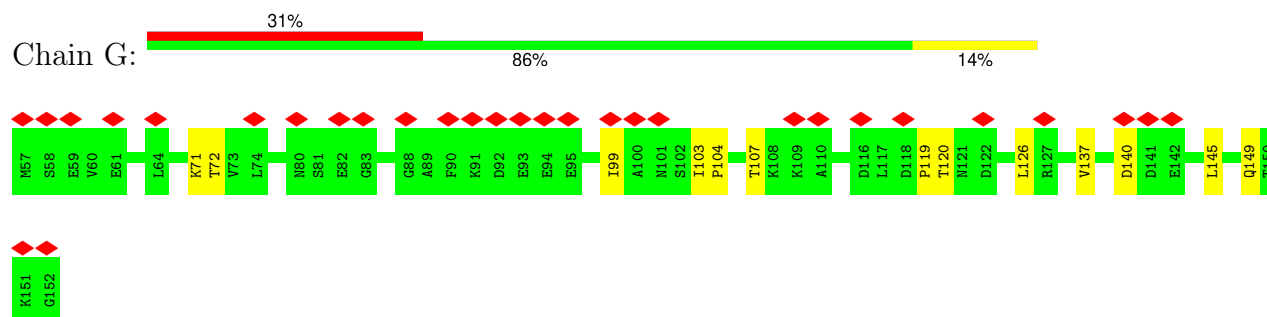
• Molecule 5: Dynein light chain



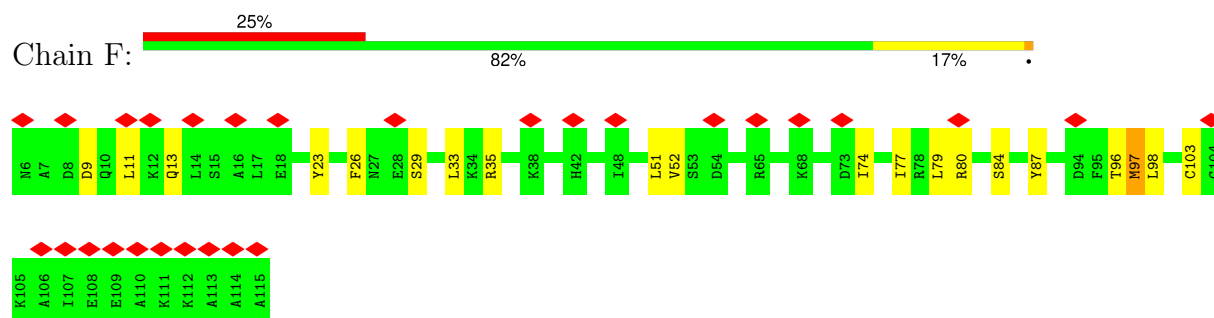
• Molecule 6: Dynein light chain



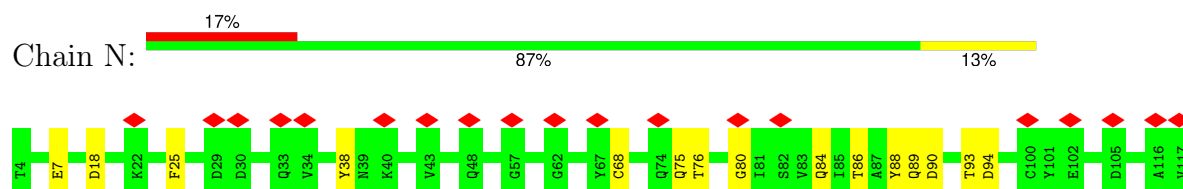
- Molecule 7: Dynein light chain roadblock



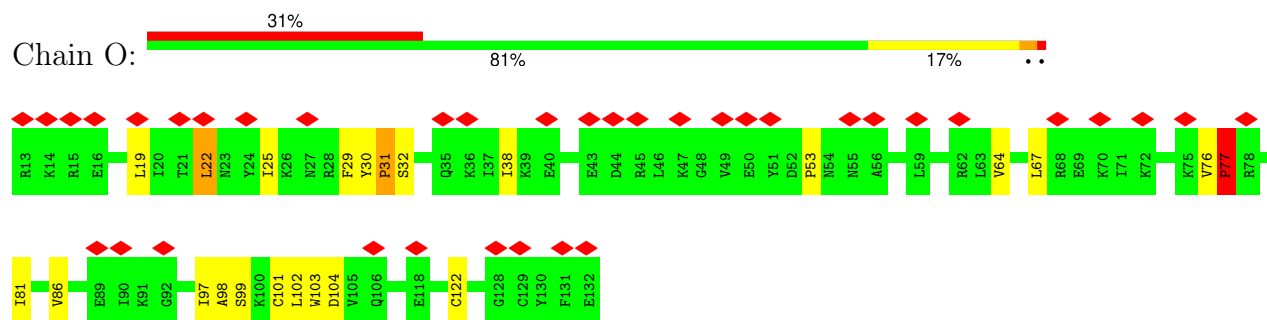
- Molecule 8: Dynein light chain roadblock-type 2 protein



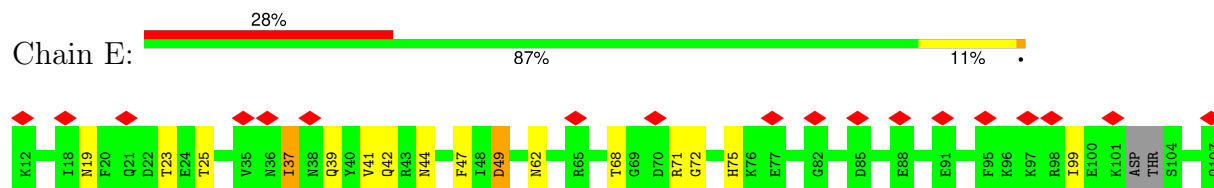
- Molecule 9: Dynein light chain tctex-type 1 protein

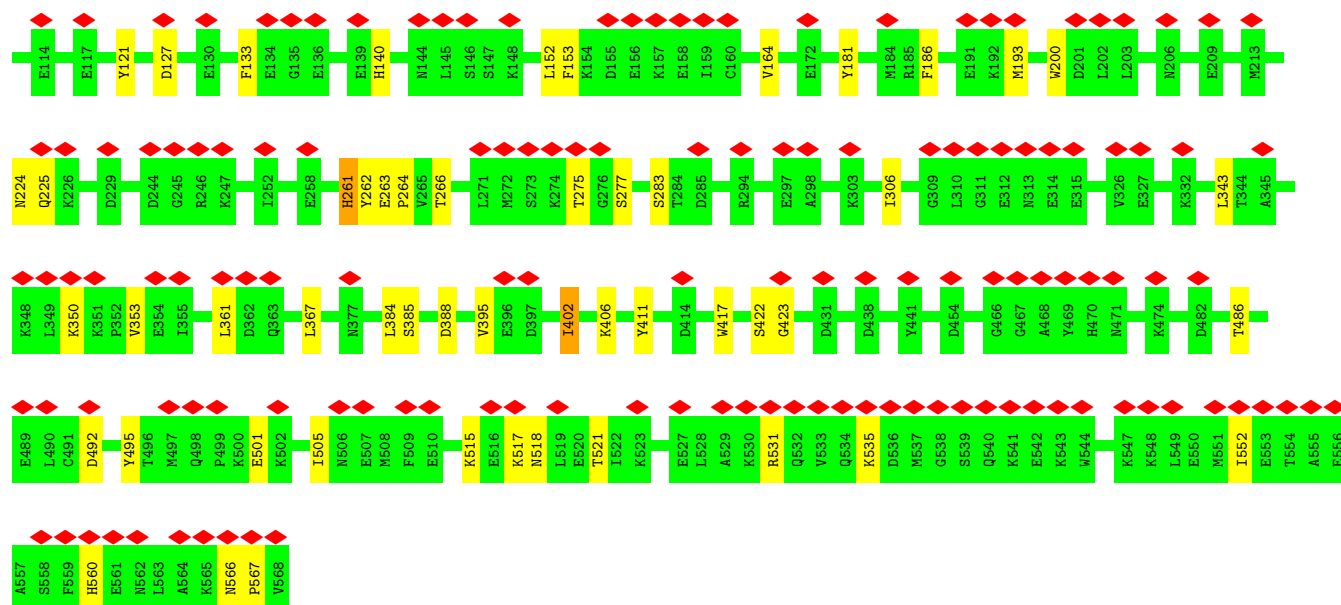


- Molecule 10: Dynein light chain 2A

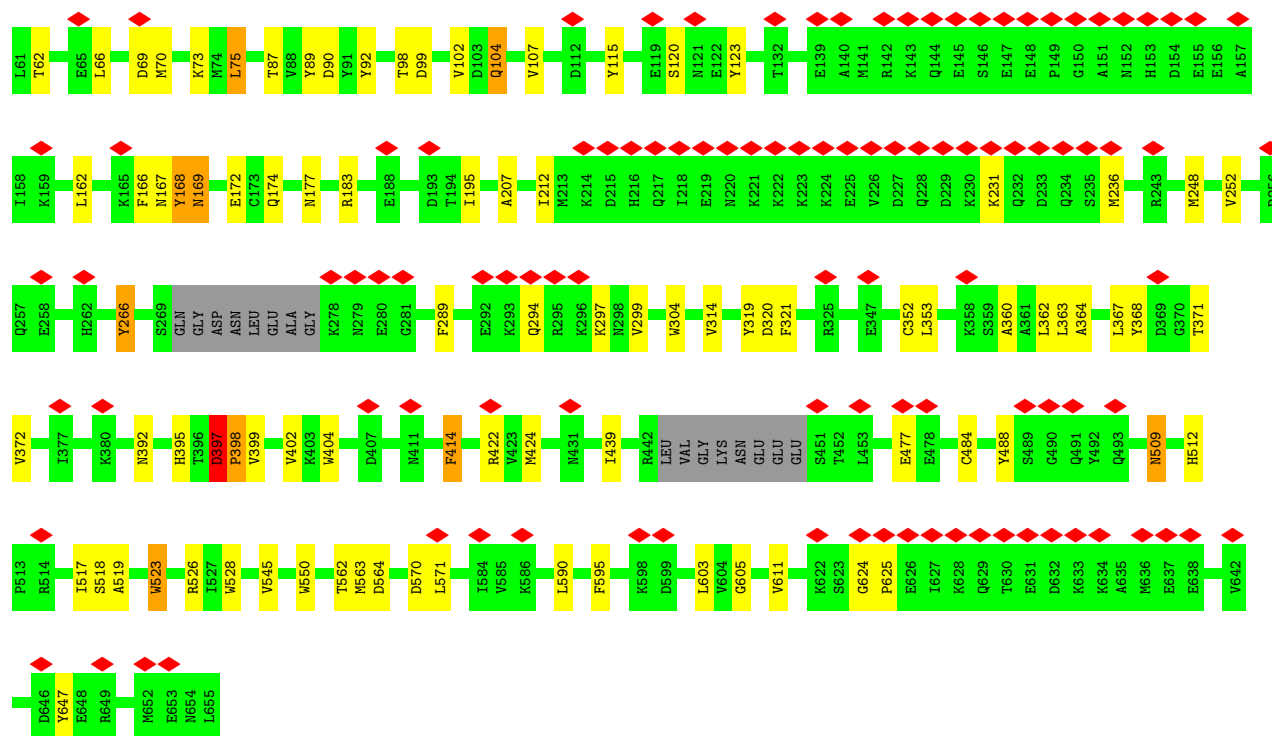
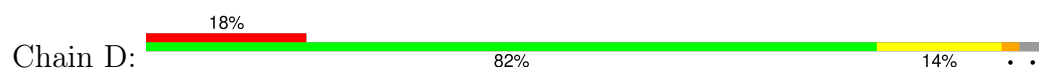


- Molecule 11: Flagellar outer dynein arm intermediate protein, putative

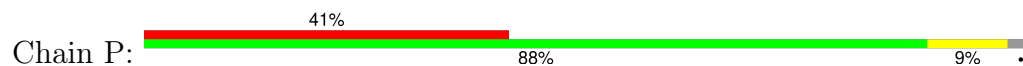


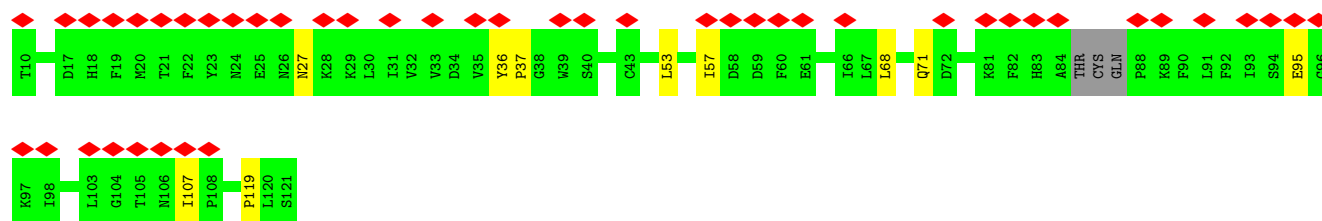


• Molecule 12: Dynein intermediate chain 2

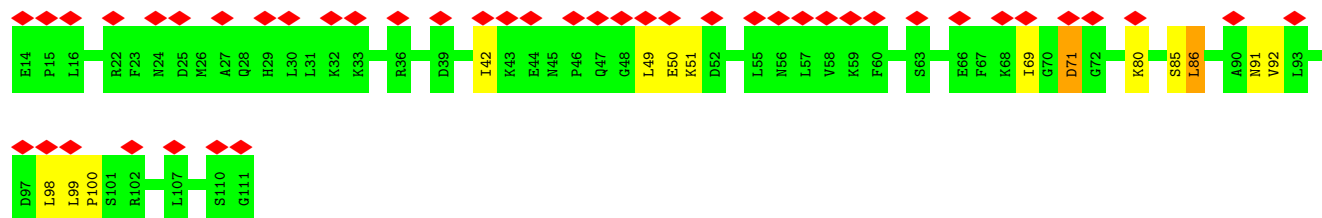
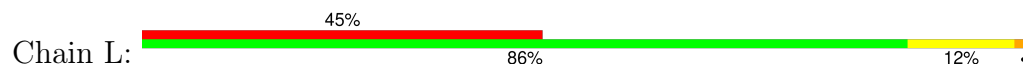


• Molecule 13: Thioredoxin

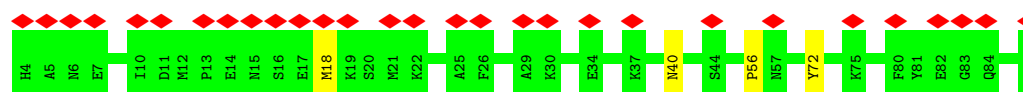




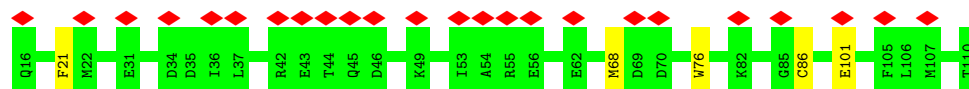
• Molecule 14: Dynein light chain



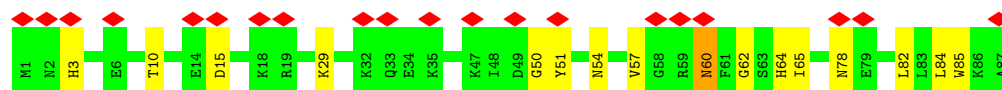
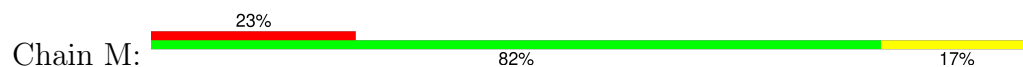
• Molecule 15: Dynein light chain



• Molecule 16: Dynein light chain



• Molecule 17: Dynein light chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191776	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.3	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	11.012	Depositor
Minimum map value	0.000	Depositor
Average map value	0.020	Depositor
Map value standard deviation	0.134	Depositor
Recommended contour level	0.8	Depositor
Map size (Å)	530.5338, 477.21387, 449.22086	wwPDB
Map dimensions	398, 358, 337	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3329996, 1.3329996, 1.3329996	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: ADP, ATP, 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	A	0.69	0/34464	0.78	1/46623 (0.0%)
2	C	0.68	0/31038	0.77	1/42003 (0.0%)
3	Q	0.86	0/1005	0.84	0/1388
4	B	0.69	1/35205 (0.0%)	0.80	3/47647 (0.0%)
5	I	0.69	0/838	0.77	0/1131
6	H	0.67	0/767	0.76	0/1031
7	G	0.69	0/755	0.77	0/1018
8	F	0.68	0/875	0.77	0/1178
9	N	0.69	0/867	0.79	0/1179
10	O	0.67	0/1004	0.80	0/1349
11	E	0.67	0/4522	0.78	0/6114
12	D	0.66	0/4772	0.78	1/6458 (0.0%)
13	P	0.87	0/538	0.86	0/746
14	L	0.66	0/800	0.76	0/1076
15	K	0.66	0/776	0.73	0/1038
16	J	0.63	0/831	0.74	0/1118
17	M	0.65	0/752	0.76	0/1006
All	All	0.69	1/119809 (0.0%)	0.78	6/162103 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	C	0	3
4	B	0	4
11	E	0	1
All	All	0	10

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	730	LEU	C-O	5.23	1.33	1.23

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3248	PRO	N-CA-CB	-6.26	95.71	102.60
4	B	533	ARG	CB-CA-C	6.19	122.77	110.40
4	B	1127	ASN	CB-CA-C	5.71	121.82	110.40
12	D	397	ASP	CB-CA-C	5.18	120.76	110.40
1	A	1016	PHE	CB-CA-C	5.13	120.66	110.40

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	35	GLU	Peptide
1	A	4250	ARG	Peptide
2	C	2717	ALA	Peptide
2	C	2746	PRO	Peptide
2	C	528	GLU	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	33894	0	32288	250	0
2	C	30436	0	29392	239	0
3	Q	1002	0	501	6	0
4	B	34604	0	33094	332	0
5	I	827	0	829	17	0
6	H	750	0	735	7	0
7	G	749	0	772	10	0
8	F	863	0	881	9	0
9	N	855	0	800	12	0
10	O	986	0	1002	12	0
11	E	4423	0	4291	40	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	D	4664	0	4484	57	0
13	P	541	0	220	2	0
14	L	783	0	811	10	0
15	K	754	0	716	3	0
16	J	806	0	772	1	0
17	M	735	0	738	9	0
18	A	54	0	24	2	0
18	B	54	0	24	0	0
18	C	54	0	24	3	0
19	A	31	0	12	0	0
19	B	31	0	12	1	0
19	C	31	0	12	0	0
20	A	3	0	0	0	0
20	B	3	0	0	0	0
20	C	3	0	0	0	0
All	All	117936	0	112434	961	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 961 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:764:GLN:O	4:B:765:PHE:C	1.73	1.26
4:B:764:GLN:O	4:B:766:ILE:N	1.79	1.12
4:B:750:PRO:O	4:B:752:ILE:N	1.89	1.05
4:B:3255:THR:OG1	4:B:3337:CYS:SG	2.13	1.02
2:C:2826:VAL:O	2:C:2829:ASP:N	1.96	0.97

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4381/4615 (95%)	4081 (93%)	257 (6%)	43 (1%)	13	47
2	C	3915/3943 (99%)	3583 (92%)	283 (7%)	49 (1%)	10	42
3	Q	190/192 (99%)	163 (86%)	24 (13%)	3 (2%)	8	38
4	B	4488/4588 (98%)	4019 (90%)	382 (8%)	87 (2%)	6	35
5	I	104/106 (98%)	95 (91%)	8 (8%)	1 (1%)	13	47
6	H	89/91 (98%)	83 (93%)	6 (7%)	0	100	100
7	G	92/96 (96%)	87 (95%)	5 (5%)	0	100	100
8	F	108/110 (98%)	96 (89%)	11 (10%)	1 (1%)	14	49
9	N	112/114 (98%)	92 (82%)	17 (15%)	3 (3%)	4	29
10	O	118/120 (98%)	104 (88%)	9 (8%)	5 (4%)	2	22
11	E	551/557 (99%)	496 (90%)	51 (9%)	4 (1%)	19	55
12	D	569/595 (96%)	510 (90%)	51 (9%)	8 (1%)	9	40
13	P	103/112 (92%)	86 (84%)	11 (11%)	6 (6%)	1	17
14	L	96/98 (98%)	91 (95%)	4 (4%)	1 (1%)	13	47
15	K	88/90 (98%)	79 (90%)	9 (10%)	0	100	100
16	J	93/95 (98%)	84 (90%)	8 (9%)	1 (1%)	12	45
17	M	85/87 (98%)	72 (85%)	11 (13%)	2 (2%)	5	31
All	All	15182/15609 (97%)	13821 (91%)	1147 (8%)	214 (1%)	12	40

5 of 214 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	PRO
1	A	197	ILE
1	A	871	LEU
1	A	973	ASP
1	A	3251	ILE

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	3420/4191 (82%)	3338 (98%)	82 (2%)	44	63
2	C	3149/3501 (90%)	3095 (98%)	54 (2%)	56	72
3	Q	10/176 (6%)	10 (100%)	0	100	100
4	B	3497/4138 (84%)	3399 (97%)	98 (3%)	38	59
5	I	91/91 (100%)	87 (96%)	4 (4%)	24	47
6	H	82/82 (100%)	81 (99%)	1 (1%)	67	78
7	G	86/87 (99%)	85 (99%)	1 (1%)	67	78
8	F	93/93 (100%)	86 (92%)	7 (8%)	11	33
9	N	85/102 (83%)	84 (99%)	1 (1%)	67	78
10	O	106/108 (98%)	99 (93%)	7 (7%)	14	37
11	E	484/496 (98%)	467 (96%)	17 (4%)	31	53
12	D	507/545 (93%)	482 (95%)	25 (5%)	21	44
14	L	87/87 (100%)	83 (95%)	4 (5%)	23	46
15	K	80/80 (100%)	79 (99%)	1 (1%)	65	77
16	J	81/81 (100%)	79 (98%)	2 (2%)	42	62
17	M	78/78 (100%)	74 (95%)	4 (5%)	20	43
All	All	11936/13936 (86%)	11628 (97%)	308 (3%)	42	61

5 of 308 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	B	4540	LYS
12	D	392	ASN
6	H	68	PHE
11	E	193	MET
14	L	86	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 143 such sidechains are listed below:

Mol	Chain	Res	Type
4	B	4176	ASN
7	G	129	GLN
11	E	481	GLN
2	C	1428	ASN
2	C	1300	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	$\# Z > 2$
18	ADP	C	4801	20	24,29,29	0.72	0	29,45,45	1.04	2 (6%)
18	ADP	B	5501	20	24,29,29	0.75	0	29,45,45	0.93	2 (6%)
19	ATP	C	4201	20	28,33,33	0.70	0	34,52,52	0.78	1 (2%)
18	ADP	A	4701	20	24,29,29	0.74	0	29,45,45	0.79	1 (3%)
18	ADP	C	4401	20	24,29,29	0.75	1 (4%)	29,45,45	1.25	3 (10%)
18	ADP	A	4901	-	24,29,29	0.75	0	29,45,45	1.04	2 (6%)
18	ADP	B	5601	20	24,29,29	0.74	0	29,45,45	0.69	1 (3%)
19	ATP	B	4701	20	28,33,33	0.71	0	34,52,52	0.85	1 (2%)
19	ATP	A	4801	20	28,33,33	0.70	0	34,52,52	0.79	1 (2%)

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
18	ADP	C	4801	20	-	4/12/32/32	0/3/3/3
18	ADP	B	5501	20	-	5/12/32/32	0/3/3/3
19	ATP	C	4201	20	-	4/18/38/38	0/3/3/3
18	ADP	A	4701	20	-	5/12/32/32	0/3/3/3
18	ADP	C	4401	20	-	5/12/32/32	0/3/3/3
18	ADP	A	4901	-	-	1/12/32/32	0/3/3/3
18	ADP	B	5601	20	-	2/12/32/32	0/3/3/3
19	ATP	B	4701	20	-	0/18/38/38	0/3/3/3
19	ATP	A	4801	20	-	5/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	C	4401	ADP	C8-N7	-2.02	1.31	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	C	4401	ADP	C4'-O4'-C1'	-4.32	105.97	109.92
18	A	4901	ADP	C4'-O4'-C1'	-3.85	106.40	109.92
18	C	4801	ADP	C4'-O4'-C1'	-3.63	106.60	109.92
18	C	4401	ADP	C1'-N9-C4	2.72	131.41	126.64
19	B	4701	ATP	C5-C6-N6	2.45	124.04	120.31

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	A	4701	ADP	PA-O3A-PB-O3B
18	C	4401	ADP	C5'-O5'-PA-O1A
18	C	4401	ADP	C5'-O5'-PA-O2A
18	C	4401	ADP	C5'-O5'-PA-O3A
18	C	4801	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

5 monomers are involved in 6 short contacts:

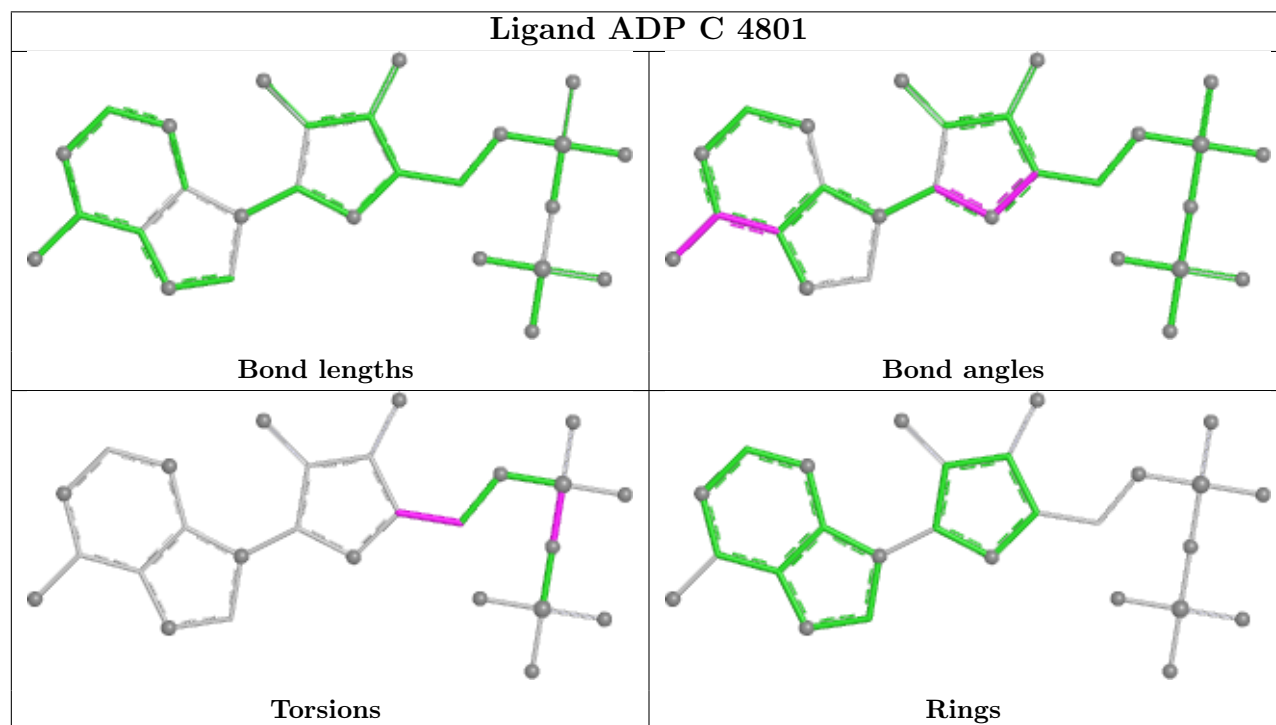
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4801	ADP	2	0
18	A	4701	ADP	1	0

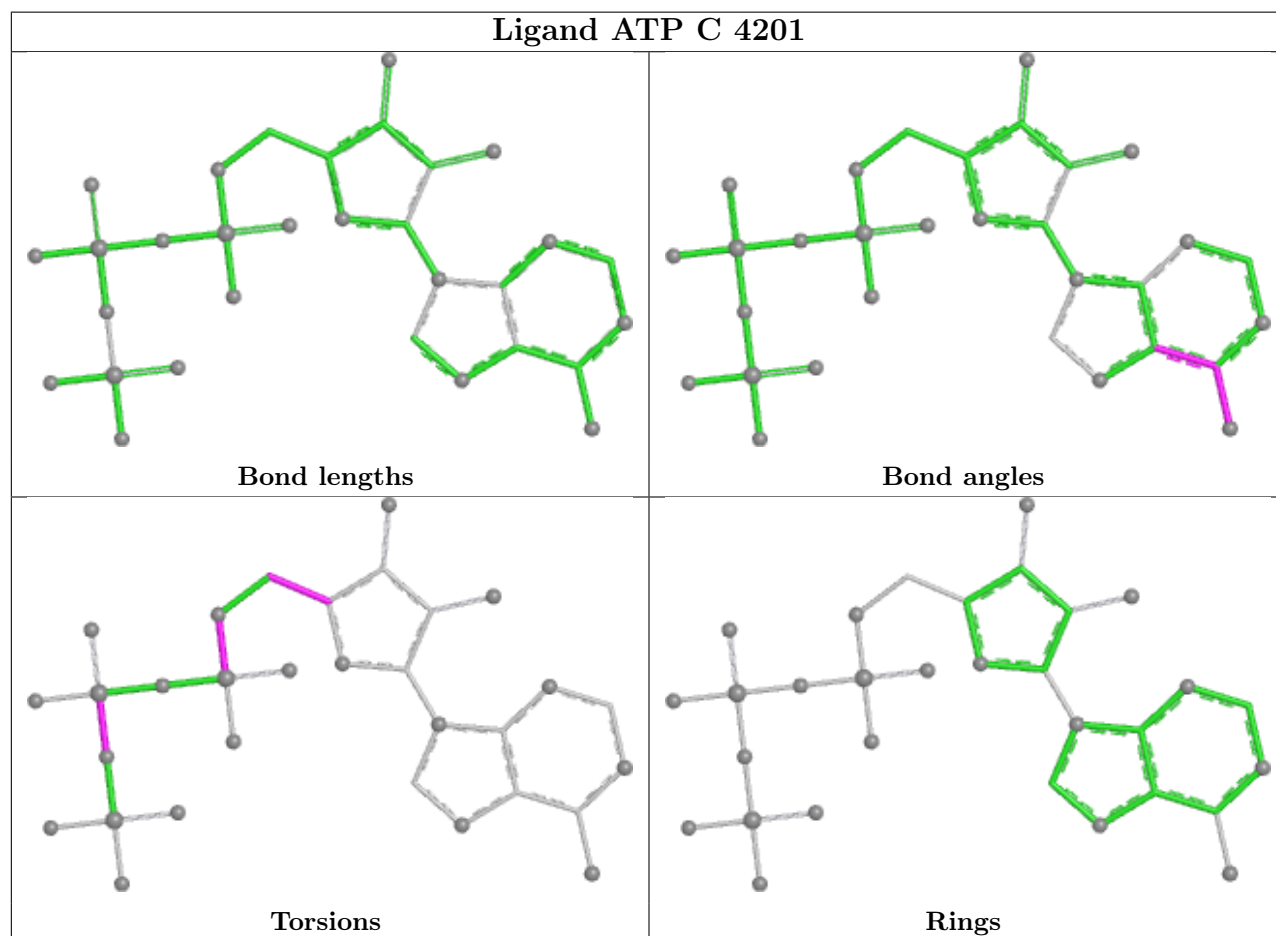
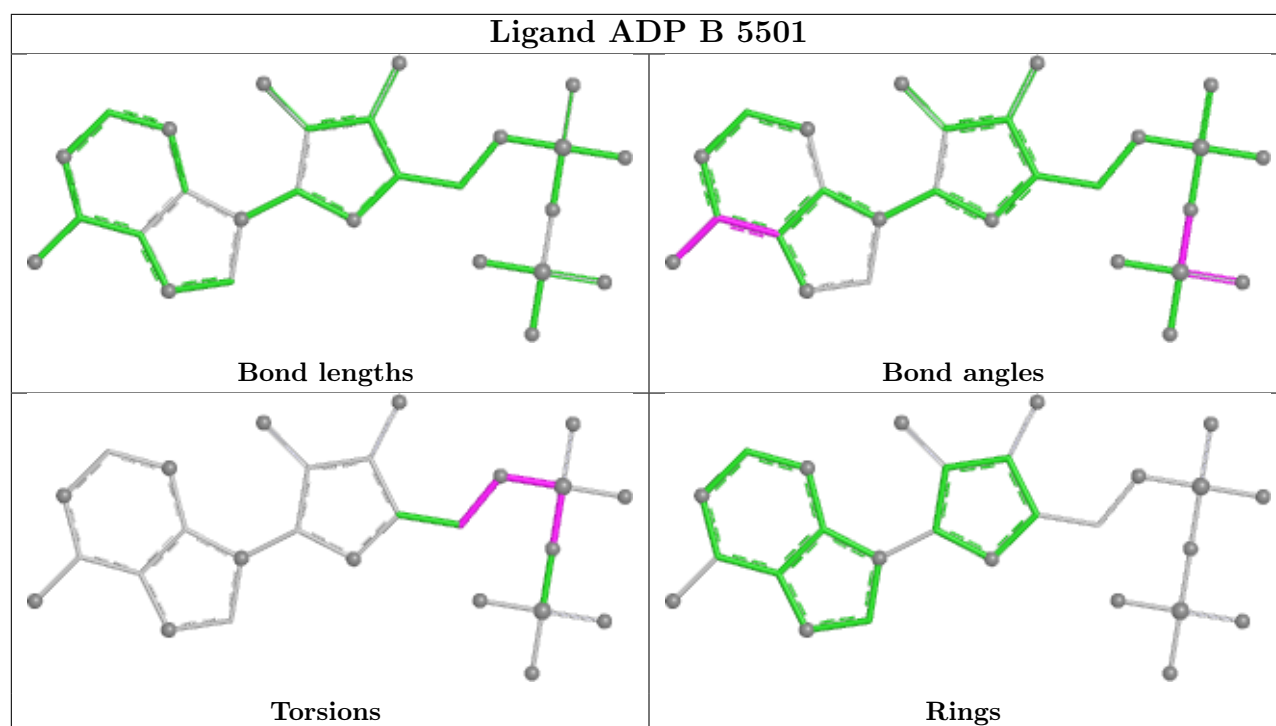
Continued on next page...

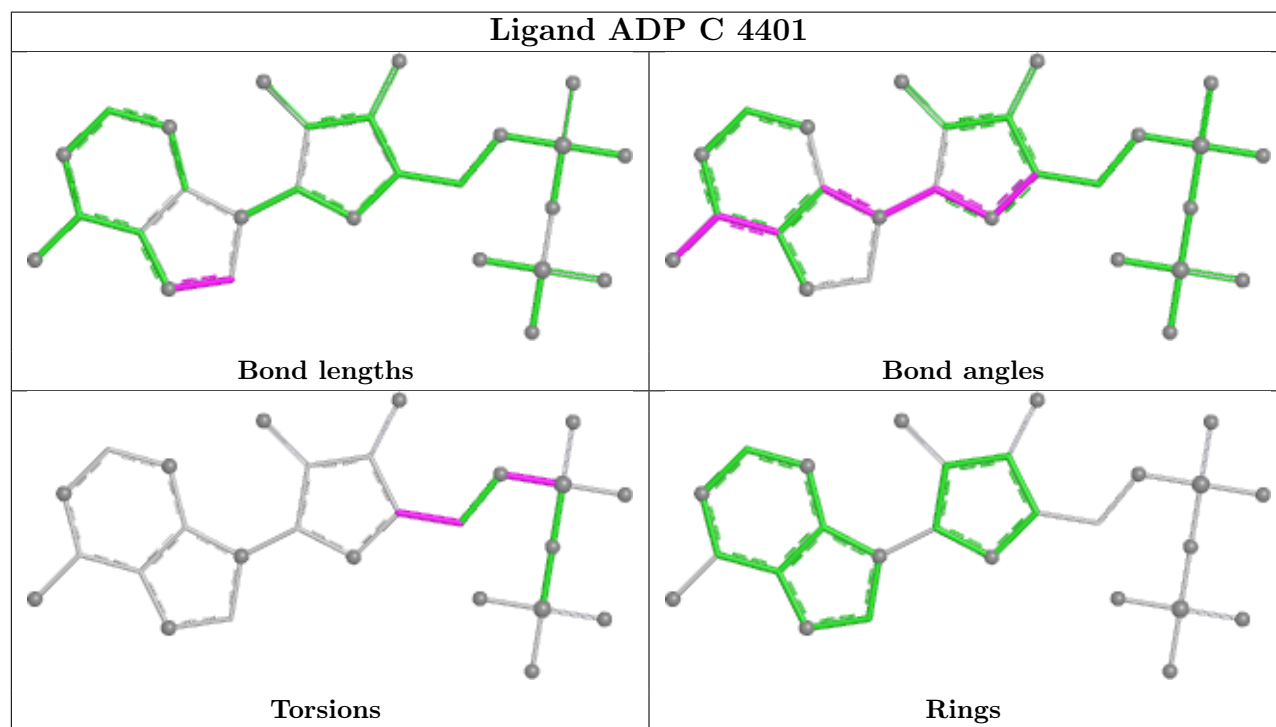
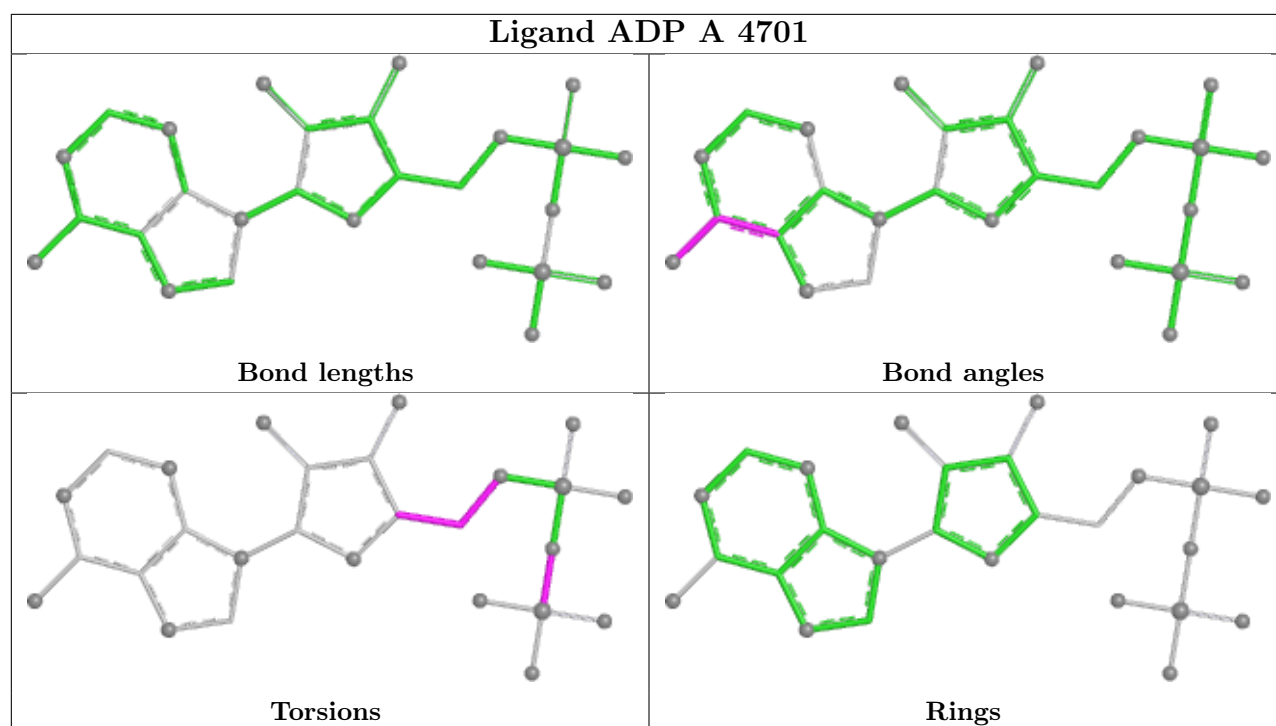
Continued from previous page...

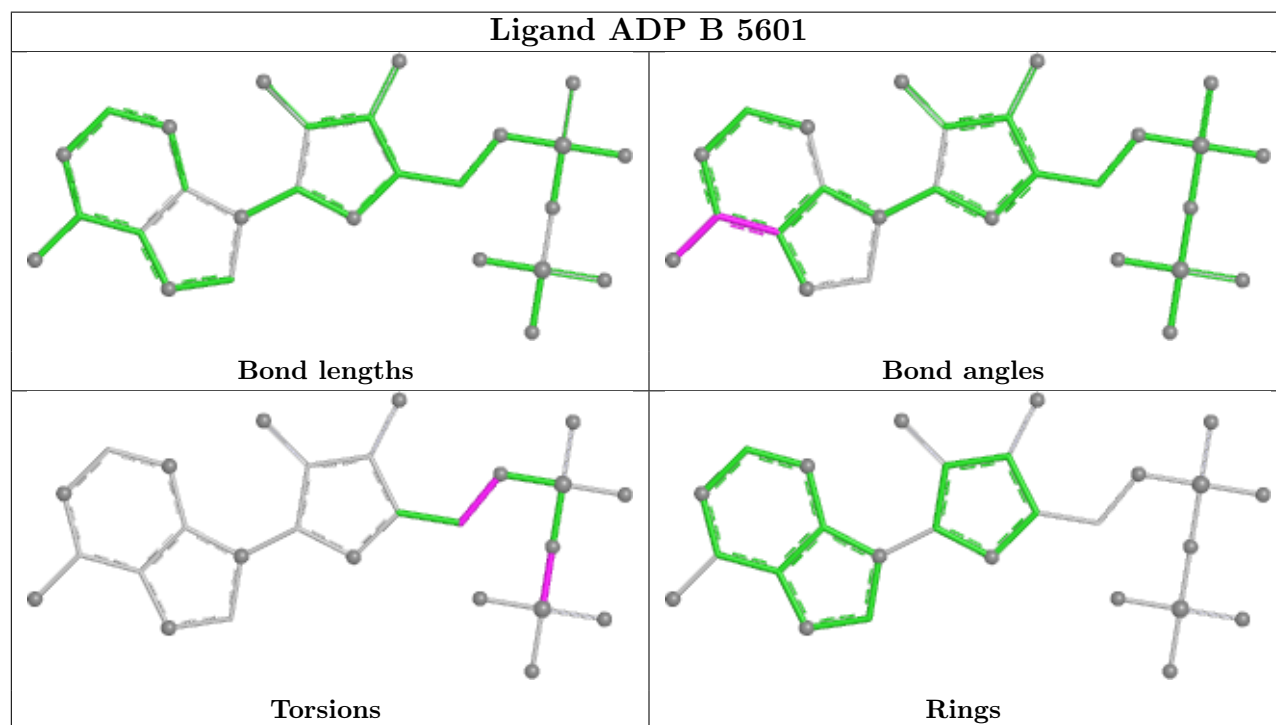
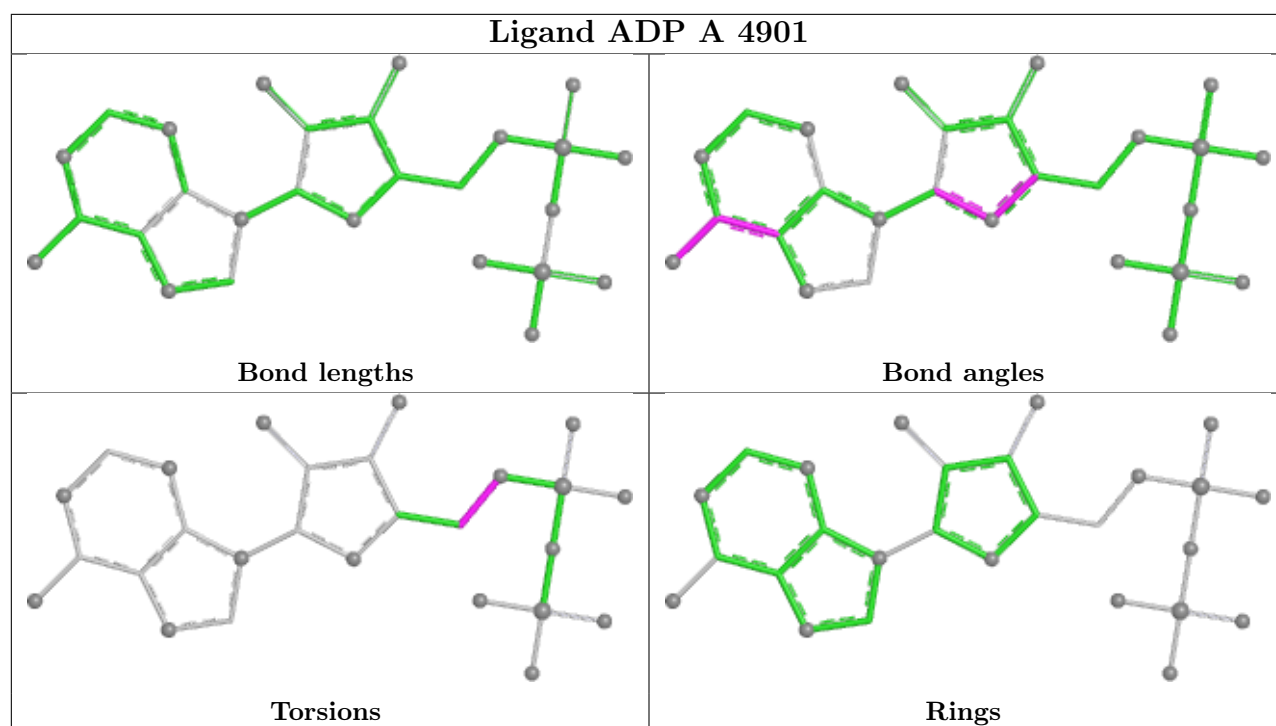
Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	C	4401	ADP	1	0
18	A	4901	ADP	1	0
19	B	4701	ATP	1	0

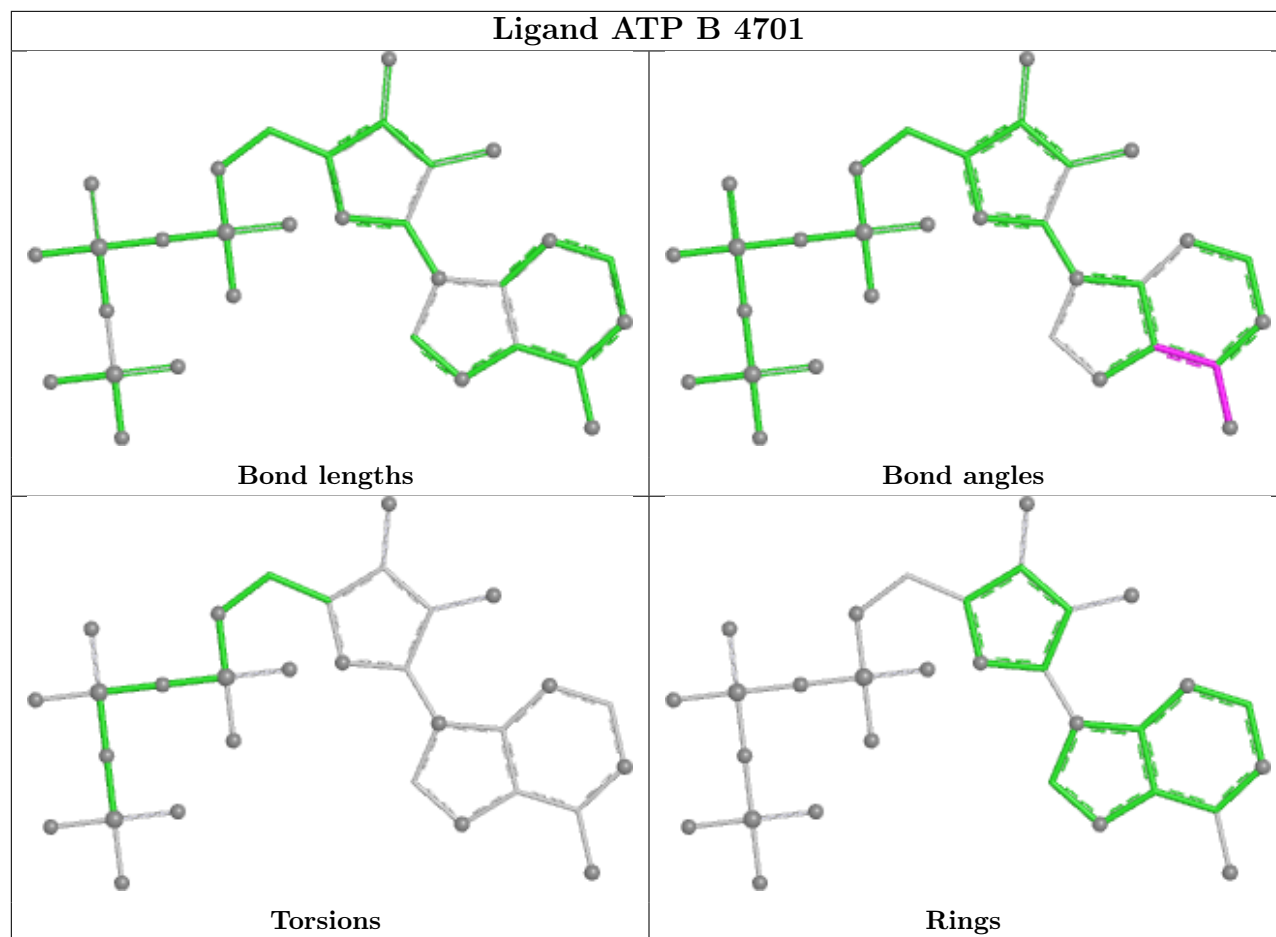
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

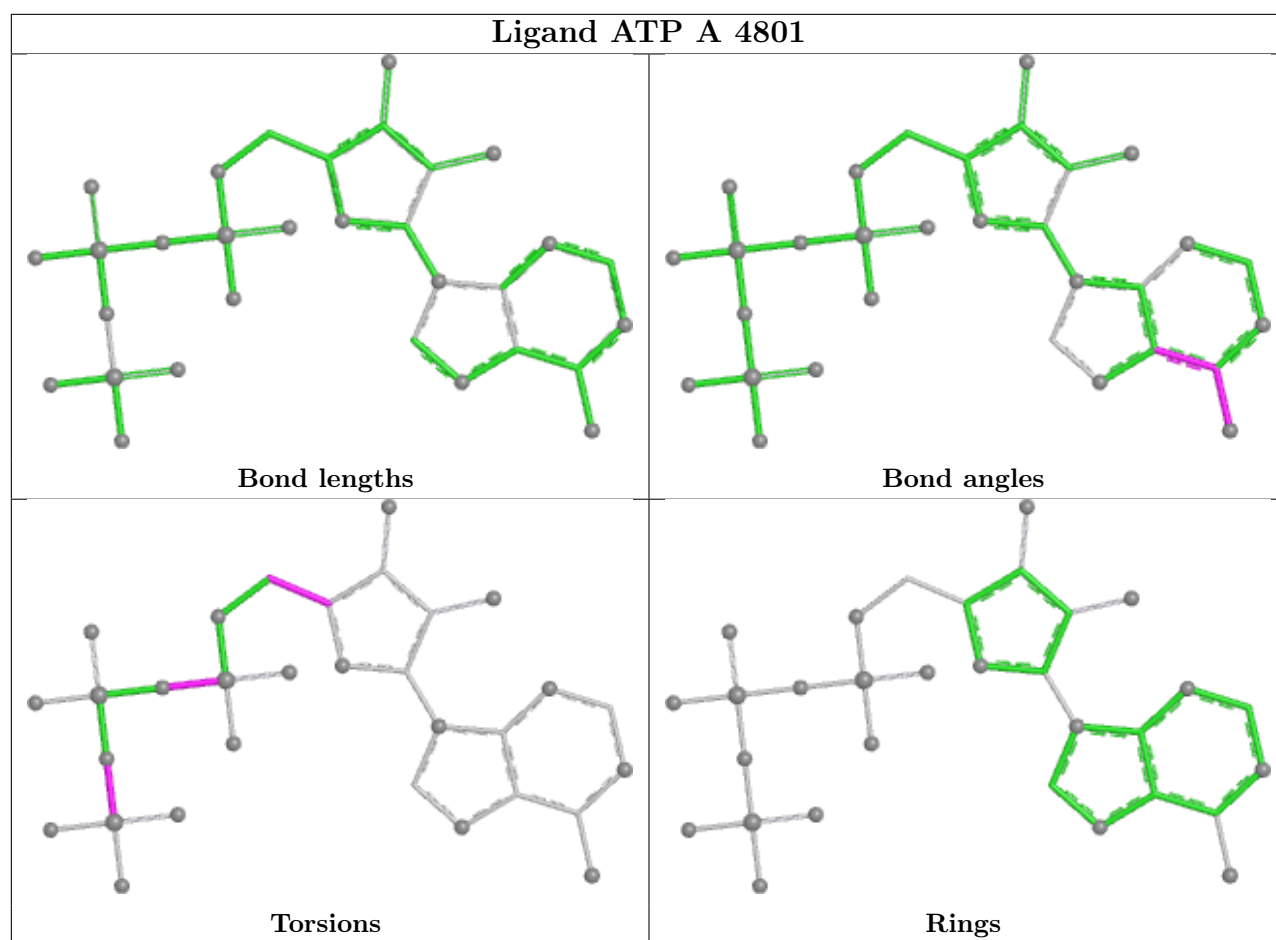












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	C	13
1	A	6
4	B	2
12	D	2
13	P	1
7	G	1

The worst 5 of 25 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	3277:MET	C	3380:MET	N	42.35
1	C	809:ARG	C	818:ILE	N	14.24
1	A	1235:PRO	C	1246:MET	N	12.91
1	C	665:ILE	C	670:SER	N	11.42
1	C	449:TYR	C	453:THR	N	10.61

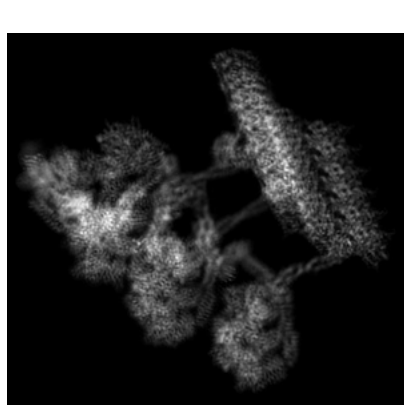
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22677. These allow visual inspection of the internal detail of the map and identification of artifacts.

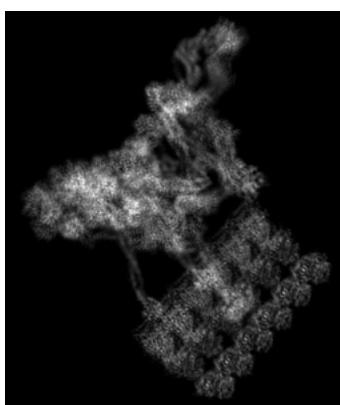
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

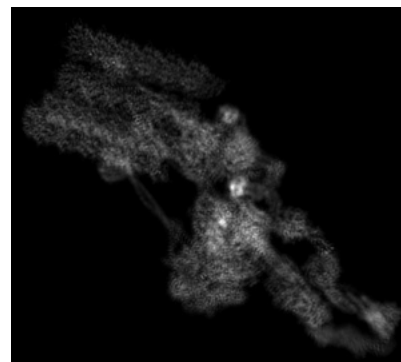
6.1.1 Primary map



X



Y



Z

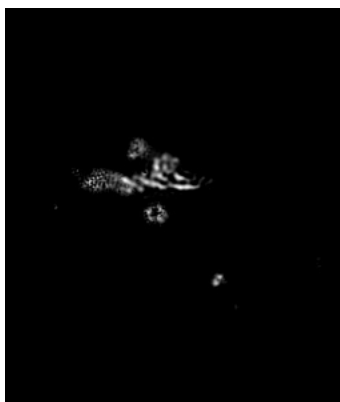
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 199



Y Index: 179



Z Index: 168

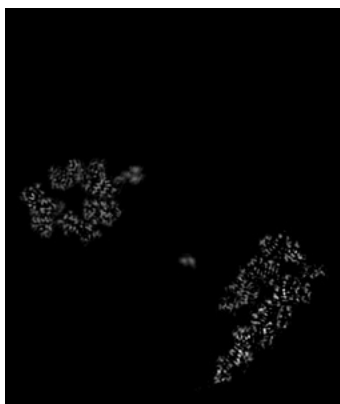
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

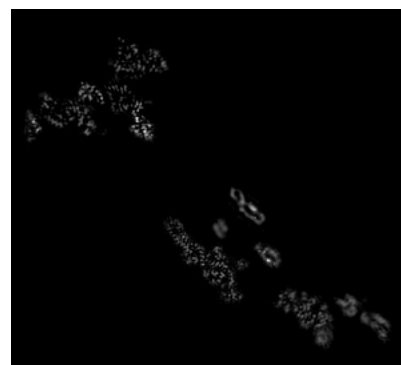
6.3.1 Primary map



X Index: 222



Y Index: 223

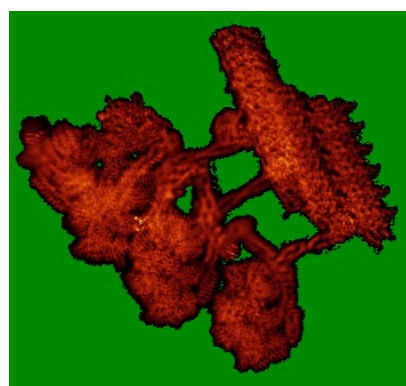


Z Index: 191

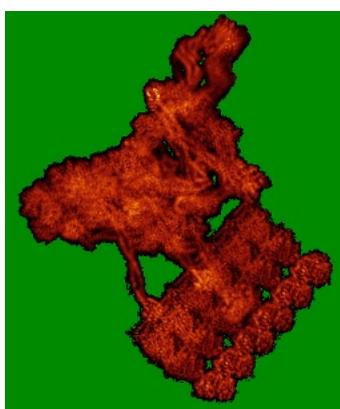
The images above show the largest variance slices of the map in three orthogonal directions.

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

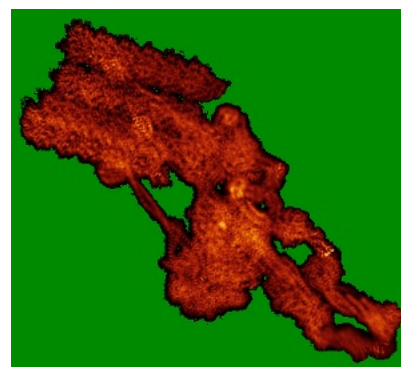
6.4.1 Primary map



X



Y

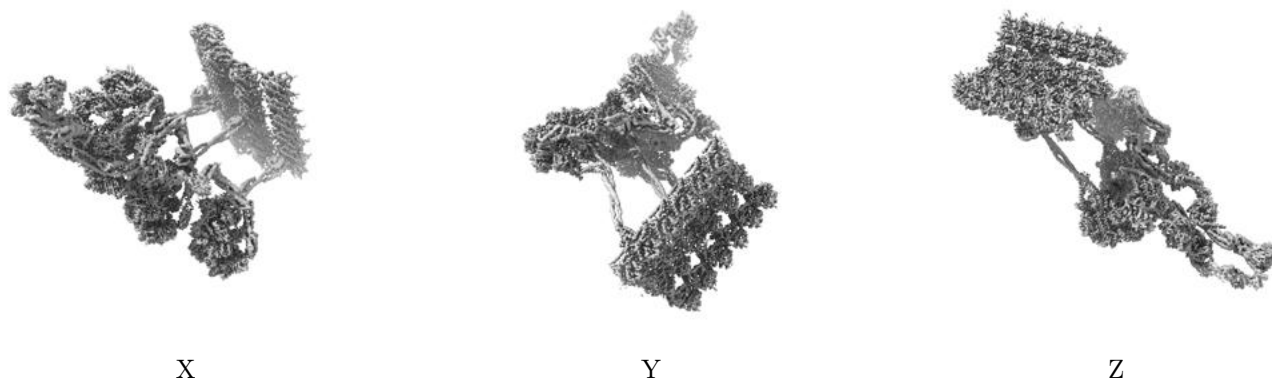


Z

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

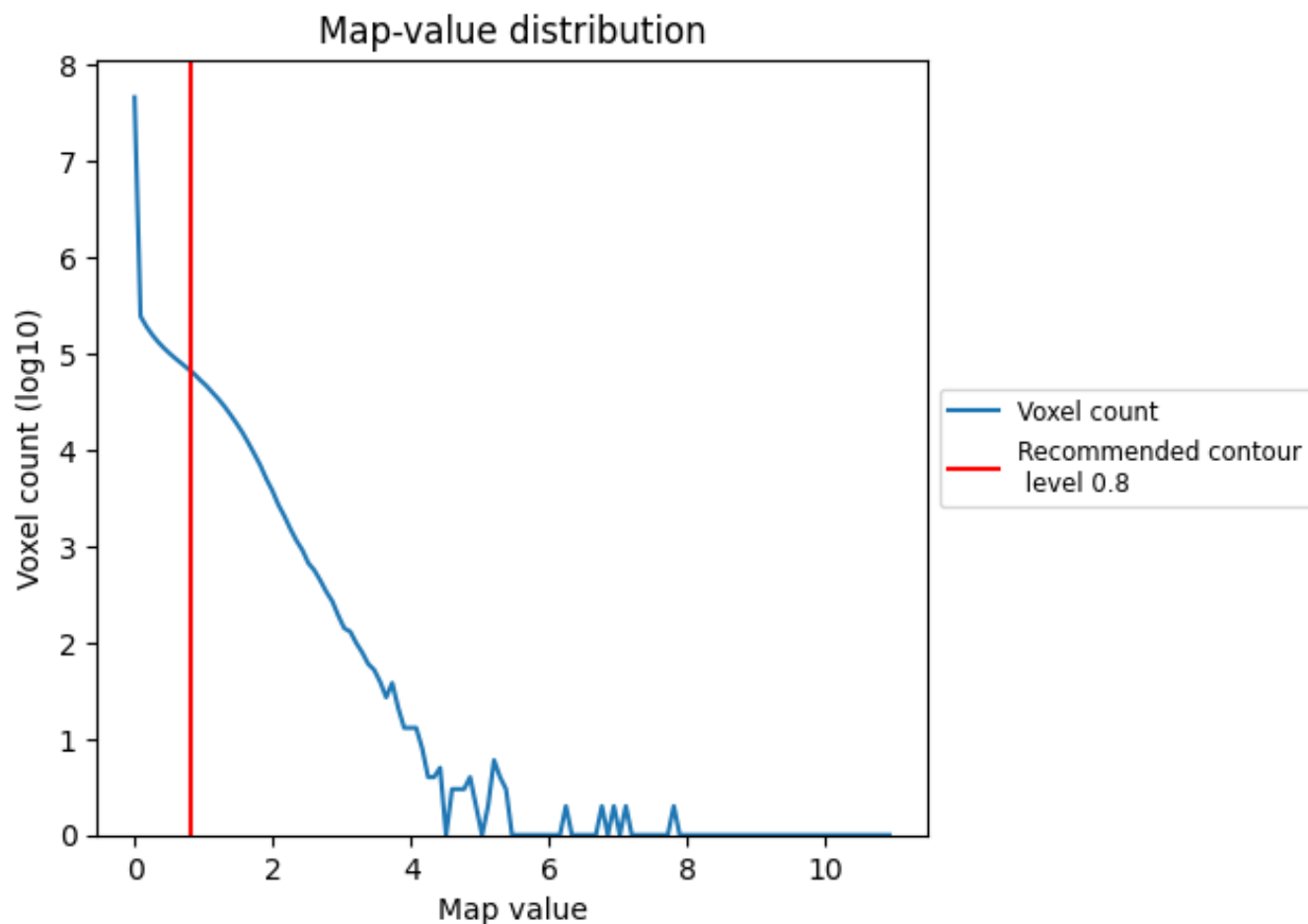
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

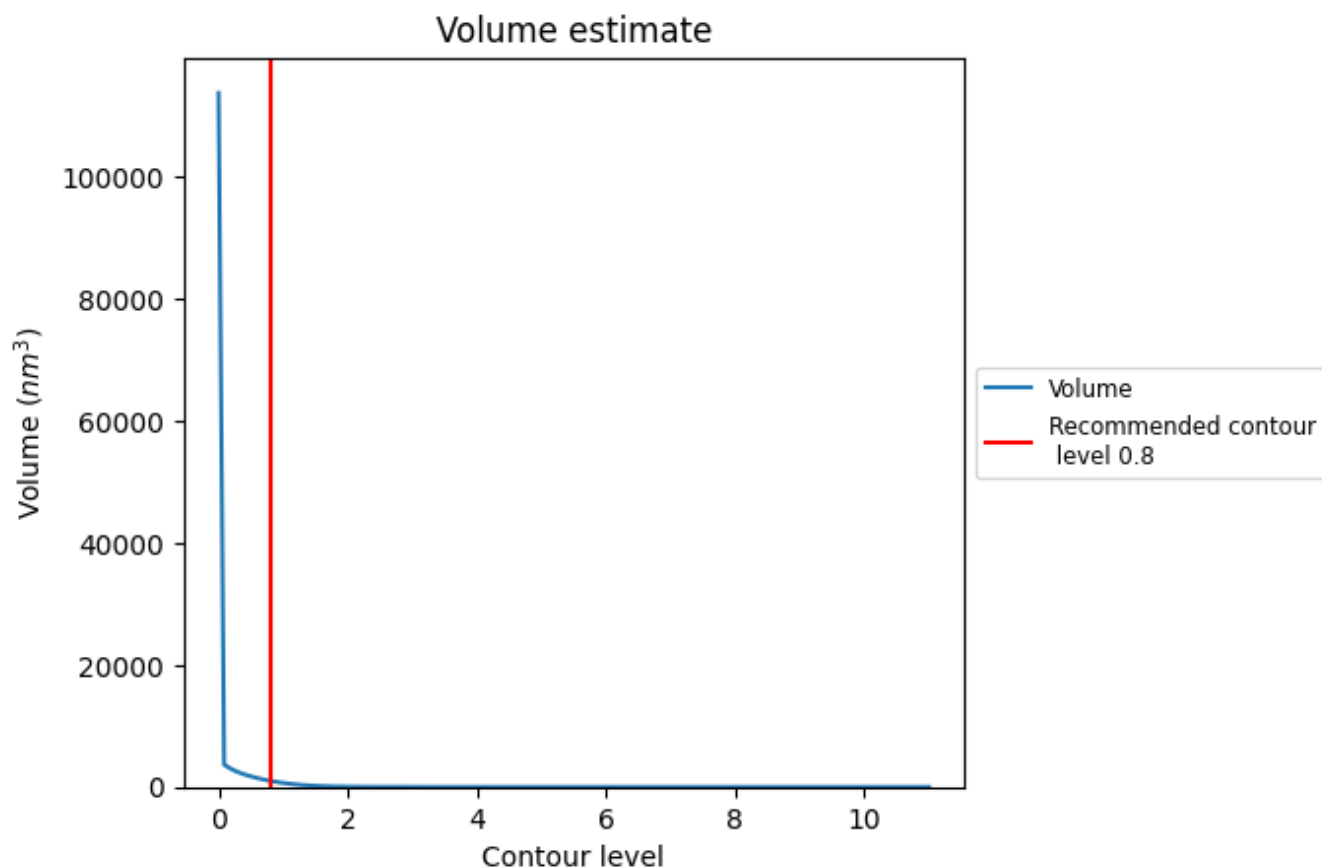
This section contains the results of statistical analysis of the map.

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 1003 nm³; this corresponds to an approximate mass of 906 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

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

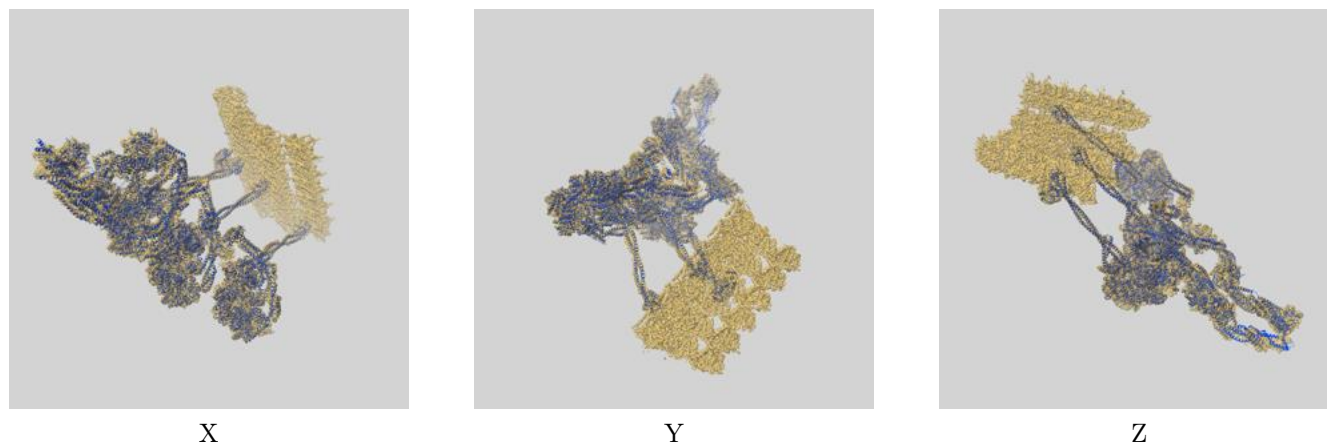
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

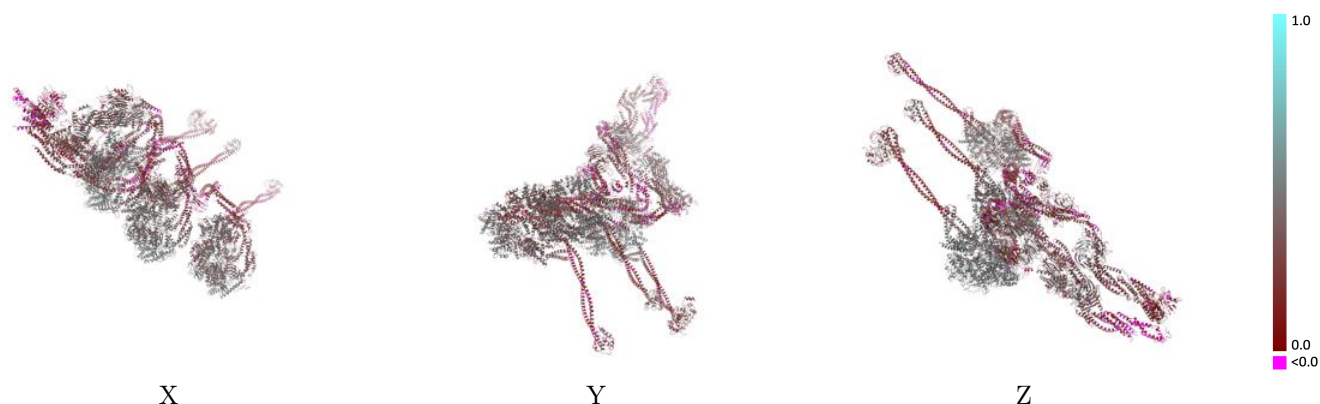
This section contains information regarding the fit between EMDB map EMD-22677 and PDB model 7K58. Per-residue inclusion information can be found in section [3](#) on page [9](#).

9.1 Map-model overlay [i](#)



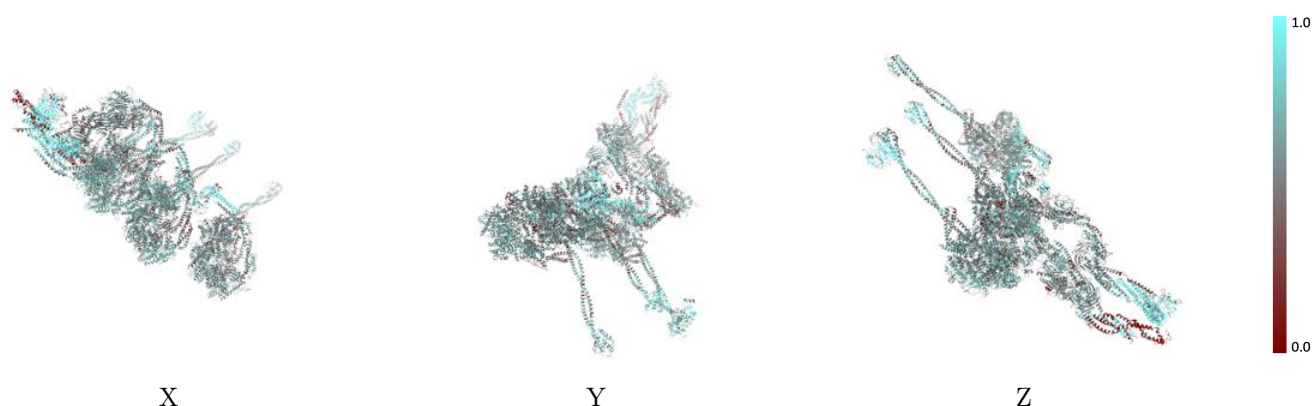
The images above show the 3D surface view of the map at the recommended contour level 0.8 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



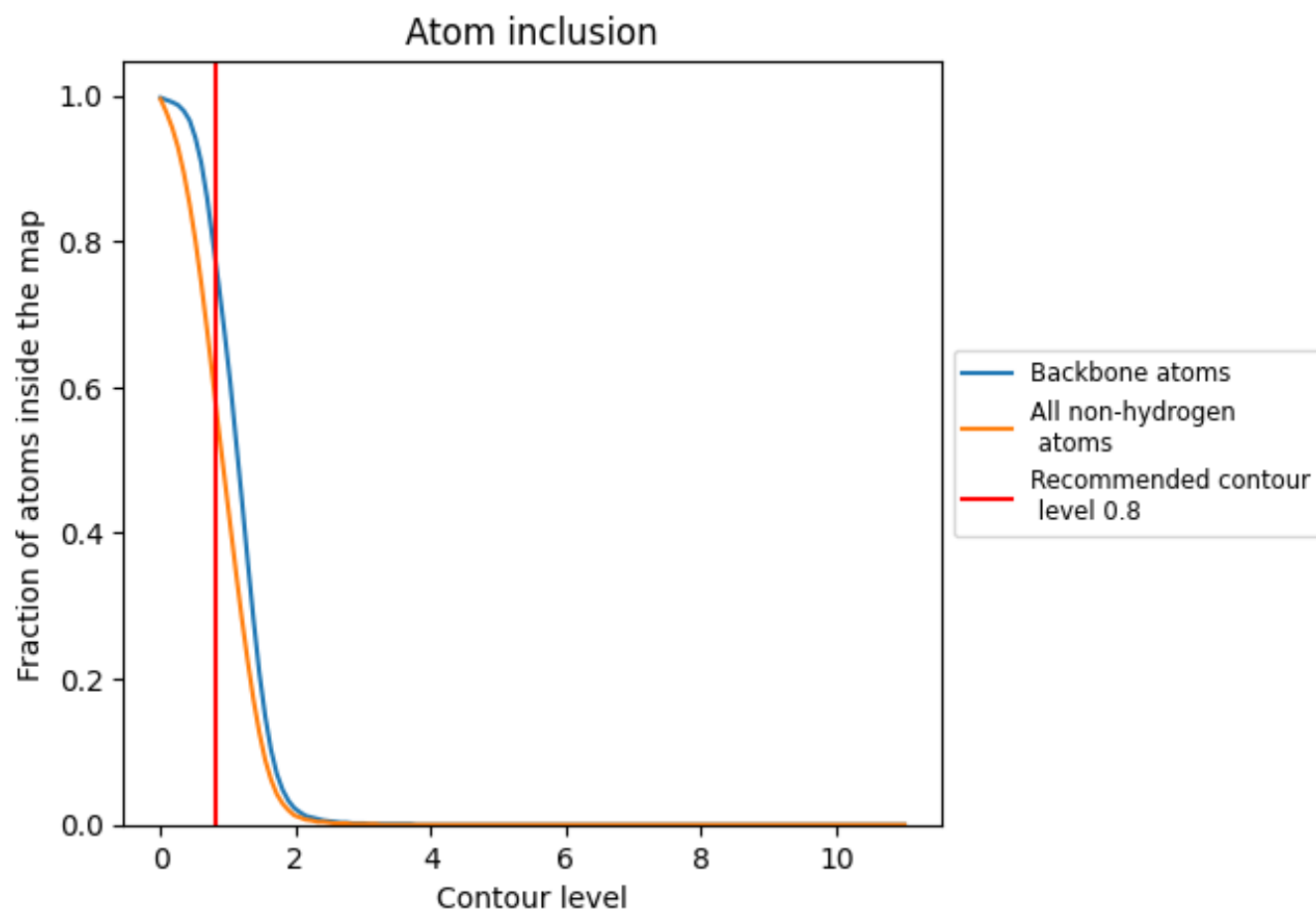
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.8).





































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 59% 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 (0.8) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5890	 0.3570
A	 0.6020	 0.3820
B	 0.6170	 0.3590
C	 0.5700	 0.3380
D	 0.5990	 0.3420
E	 0.5230	 0.3550
F	 0.5180	 0.3830
G	 0.4550	 0.3710
H	 0.4860	 0.3550
I	 0.5260	 0.3180
J	 0.5370	 0.3860
K	 0.4750	 0.3630
L	 0.4140	 0.3650
M	 0.5180	 0.3810
N	 0.5700	 0.2740
O	 0.5110	 0.2540
P	 0.5560	 0.1490
Q	 0.7990	 0.3230

