wwPDB EM Validation Summary Report

Aug 26, 2026 – 09:35 pm BST

PDB ID	:	9H5K / pdb_00009h5k
EMDB ID	:	EMD-51887
Title	:	Cryo-EM structure of the SEAC-EGOC supercomplex
Authors	:	Tafur, L.; Loewith, R.
Deposited on	:	2024-10-22
Resolution	:	3.20 Å(reported)
Based on initial models	:	6jwp, ., 8adl

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

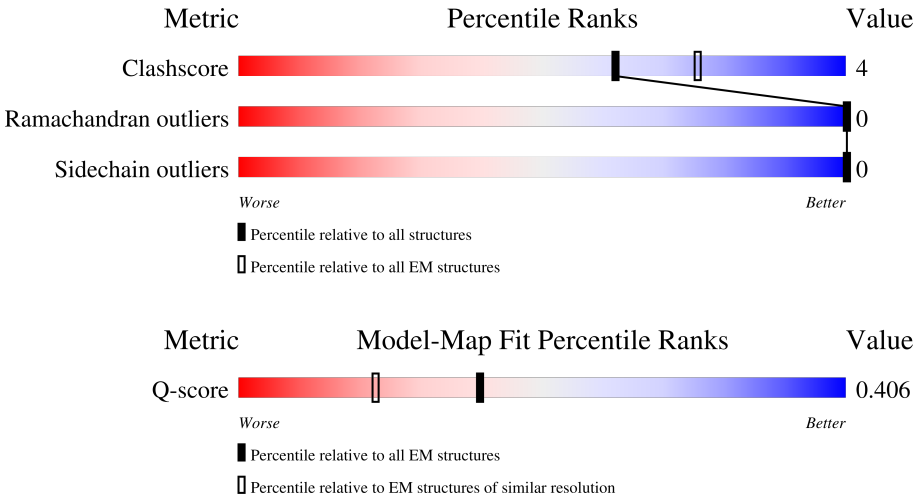
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 <=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	C	1148	58% 11% 31%
1	K	1148	59% 10% 31%
2	H	297	83% 12% 5%
2	P	297	83% 12% 5%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	A	1341	42% 6% 53%
3	I	1341	42% 6% 53%
4	D	349	78% 11% 11%
4	E	349	75% 13% 12%
4	F	349	77% 12% 11%
4	L	349	77% 12% 11%
4	M	349	76% 12% 12%
4	N	349	77% 12% 11%
5	B	1038	69% 8% 23%
5	G	1038	67% 9% 25%
5	J	1038	69% 8% 23%
5	O	1038	66% 9% 25%
6	a	310	87% 7% 6%
6	b	310	87% 7% 6%
7	c	341	71% 11% 18%
7	d	341	74% 8% 18%
8	T	615	57% 9% 34%
8	g	615	58% 8% 34%
9	h	1146	45% 5% 50%
9	i	1146	44% 6% 50%
10	X	1584	56% 7% 38%
10	j	1584	55% 7% 38%
11	R	184	47% 48%
11	S	184	47% 48%
12	U	75	76% 13% 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	W	75	
13	Y	162	
13	Z	162	

2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 114318 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 Maintenance of telomere capping protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	791	Total	C	N	O	S	0	0
			6414	4095	1090	1191	38		
1	K	791	Total	C	N	O	S	0	0
			6414	4095	1090	1191	38		

- Molecule 2 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	282	Total	C	N	O	S	0	0
			2226	1423	380	420	3		
2	P	282	Total	C	N	O	S	0	0
			2226	1423	380	420	3		

- Molecule 3 is a protein called Restriction of telomere capping protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	632	Total	C	N	O	S	0	0
			5036	3226	835	948	27		
3	I	632	Total	C	N	O	S	0	0
			5036	3226	835	948	27		

- Molecule 4 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	311	Total	C	N	O	S	0	0
			2469	1562	427	469	11		
4	E	307	Total	C	N	O	S	0	0
			2438	1543	422	462	11		
4	D	310	Total	C	N	O	S	0	0
			2457	1554	425	467	11		
4	N	311	Total	C	N	O	S	0	0
			2469	1562	427	469	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	307	Total	C	N	O	S	0	0
			2438	1543	422	462	11		
4	L	310	Total	C	N	O	S	0	0
			2457	1554	425	467	11		

- Molecule 5 is a protein called SEH-associated protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	783	Total	C	N	O	S	0	0
			6303	3980	1097	1184	42		
5	B	800	Total	C	N	O	S	0	0
			6439	4065	1124	1208	42		
5	O	783	Total	C	N	O	S	0	0
			6303	3980	1097	1184	42		
5	J	800	Total	C	N	O	S	0	0
			6439	4065	1124	1208	42		

- Molecule 6 is a protein called GTP-binding protein GTR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	a	292	Total	C	N	O	S	0	0
			2375	1531	397	429	18		
6	b	292	Total	C	N	O	S	0	0
			2375	1531	397	429	18		

- Molecule 7 is a protein called GTP-binding protein GTR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	c	280	Total	C	N	O	S	0	0
			2230	1434	355	428	13		
7	d	280	Total	C	N	O	S	0	0
			2230	1434	355	428	13		

- Molecule 8 is a protein called Nitrogen permease regulator 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	T	405	Total	C	N	O	S	0	0
			3312	2166	524	603	19		
8	g	405	Total	C	N	O	S	0	0
			3312	2166	524	603	19		

- Molecule 9 is a protein called Nitrogen permease regulator 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	h	573	Total	C	N	O	S	0	0
			4727	3042	787	872	26		
9	i	573	Total	C	N	O	S	0	0
			4727	3042	787	872	26		

- Molecule 10 is a protein called Vacuolar membrane-associated protein IML1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	990	Total	C	N	O	S	0	0
			8187	5269	1381	1501	36		
10	j	990	Total	C	N	O	S	0	0
			8187	5269	1381	1501	36		

- Molecule 11 is a protein called Protein MEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	95	Total	C	N	O	S	0	0
			765	475	135	154	1		
11	S	95	Total	C	N	O	S	0	0
			765	475	135	154	1		

- Molecule 12 is a protein called Protein EGO2.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	U	67	Total	C	N	O	0	0
			505	315	86	104		
12	W	67	Total	C	N	O	0	0
			505	315	86	104		

- Molecule 13 is a protein called Protein SLM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Y	151	Total	C	N	O	S	0	0
			1201	764	190	239	8		
13	Z	151	Total	C	N	O	S	0	0
			1201	764	190	239	8		

- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
14	C	3	Total	Zn	0
			3	3	

Continued on next page...

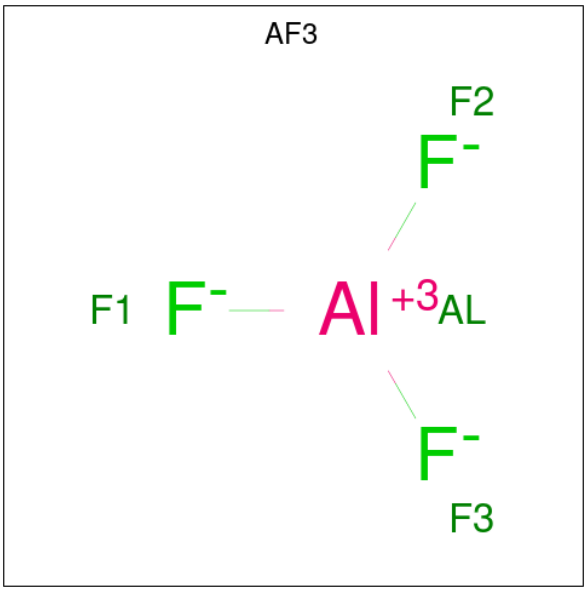
Continued from previous page...

Mol	Chain	Residues	Atoms	AltConf
14	A	3	Total Zn 3 3	0
14	G	4	Total Zn 4 4	0
14	B	4	Total Zn 4 4	0
14	K	3	Total Zn 3 3	0
14	I	3	Total Zn 3 3	0
14	O	4	Total Zn 4 4	0
14	J	4	Total Zn 4 4	0

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

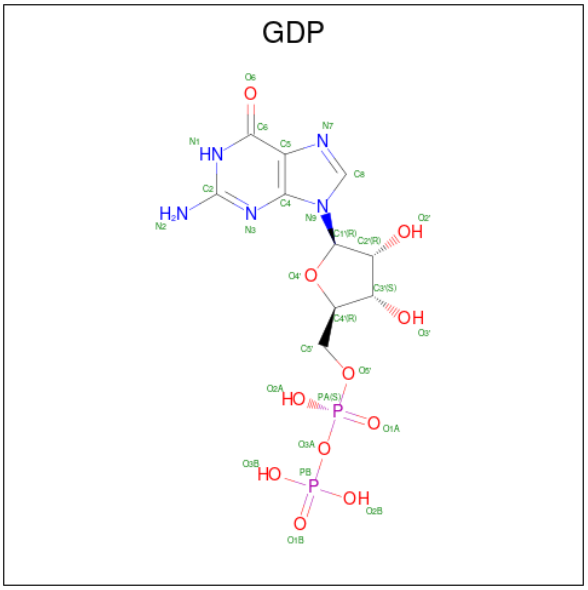
Mol	Chain	Residues	Atoms	AltConf
15	a	1	Total Mg 1 1	0
15	b	1	Total Mg 1 1	0

- Molecule 16 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
16	a	1	Total 4	Al 1	F 3	0
16	b	1	Total 4	Al 1	F 3	0

- Molecule 17 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
17	a	1	Total 28	C 10	N 5	O 11	P 2	0
17	c	1	Total 28	C 10	N 5	O 11	P 2	0
17	b	1	Total 28	C 10	N 5	O 11	P 2	0
17	d	1	Total 28	C 10	N 5	O 11	P 2	0

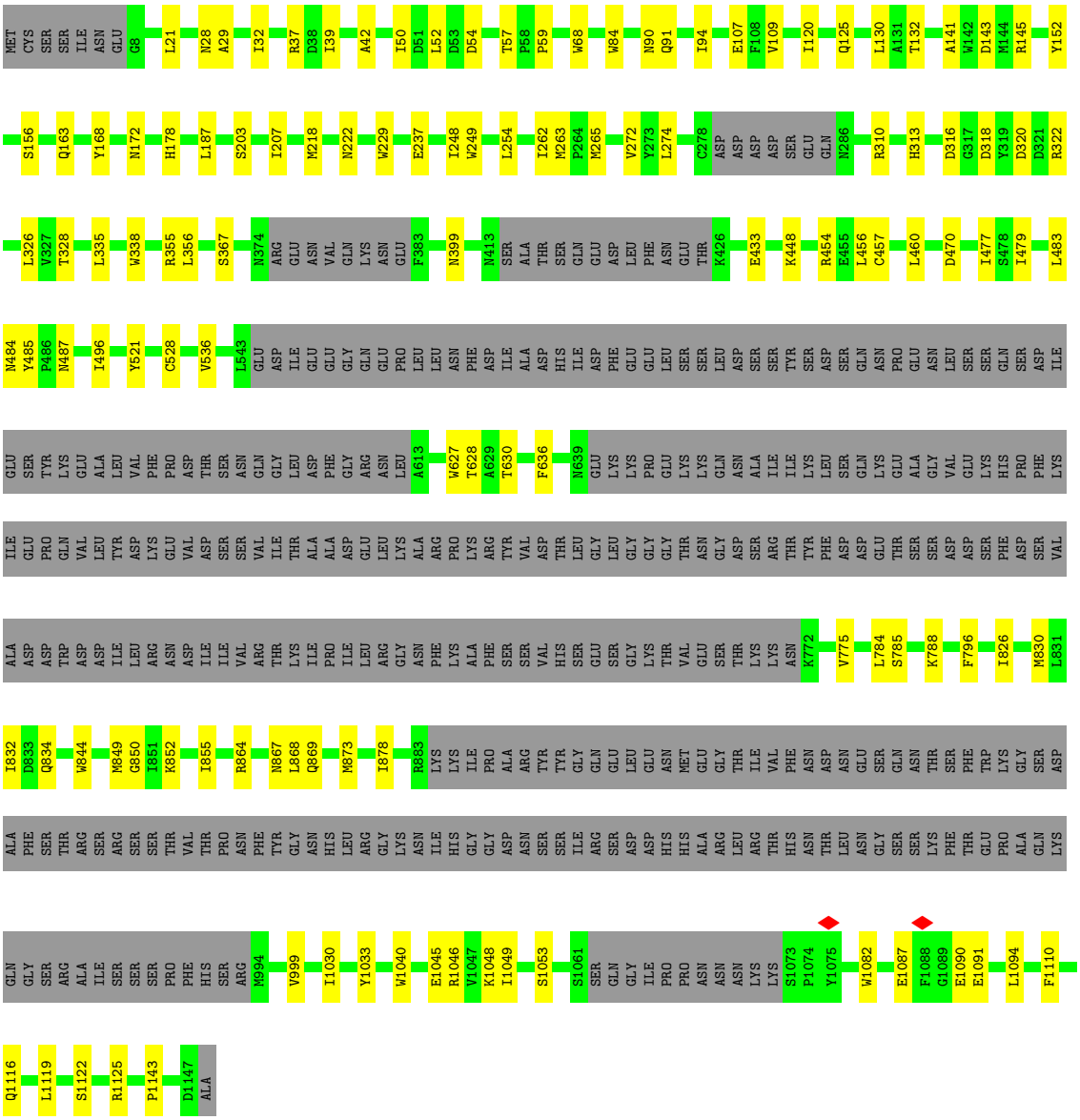
3 Residue-property plots (i)

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: Maintenance of telomere capping protein 5

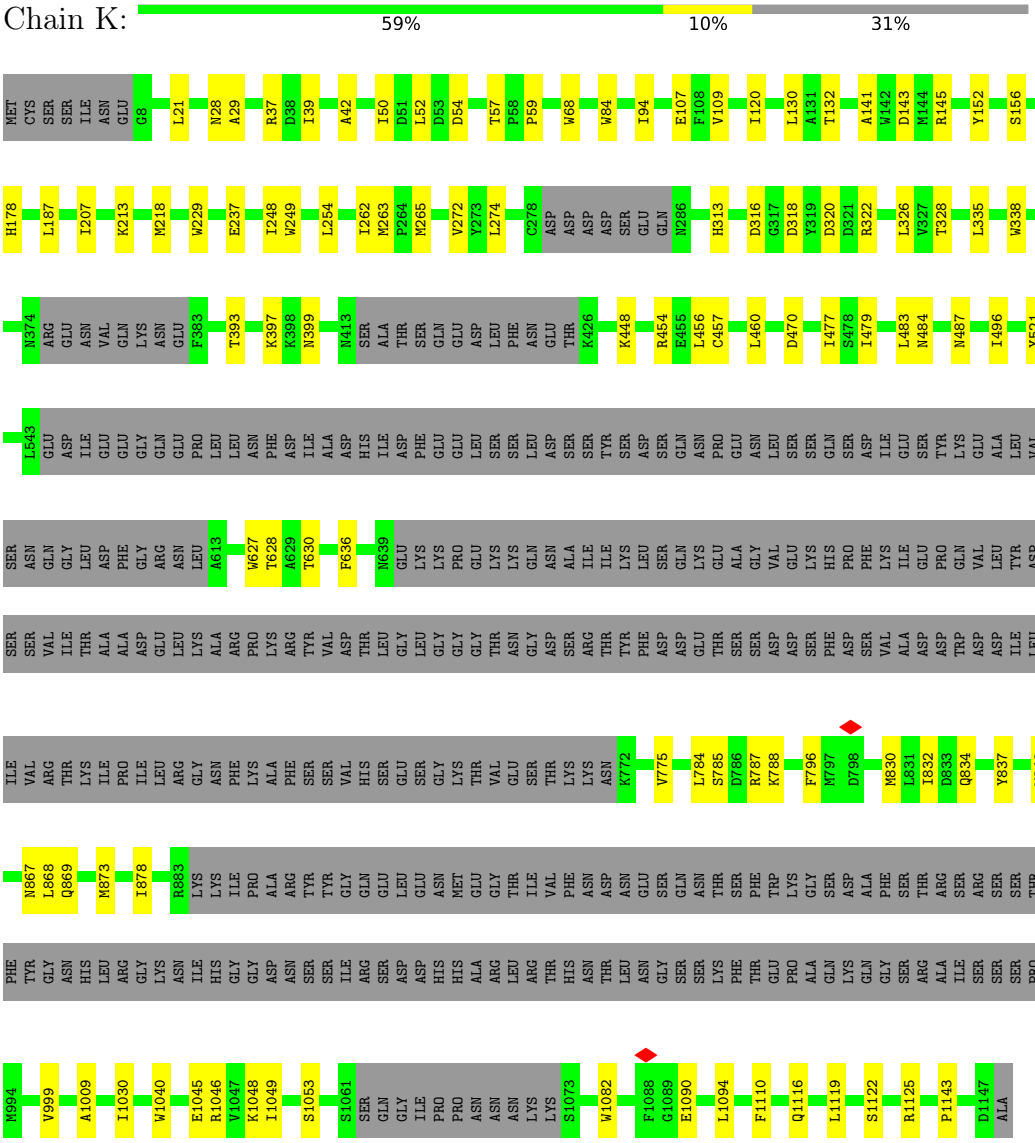
Chain C:





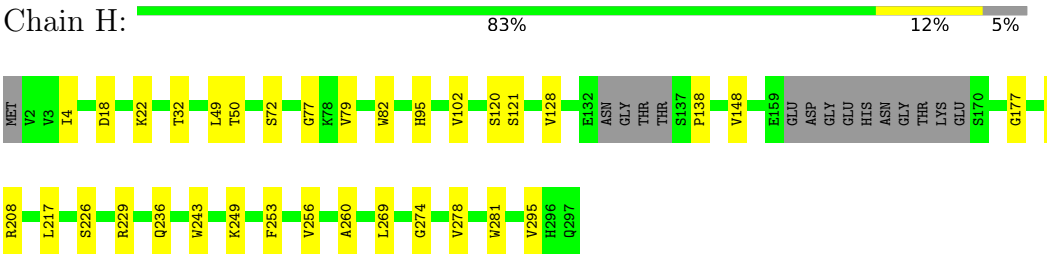
• Molecule 1: Maintenance of telomere capping protein 5

Chain K:



• Molecule 2: Protein transport protein SEC13

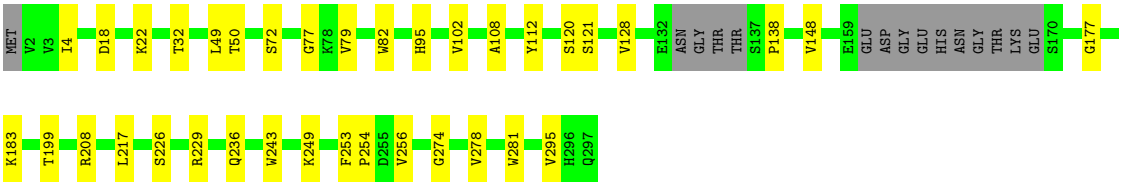
Chain H:



• Molecule 2: Protein transport protein SEC13

Chain P:

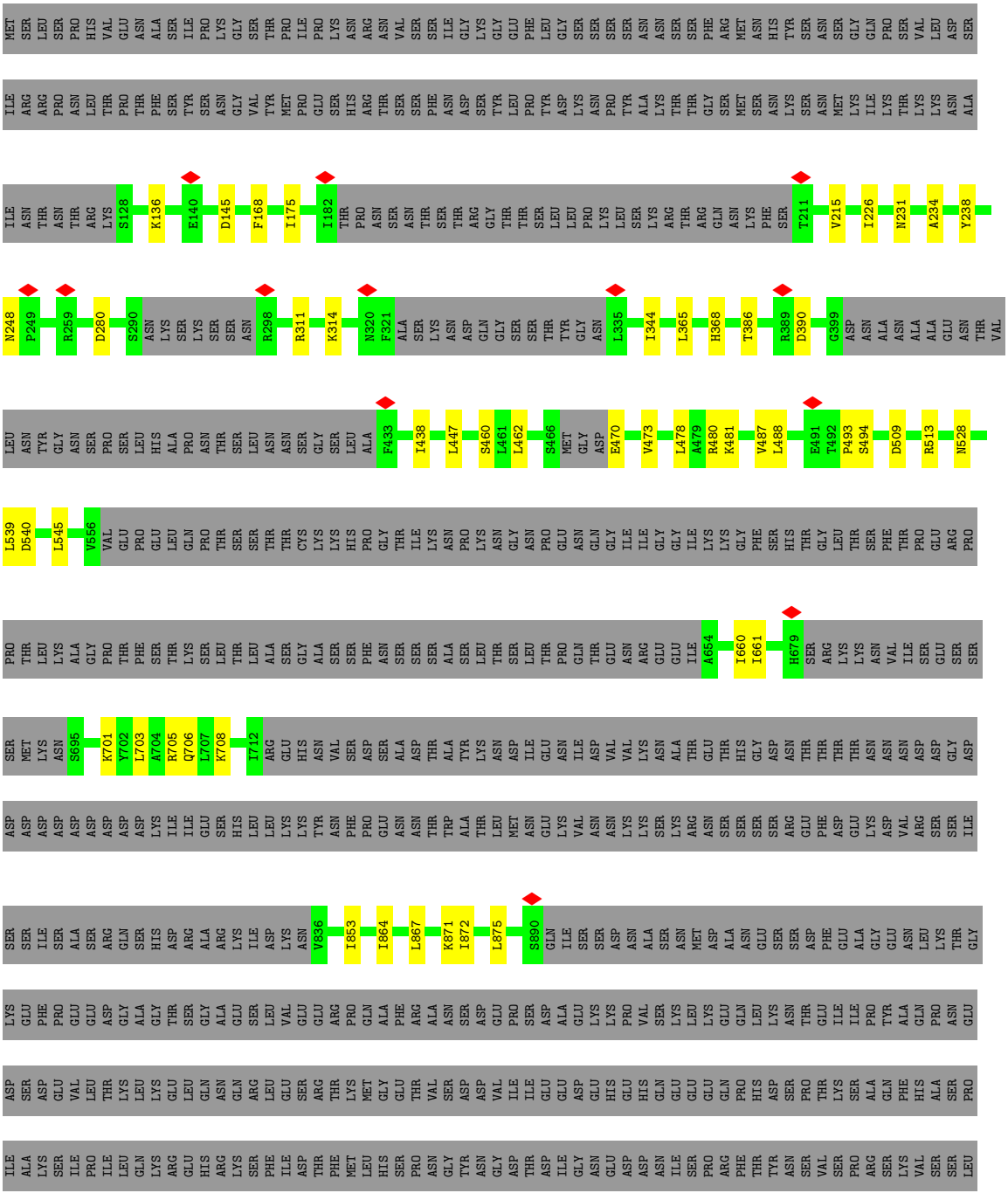


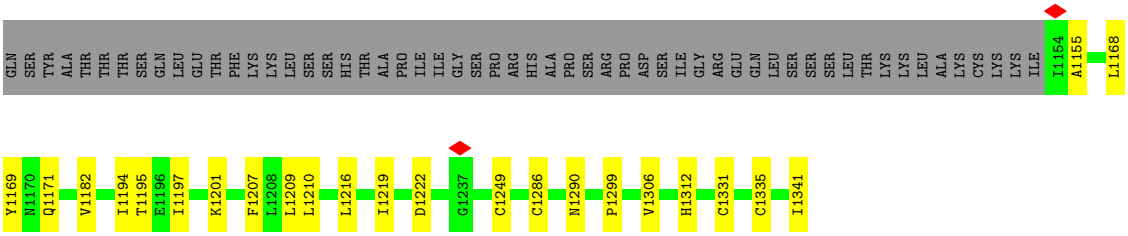


• Molecule 3: Restriction of telomere capping protein 1

Chain A:



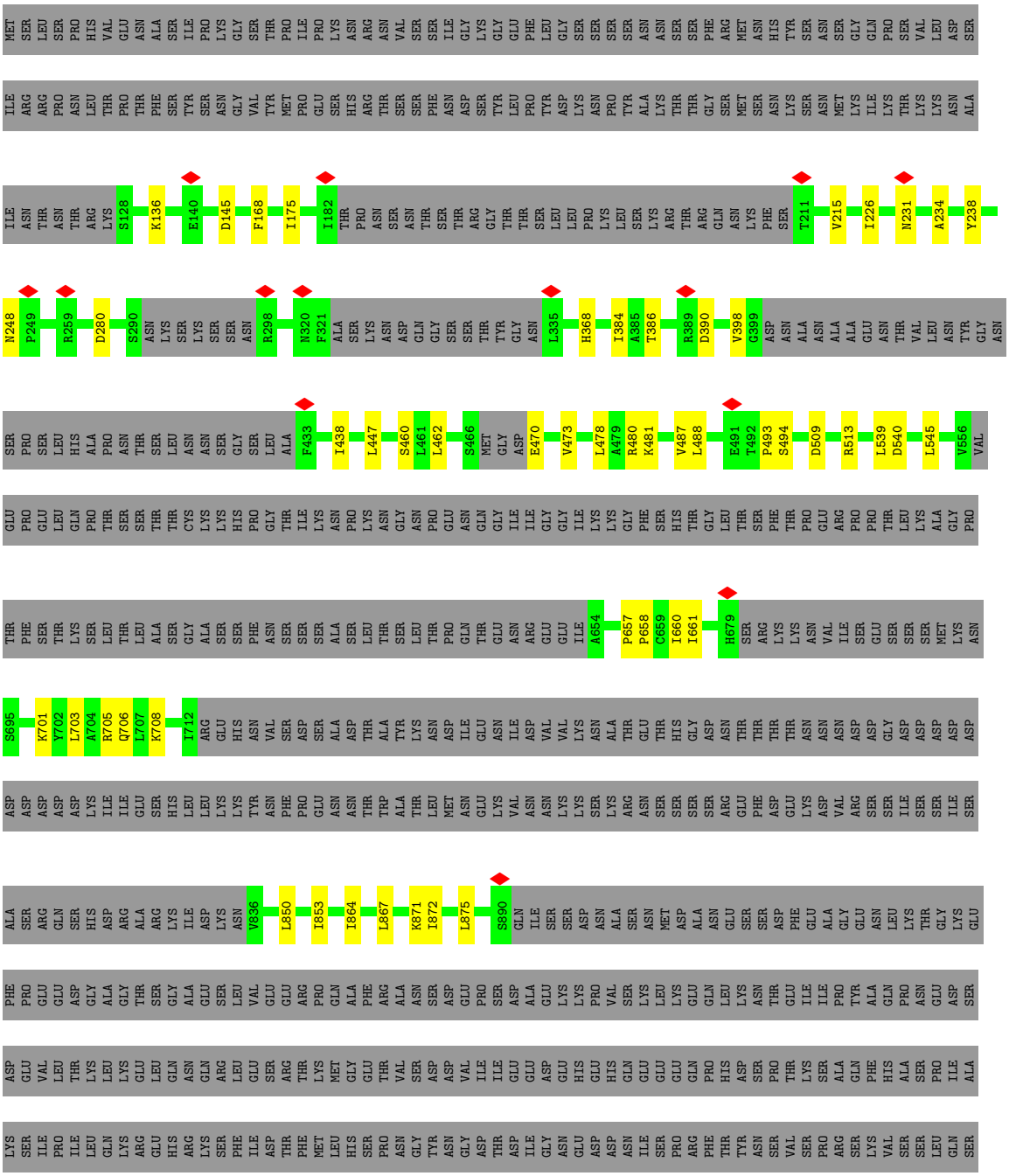


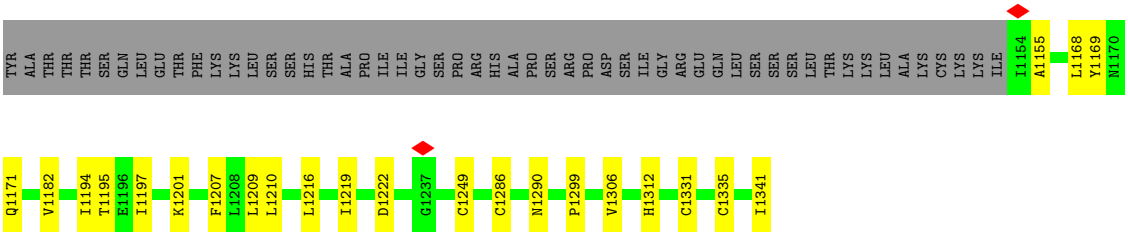


• Molecule 3: Restriction of telomere capping protein 1

Chain I:



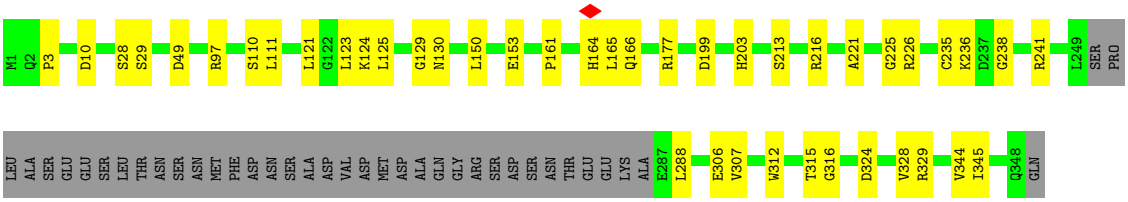




• Molecule 4: Nucleoporin SEH1

Chain F:

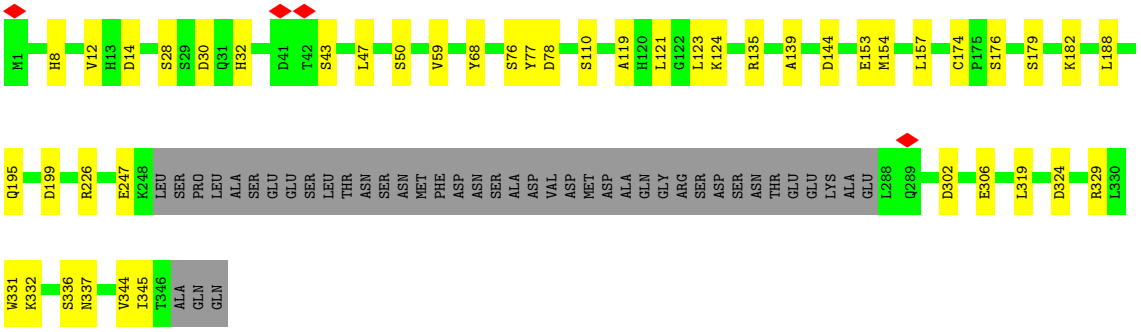




• Molecule 4: Nucleoporin SEH1

Chain E:

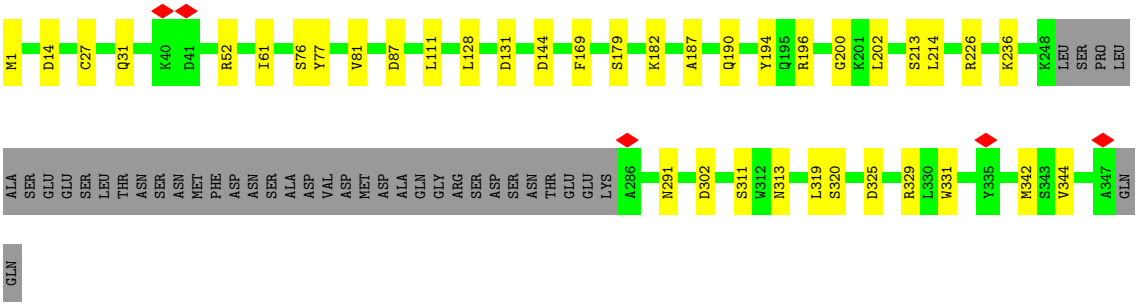




• Molecule 4: Nucleoporin SEH1

Chain D:

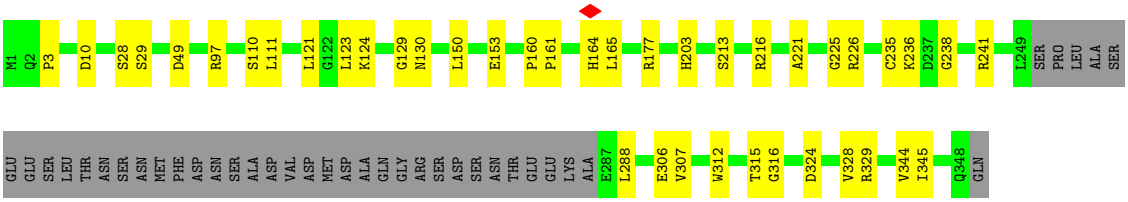




• Molecule 4: Nucleoporin SEH1

Chain N:

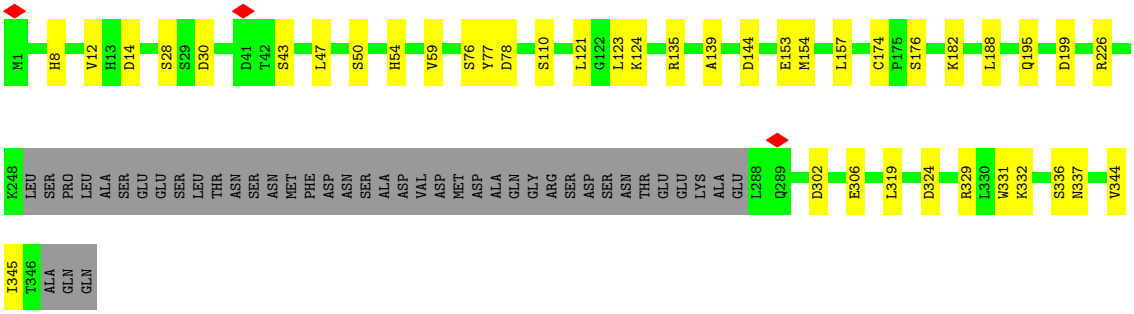




• Molecule 4: Nucleoporin SEH1

Chain M:

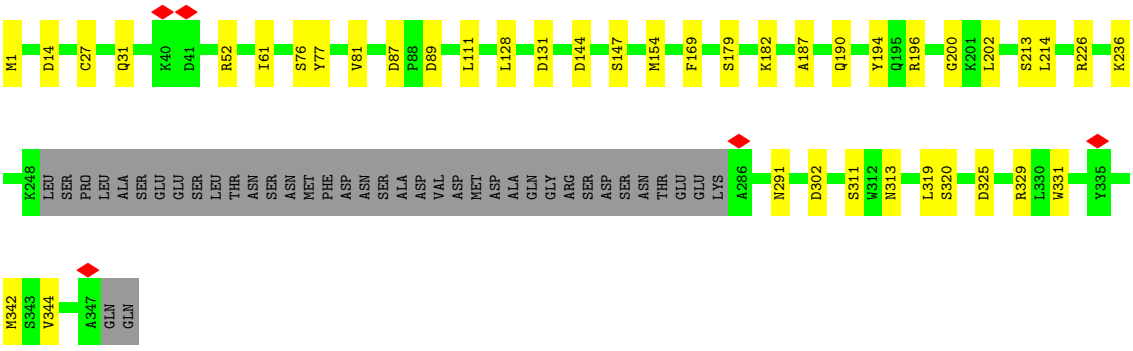




• Molecule 4: Nucleoporin SEH1

Chain L:

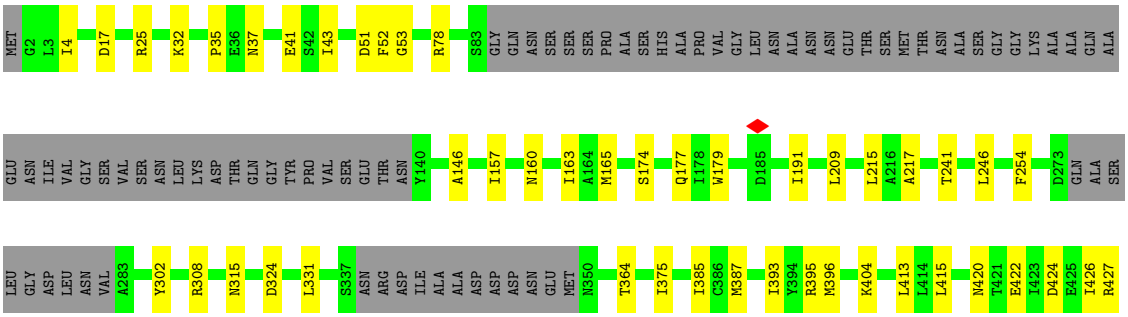


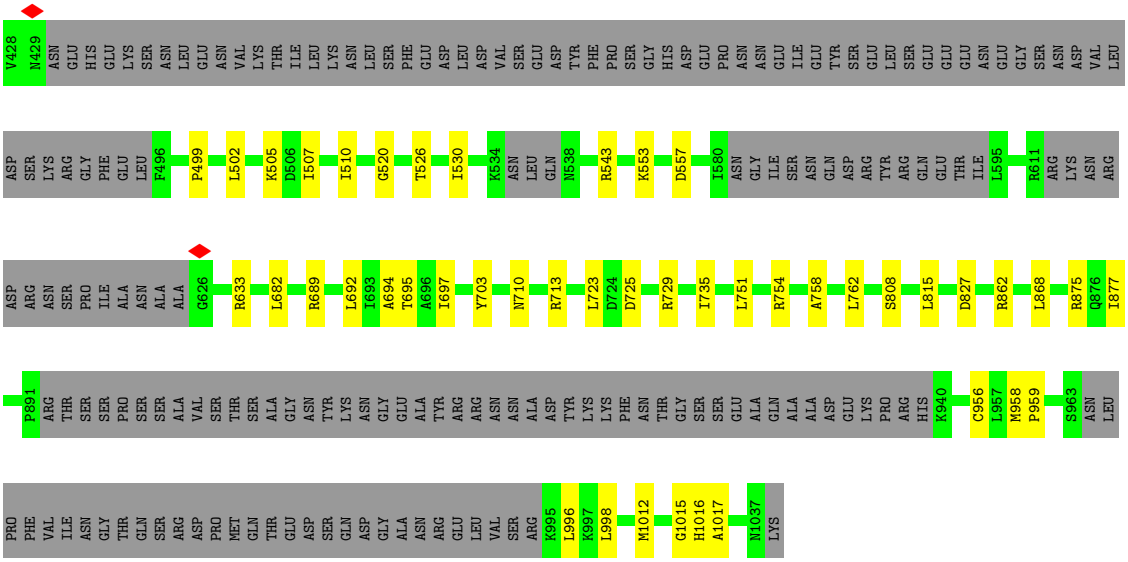


• Molecule 5: SEH-associated protein 4

Chain G:



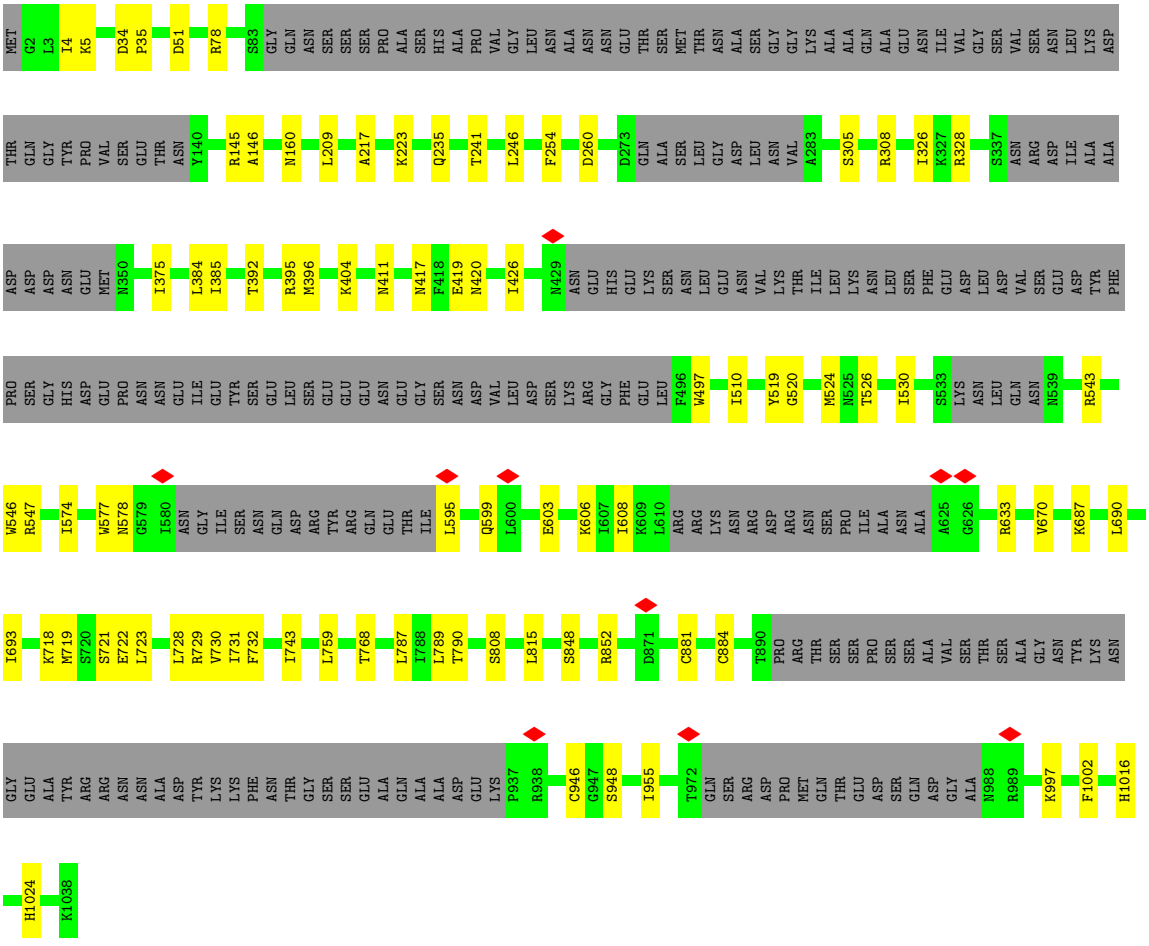




• Molecule 5: SEH-associated protein 4

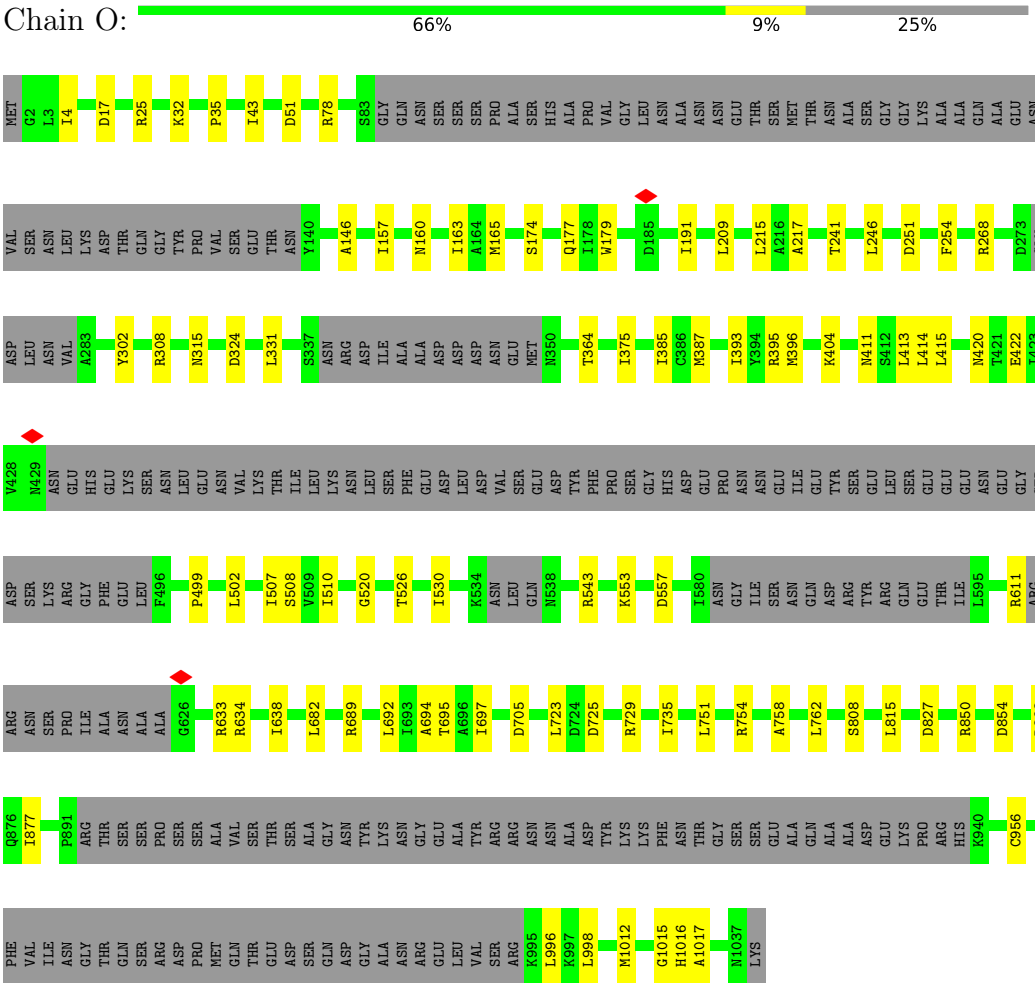
Chain B:





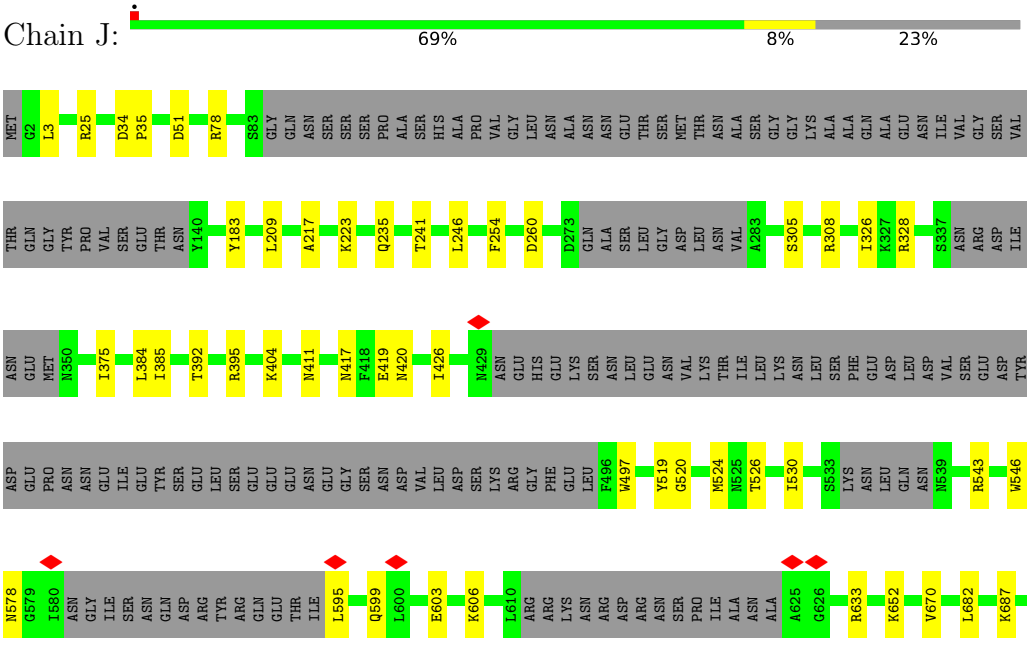
• Molecule 5: SEH-associated protein 4

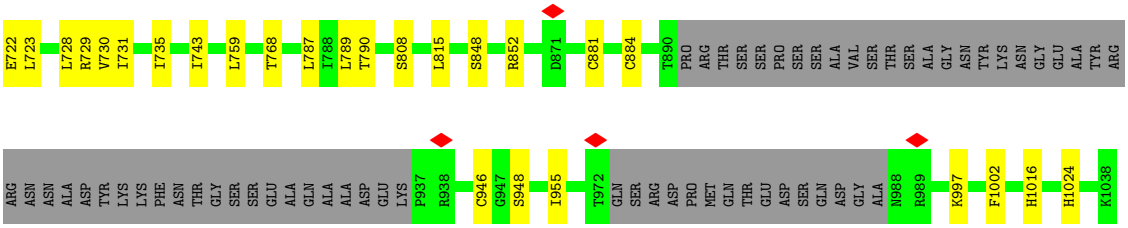
Chain O:



• Molecule 5: SEH-associated protein 4

Chain J:





• Molecule 6: GTP-binding protein GTR1

Chain a:





• Molecule 6: GTP-binding protein GTR1

Chain b:

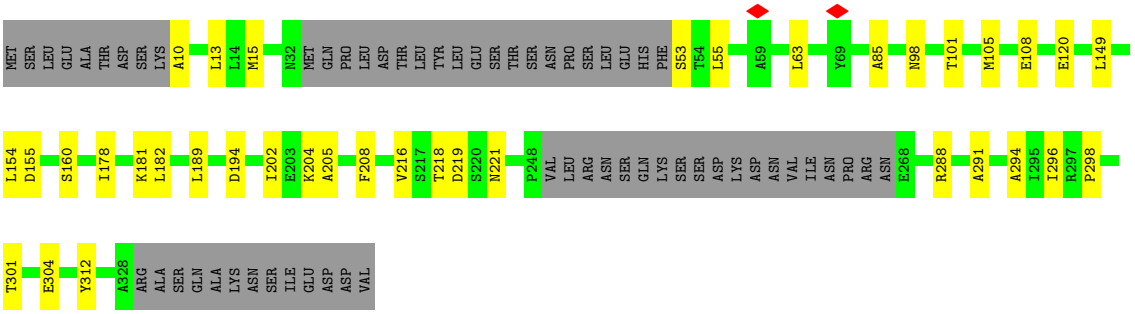




• Molecule 7: GTP-binding protein GTR2

Chain c:

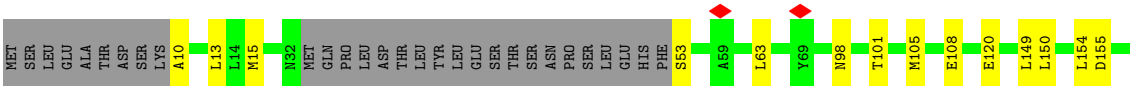


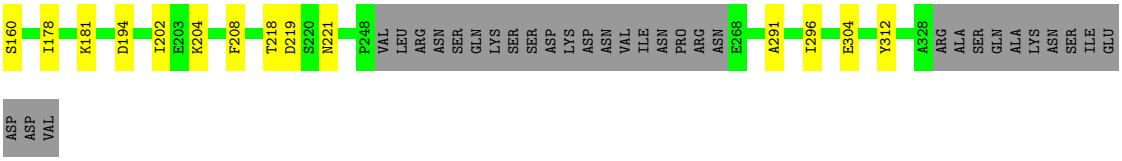


• Molecule 7: GTP-binding protein GTR2

Chain d:



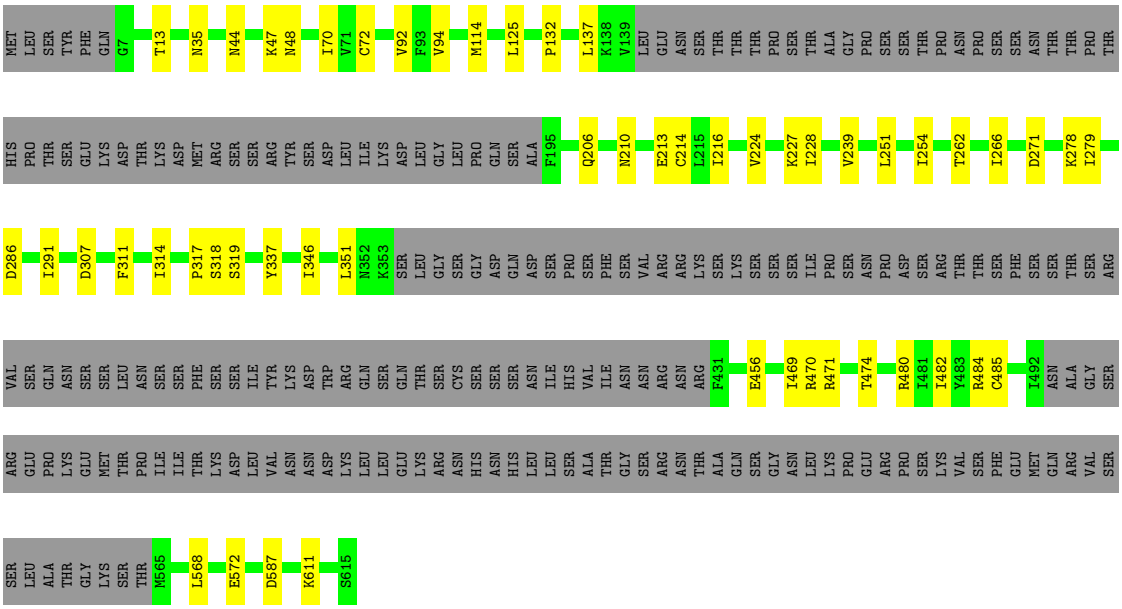




• Molecule 8: Nitrogen permease regulator 2

Chain T:

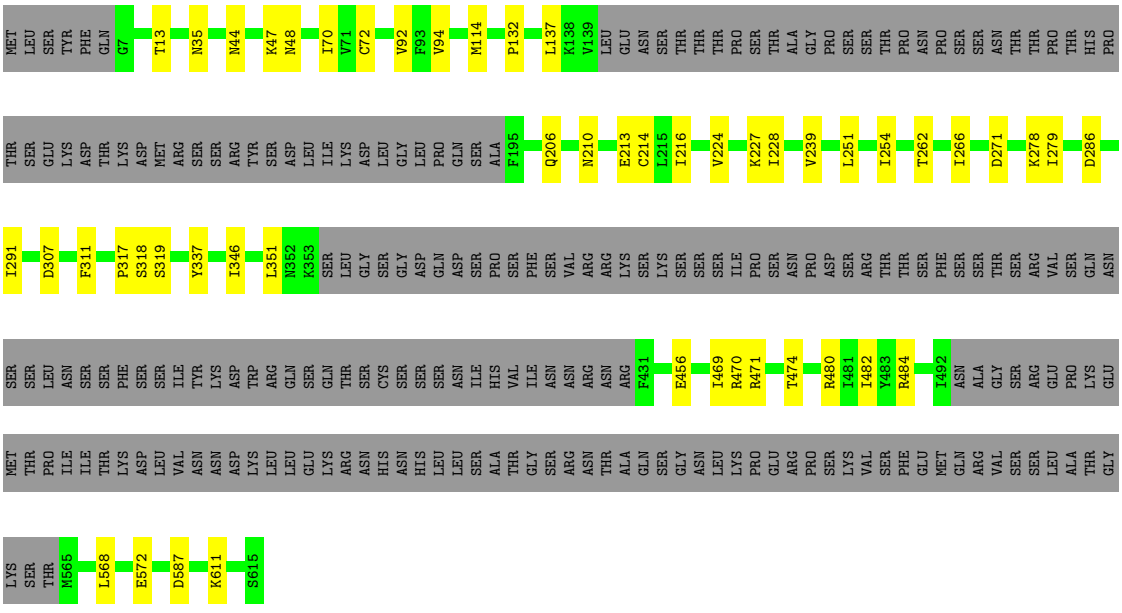




• Molecule 8: Nitrogen permease regulator 2

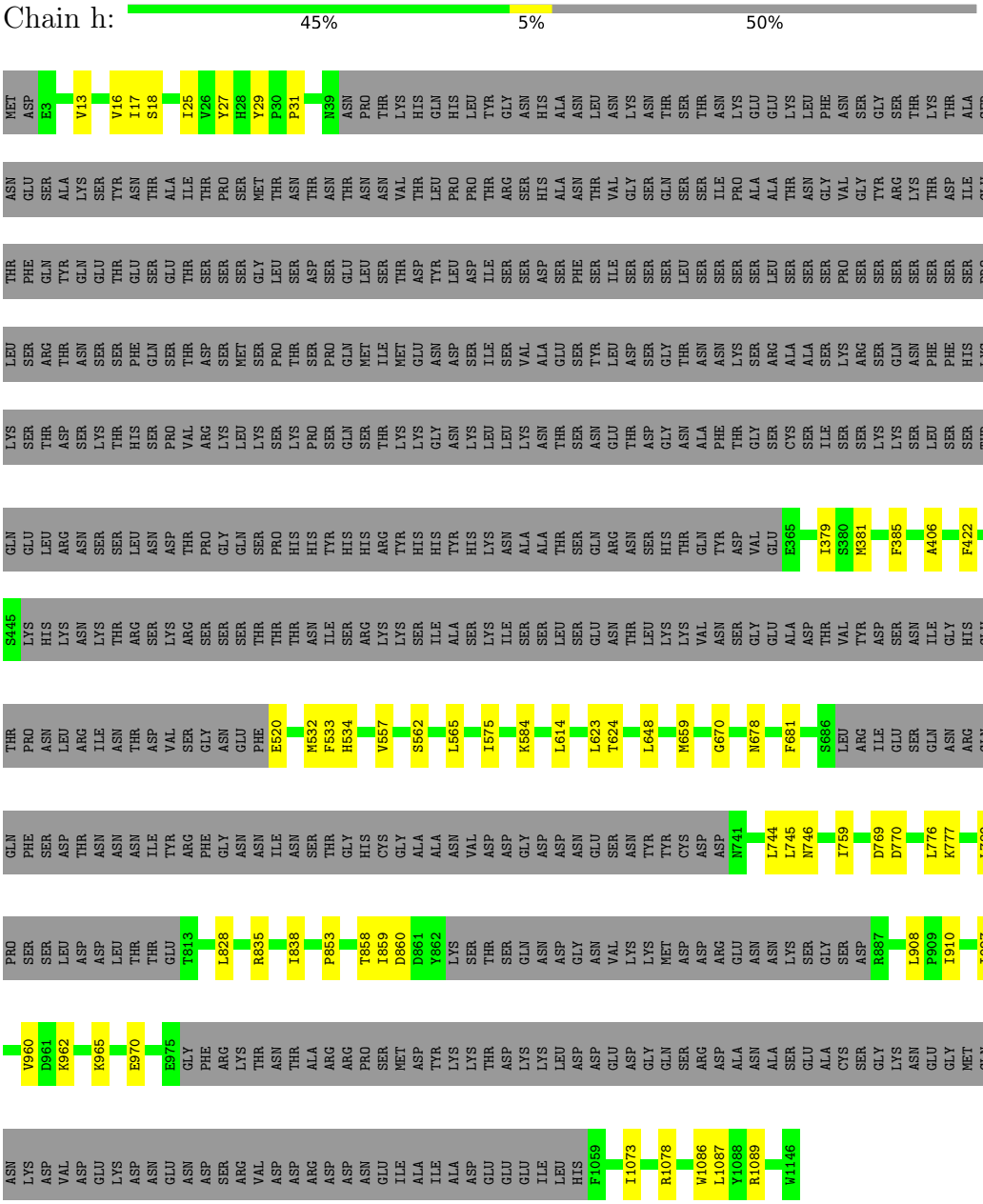
Chain g:





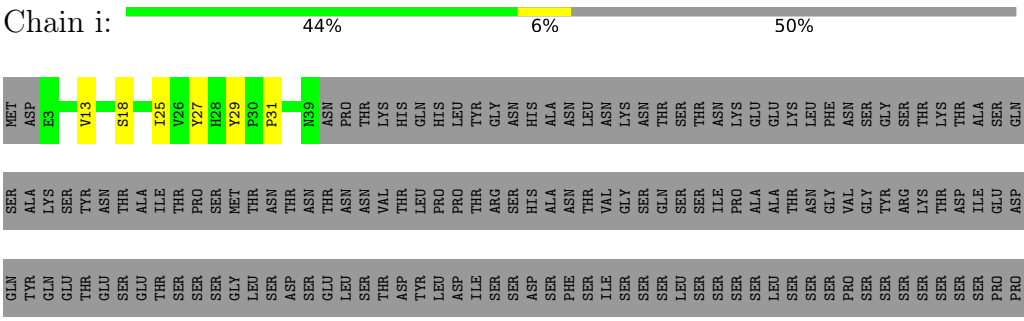
• Molecule 9: Nitrogen permease regulator 3

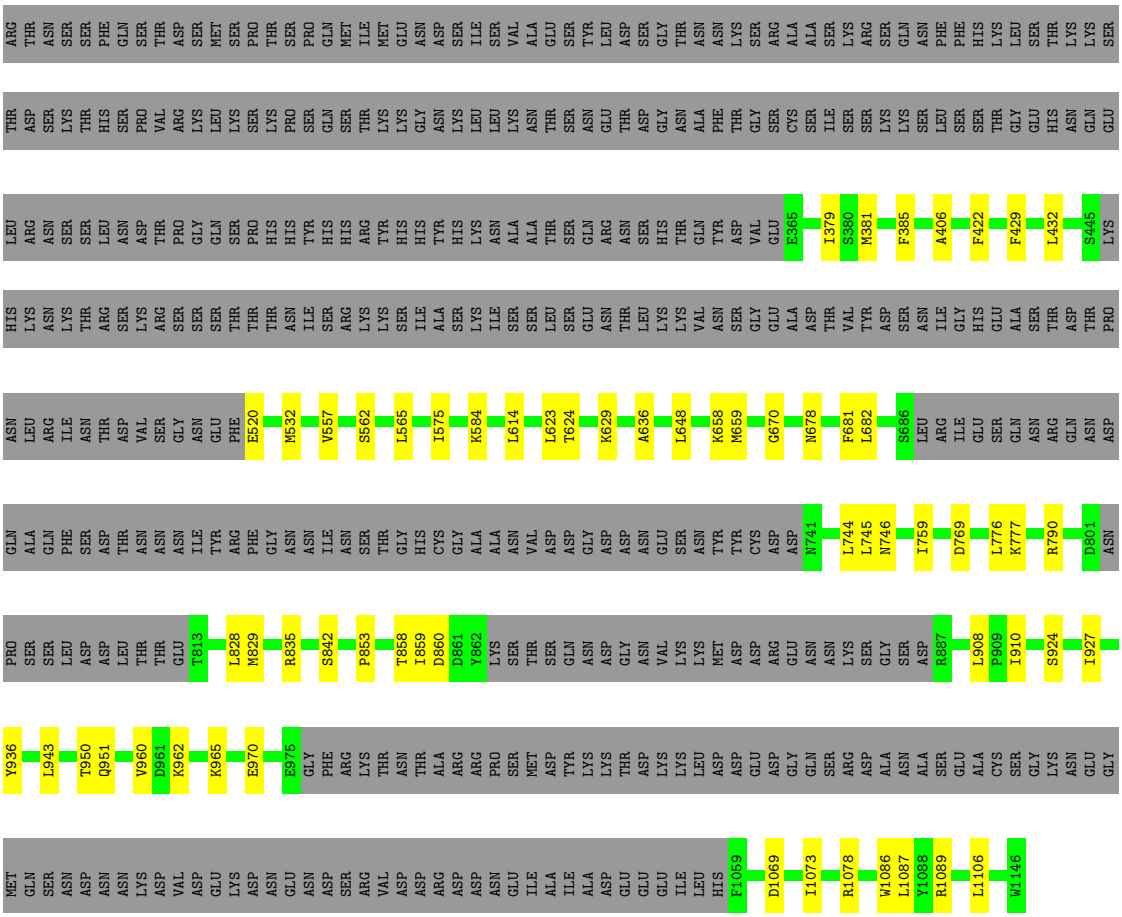
Chain h:



• Molecule 9: Nitrogen permease regulator 3

Chain i:

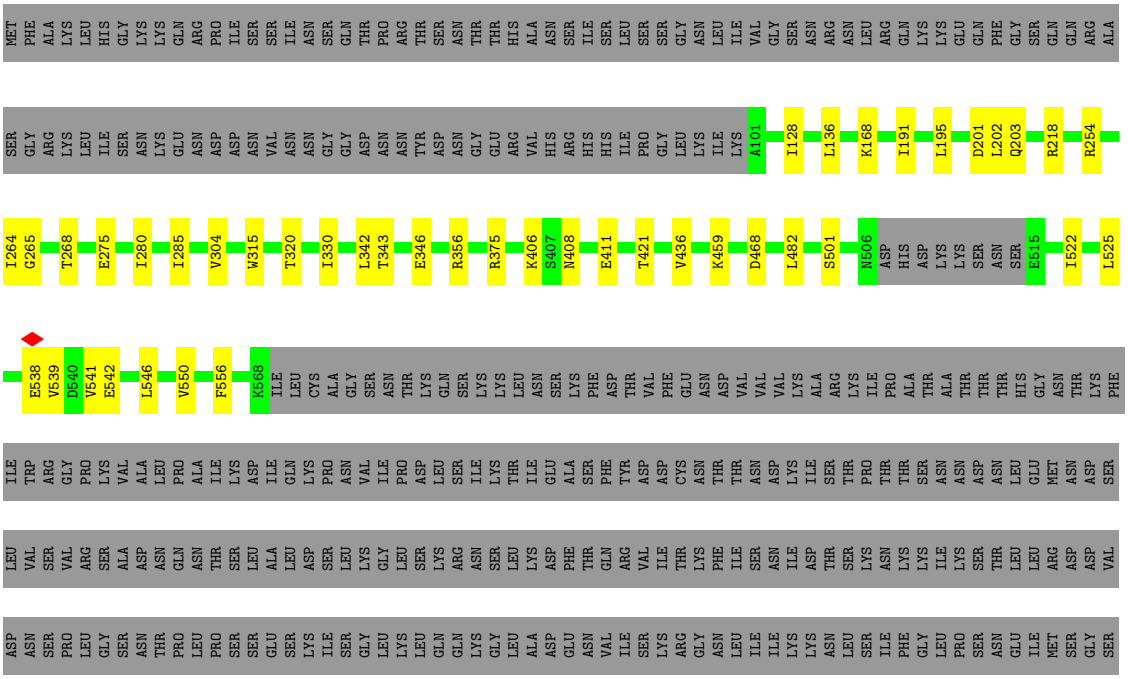


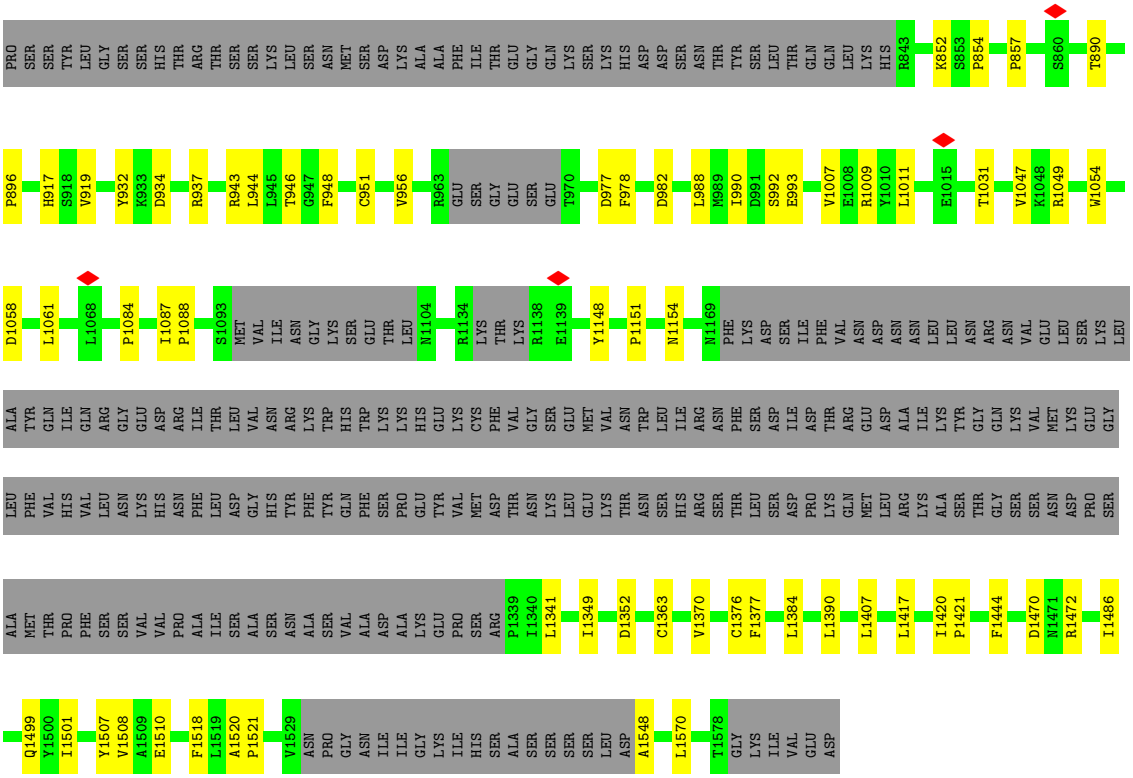


• Molecule 10: Vacuolar membrane-associated protein IML1

Chain X:



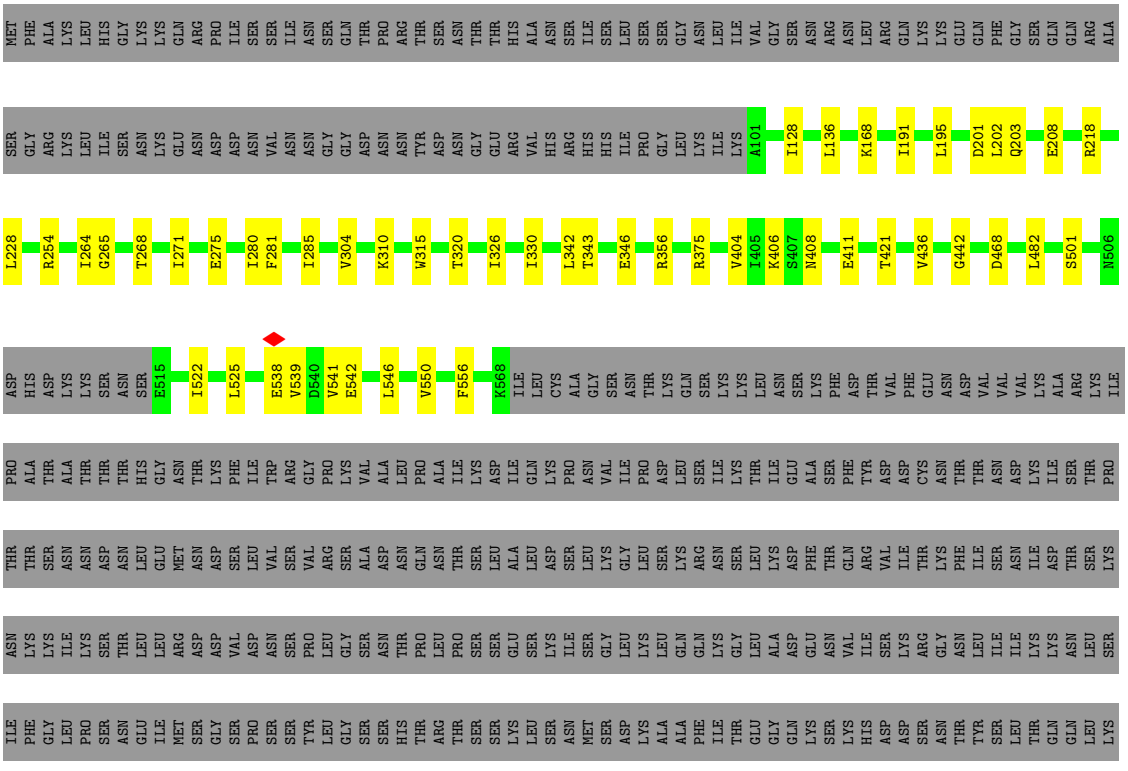


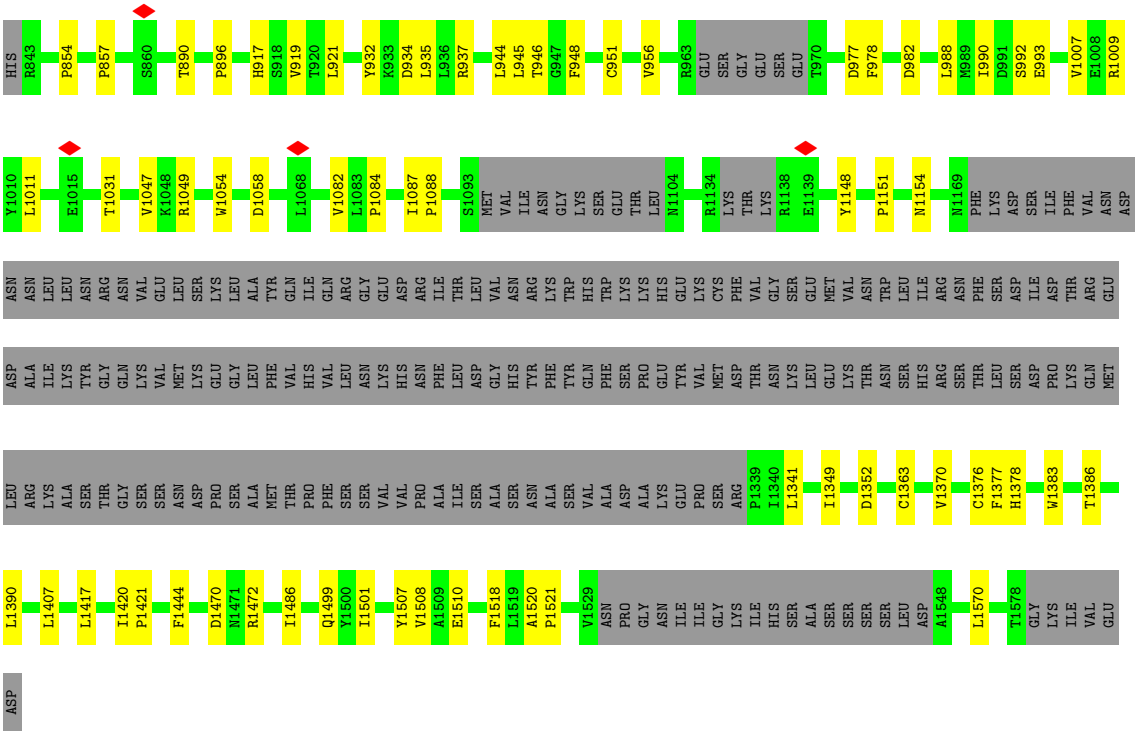


• Molecule 10: Vacuolar membrane-associated protein IML1

Chain j:



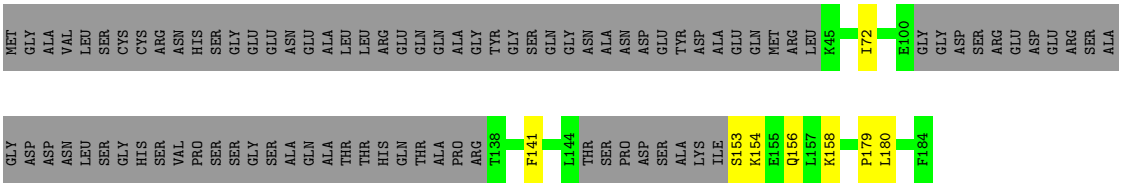




• Molecule 11: Protein MEH1

Chain R:

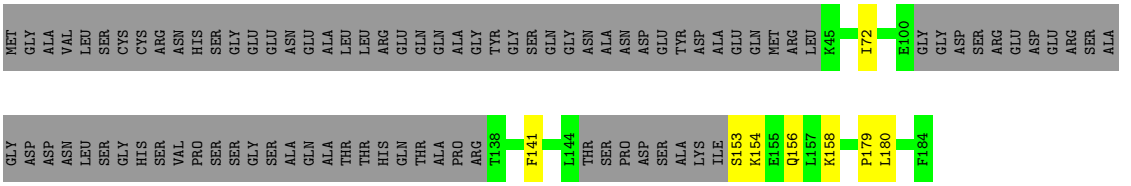




• Molecule 11: Protein MEH1

Chain S:

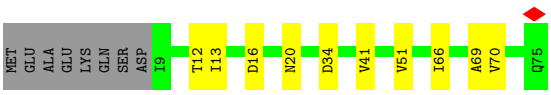




• Molecule 12: Protein EGO2

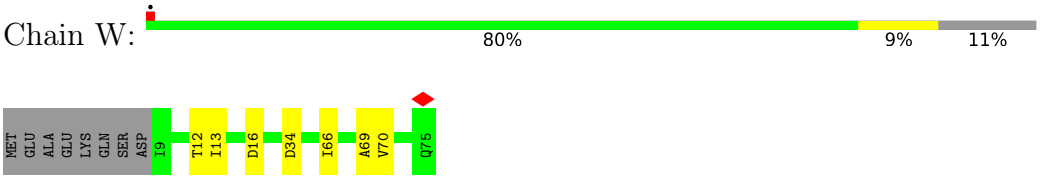
Chain U:





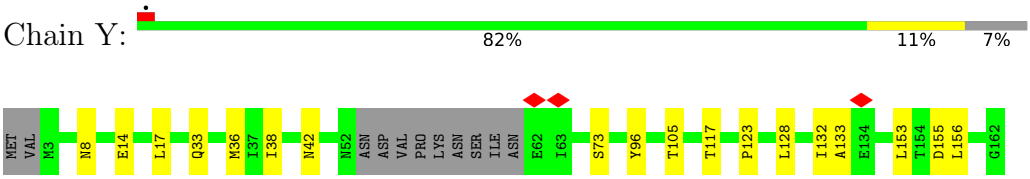
• Molecule 12: Protein EGO2

Chain W:



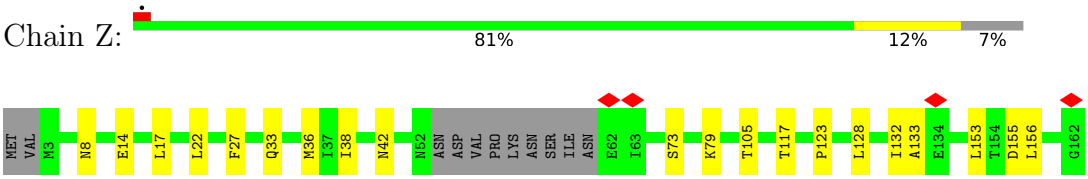
• Molecule 13: Protein SLM4

Chain Y:



• Molecule 13: Protein SLM4

Chain Z:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	208039	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 ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k)	Depositor
Maximum map value	1.546	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.0426	Depositor
Map size (Å)	522.7008, 522.7008, 522.7008	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0209, 1.0209, 1.0209	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: ZN, AF3, GDP, 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	C	0.14	0/6589	0.34	0/8940
1	K	0.14	0/6589	0.34	0/8940
2	H	0.13	0/2286	0.31	0/3117
2	P	0.12	0/2286	0.31	0/3117
3	A	0.15	0/5141	0.34	0/6957
3	I	0.15	0/5141	0.34	0/6957
4	D	0.17	0/2518	0.31	0/3414
4	E	0.18	0/2499	0.35	0/3388
4	F	0.15	0/2530	0.32	0/3430
4	L	0.17	0/2518	0.31	0/3414
4	M	0.18	0/2499	0.36	0/3388
4	N	0.16	0/2530	0.32	0/3430
5	B	0.17	0/6572	0.36	0/8881
5	G	0.16	0/6433	0.35	0/8694
5	J	0.18	0/6572	0.36	0/8881
5	O	0.16	0/6433	0.35	0/8694
6	a	0.12	0/2418	0.32	0/3243
6	b	0.12	0/2418	0.32	0/3243
7	c	0.13	0/2266	0.35	0/3067
7	d	0.14	0/2266	0.36	0/3067
8	T	0.15	0/3396	0.36	0/4602
8	g	0.15	0/3396	0.35	0/4602
9	h	0.14	0/4829	0.37	0/6527
9	i	0.14	0/4829	0.36	0/6527
10	X	0.15	0/8378	0.35	0/11323
10	j	0.15	0/8378	0.35	0/11323
11	R	0.11	0/771	0.28	0/1035
11	S	0.11	0/771	0.28	0/1035
12	U	0.11	0/510	0.29	0/690
12	W	0.11	0/510	0.29	0/690
13	Y	0.11	0/1222	0.26	0/1649
13	Z	0.10	0/1222	0.27	0/1649

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
All	All	0.15	0/116716	0.34	0/157914

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	6414	0	6196	74	0
1	K	6414	0	6196	69	0
2	H	2226	0	2164	22	0
2	P	2226	0	2164	23	0
3	A	5036	0	5003	51	0
3	I	5036	0	5003	49	0
4	D	2457	0	2394	25	0
4	E	2438	0	2378	31	0
4	F	2469	0	2408	30	0
4	L	2457	0	2394	28	0
4	M	2438	0	2378	27	0
4	N	2469	0	2408	28	0
5	B	6439	0	6323	57	0
5	G	6303	0	6184	58	0
5	J	6439	0	6323	53	0
5	O	6303	0	6184	58	0
6	a	2375	0	2433	13	0
6	b	2375	0	2433	13	0
7	c	2230	0	2234	24	0
7	d	2230	0	2234	18	0
8	T	3312	0	3337	34	0
8	g	3312	0	3337	32	0
9	h	4727	0	4738	37	0
9	i	4727	0	4738	40	0
10	X	8187	0	8161	66	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	j	8187	0	8161	71	0
11	R	765	0	770	7	0
11	S	765	0	770	7	0
12	U	505	0	499	6	0
12	W	505	0	499	4	0
13	Y	1201	0	1186	13	0
13	Z	1201	0	1186	14	0
14	A	3	0	0	0	0
14	B	4	0	0	0	0
14	C	3	0	0	0	0
14	G	4	0	0	0	0
14	I	3	0	0	0	0
14	J	4	0	0	0	0
14	K	3	0	0	0	0
14	O	4	0	0	0	0
15	a	1	0	0	0	0
15	b	1	0	0	0	0
16	a	4	0	0	1	0
16	b	4	0	0	1	0
17	a	28	0	12	0	0
17	b	28	0	12	0	0
17	c	28	0	12	0	0
17	d	28	0	12	0	0
All	All	114318	0	112864	976	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 976 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)
5:J:884:CYS:HB3	5:J:946:CYS:SG	2.23	0.78
5:B:884:CYS:HB3	5:B:946:CYS:SG	2.23	0.78
5:O:956:CYS:SG	5:O:1016:HIS:HE1	2.14	0.69
10:X:1510:GLU:HB3	10:X:1518:PHE:HB2	1.76	0.68
1:C:484:ASN:HB3	1:C:487:ASN:HB2	1.76	0.66

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	C	775/1148 (68%)	741 (96%)	34 (4%)	0	100	100
1	K	775/1148 (68%)	741 (96%)	34 (4%)	0	100	100
2	H	276/297 (93%)	267 (97%)	9 (3%)	0	100	100
2	P	276/297 (93%)	267 (97%)	9 (3%)	0	100	100
3	A	612/1341 (46%)	585 (96%)	27 (4%)	0	100	100
3	I	612/1341 (46%)	585 (96%)	27 (4%)	0	100	100
4	D	306/349 (88%)	298 (97%)	8 (3%)	0	100	100
4	E	303/349 (87%)	289 (95%)	14 (5%)	0	100	100
4	F	307/349 (88%)	298 (97%)	9 (3%)	0	100	100
4	L	306/349 (88%)	298 (97%)	8 (3%)	0	100	100
4	M	303/349 (87%)	289 (95%)	14 (5%)	0	100	100
4	N	307/349 (88%)	298 (97%)	9 (3%)	0	100	100
5	B	780/1038 (75%)	750 (96%)	30 (4%)	0	100	100
5	G	763/1038 (74%)	738 (97%)	25 (3%)	0	100	100
5	J	780/1038 (75%)	749 (96%)	31 (4%)	0	100	100
5	O	763/1038 (74%)	738 (97%)	25 (3%)	0	100	100
6	a	288/310 (93%)	282 (98%)	6 (2%)	0	100	100
6	b	288/310 (93%)	280 (97%)	8 (3%)	0	100	100
7	c	274/341 (80%)	262 (96%)	12 (4%)	0	100	100
7	d	274/341 (80%)	263 (96%)	11 (4%)	0	100	100
8	T	397/615 (65%)	383 (96%)	14 (4%)	0	100	100
8	g	397/615 (65%)	383 (96%)	14 (4%)	0	100	100
9	h	559/1146 (49%)	531 (95%)	28 (5%)	0	100	100
9	i	559/1146 (49%)	532 (95%)	27 (5%)	0	100	100
10	X	974/1584 (62%)	917 (94%)	57 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j	974/1584 (62%)	918 (94%)	56 (6%)	0	100	100
11	R	89/184 (48%)	87 (98%)	2 (2%)	0	100	100
11	S	89/184 (48%)	87 (98%)	2 (2%)	0	100	100
12	U	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
12	W	65/75 (87%)	64 (98%)	1 (2%)	0	100	100
13	Y	147/162 (91%)	143 (97%)	4 (3%)	0	100	100
13	Z	147/162 (91%)	143 (97%)	4 (3%)	0	100	100
All	All	13830/20652 (67%)	13270 (96%)	560 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	C	720/1040 (69%)	720 (100%)	0	100	100
1	K	720/1040 (69%)	720 (100%)	0	100	100
2	H	240/252 (95%)	240 (100%)	0	100	100
2	P	240/252 (95%)	240 (100%)	0	100	100
3	A	568/1207 (47%)	568 (100%)	0	100	100
3	I	568/1207 (47%)	568 (100%)	0	100	100
4	D	270/305 (88%)	270 (100%)	0	100	100
4	E	269/305 (88%)	269 (100%)	0	100	100
4	F	272/305 (89%)	272 (100%)	0	100	100
4	L	270/305 (88%)	270 (100%)	0	100	100
4	M	269/305 (88%)	269 (100%)	0	100	100
4	N	272/305 (89%)	272 (100%)	0	100	100
5	B	716/919 (78%)	716 (100%)	0	100	100
5	G	701/919 (76%)	701 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	J	716/919 (78%)	716 (100%)	0	100	100
5	O	701/919 (76%)	701 (100%)	0	100	100
6	a	273/291 (94%)	273 (100%)	0	100	100
6	b	273/291 (94%)	273 (100%)	0	100	100
7	c	252/310 (81%)	252 (100%)	0	100	100
7	d	252/310 (81%)	252 (100%)	0	100	100
8	T	386/582 (66%)	386 (100%)	0	100	100
8	g	386/582 (66%)	386 (100%)	0	100	100
9	h	539/1060 (51%)	539 (100%)	0	100	100
9	i	539/1060 (51%)	539 (100%)	0	100	100
10	X	921/1458 (63%)	921 (100%)	0	100	100
10	j	921/1458 (63%)	921 (100%)	0	100	100
11	R	89/158 (56%)	89 (100%)	0	100	100
11	S	89/158 (56%)	89 (100%)	0	100	100
12	U	55/62 (89%)	55 (100%)	0	100	100
12	W	55/62 (89%)	55 (100%)	0	100	100
13	Y	139/150 (93%)	139 (100%)	0	100	100
13	Z	139/150 (93%)	139 (100%)	0	100	100
All	All	12820/18646 (69%)	12820 (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 123 such sidechains are listed below:

Mol	Chain	Res	Type
3	I	503	ASN
8	g	58	HIS
5	O	632	GLN
7	d	274	GLN
10	j	973	ASN

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 36 ligands modelled in this entry, 30 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
17	GDP	d	401	-	28,30,30	1.14	3 (10%)	44,47,47	1.85	8 (18%)
17	GDP	b	403	15	28,30,30	1.14	3 (10%)	44,47,47	1.82	7 (15%)
16	AF3	b	402	-	0,3,3	-	-	-		
16	AF3	a	402	-	0,3,3	-	-	-		
17	GDP	a	403	15	28,30,30	1.14	3 (10%)	44,47,47	1.82	7 (15%)
17	GDP	c	401	-	28,30,30	1.14	3 (10%)	44,47,47	1.86	8 (18%)

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
17	GDP	d	401	-	-	0/16/32/32	0/3/3/3
17	GDP	a	403	15	-	0/16/32/32	0/3/3/3
17	GDP	c	401	-	-	0/16/32/32	0/3/3/3
17	GDP	b	403	15	-	0/16/32/32	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	c	401	GDP	C5-C4	3.12	1.47	1.38
17	d	401	GDP	C5-C4	3.11	1.47	1.38
17	a	403	GDP	C5-C4	3.10	1.47	1.38
17	b	403	GDP	C5-C4	3.10	1.47	1.38
17	c	401	GDP	C6-N1	-2.45	1.34	1.38

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	d	401	GDP	C5-C4-N3	-6.12	118.53	128.46
17	c	401	GDP	C5-C4-N3	-6.12	118.53	128.46
17	b	403	GDP	C5-C4-N3	-6.07	118.61	128.46
17	a	403	GDP	C5-C4-N3	-6.05	118.64	128.46
17	c	401	GDP	C2-N3-C4	4.94	121.10	112.30

There are no chirality outliers.

There are no torsion outliers.

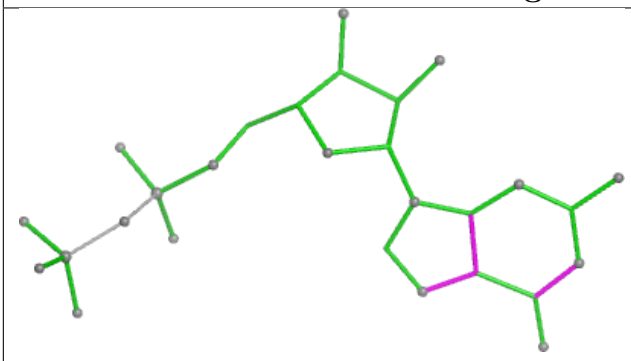
There are no ring outliers.

2 monomers are involved in 2 short contacts:

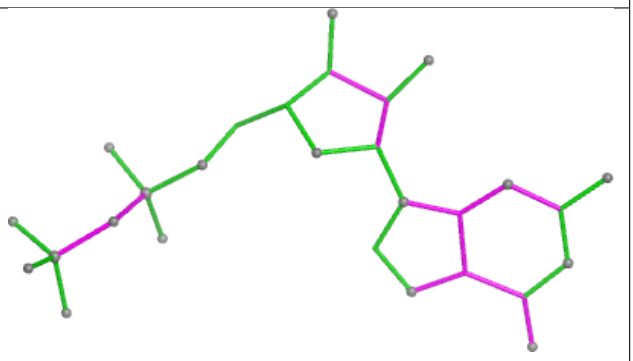
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	402	AF3	1	0
16	a	402	AF3	1	0

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 then 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.

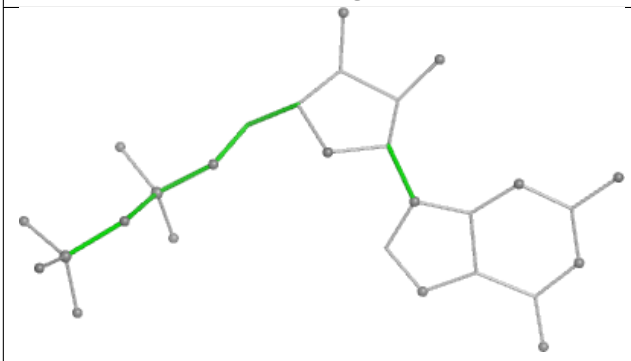
Ligand GDP d 401



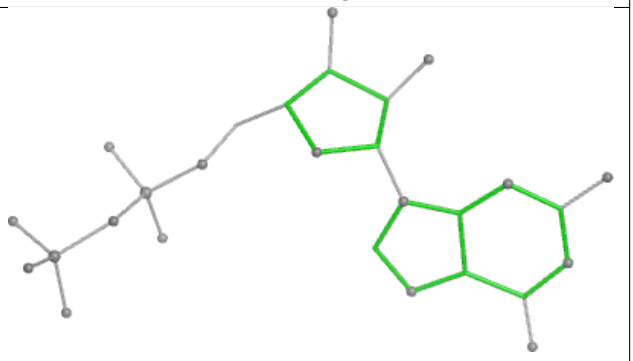
Bond lengths



Bond angles

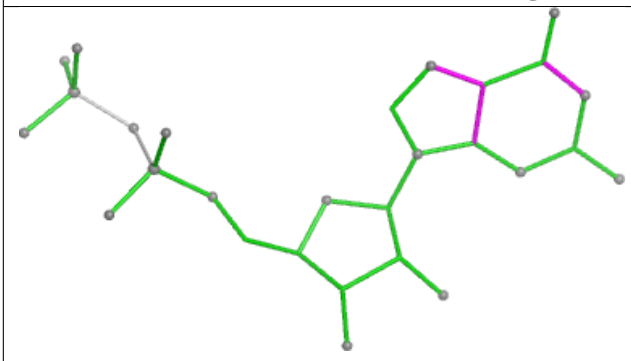


Torsions

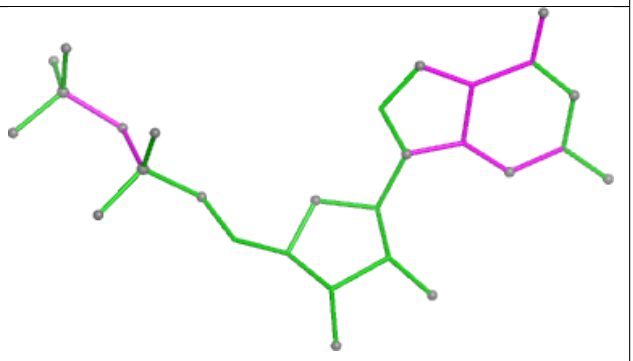


Rings

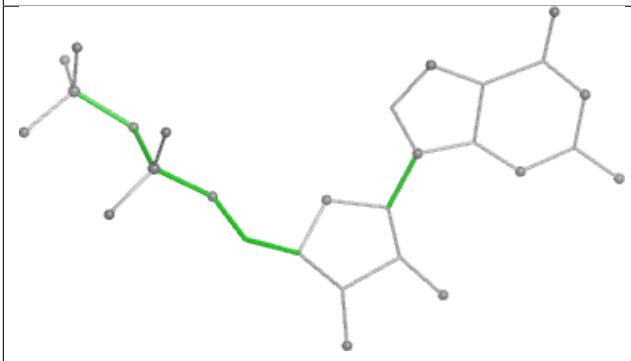
Ligand GDP b 403



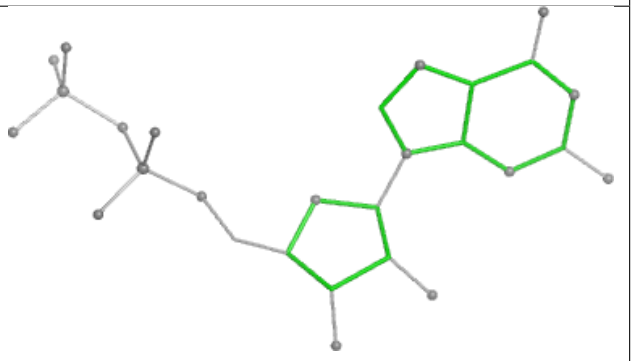
Bond lengths



Bond angles

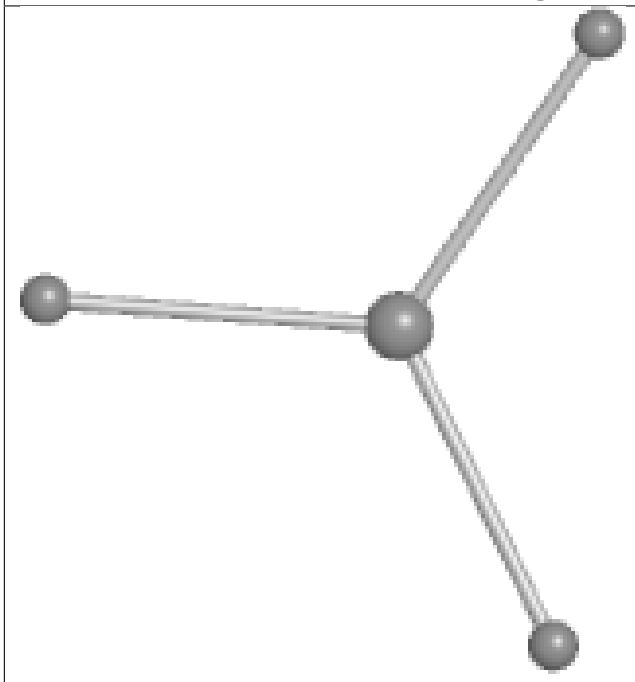


Torsions

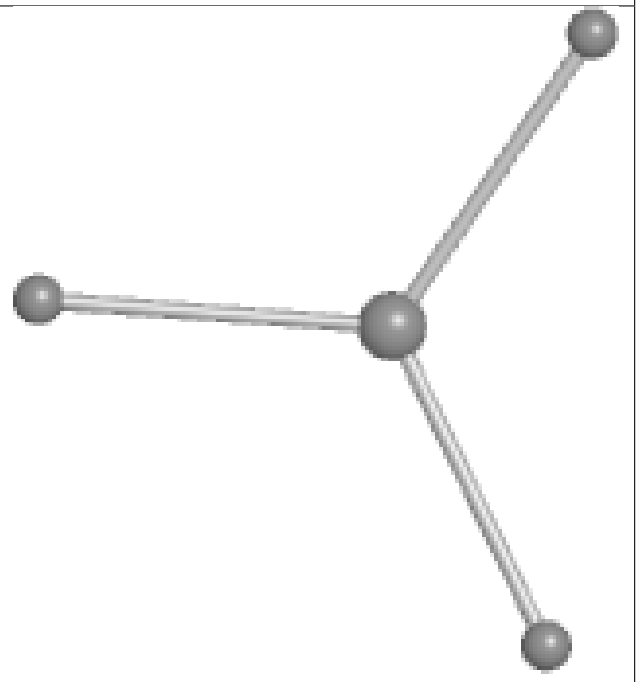


Rings

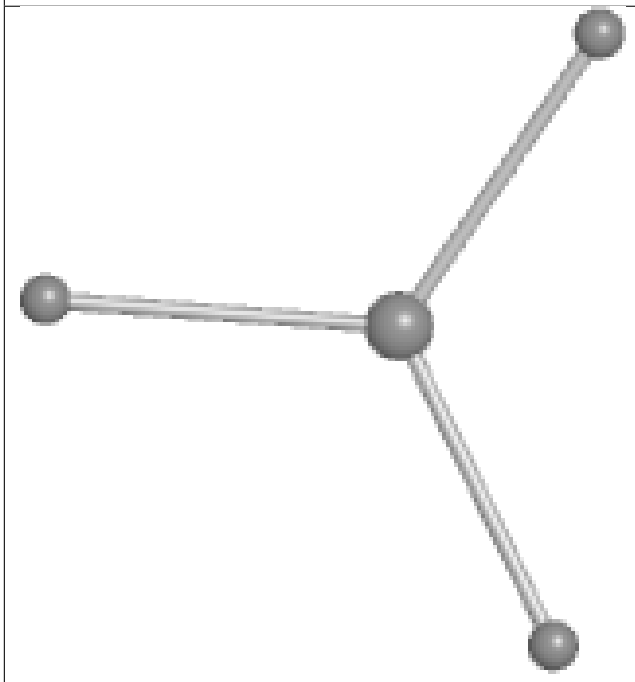
Ligand AF3 b 402



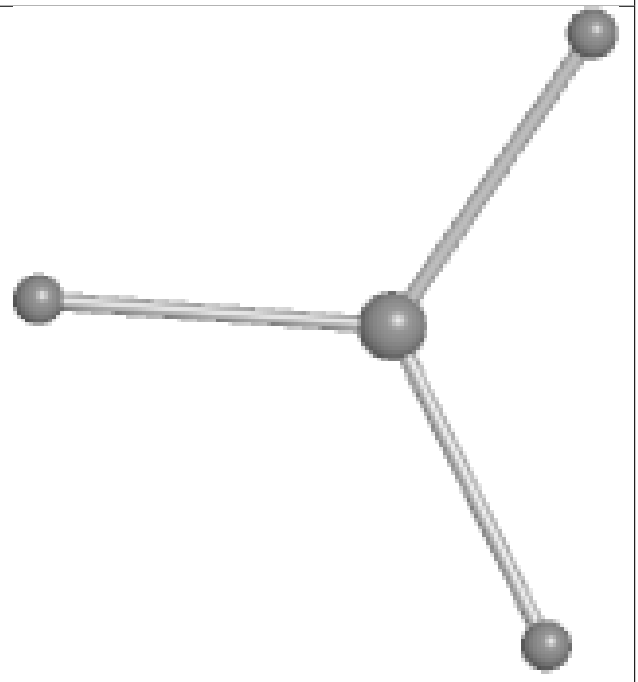
Bond lengths



Bond angles

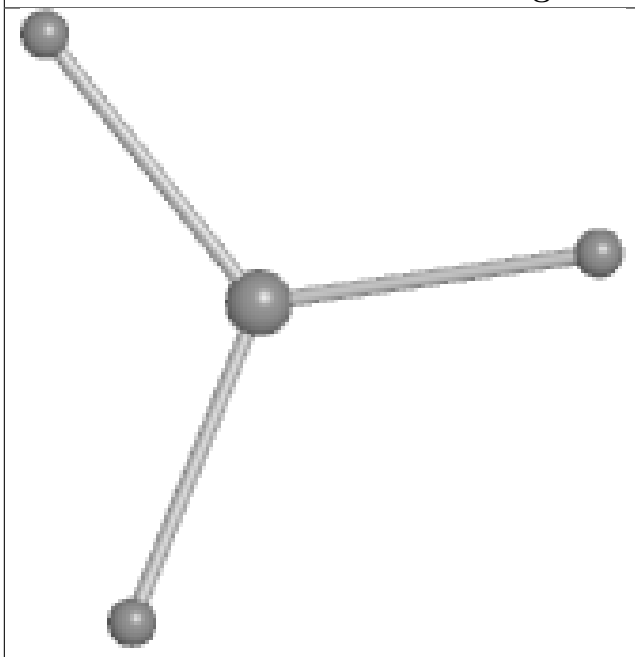


Torsions

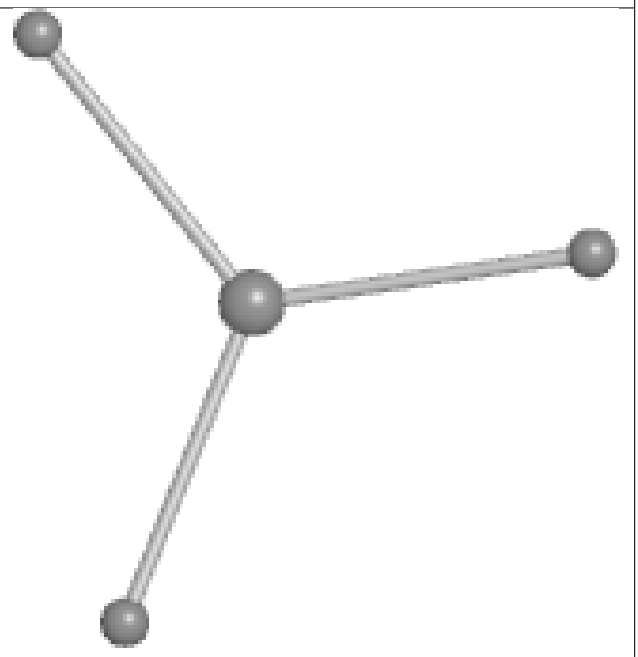


Rings

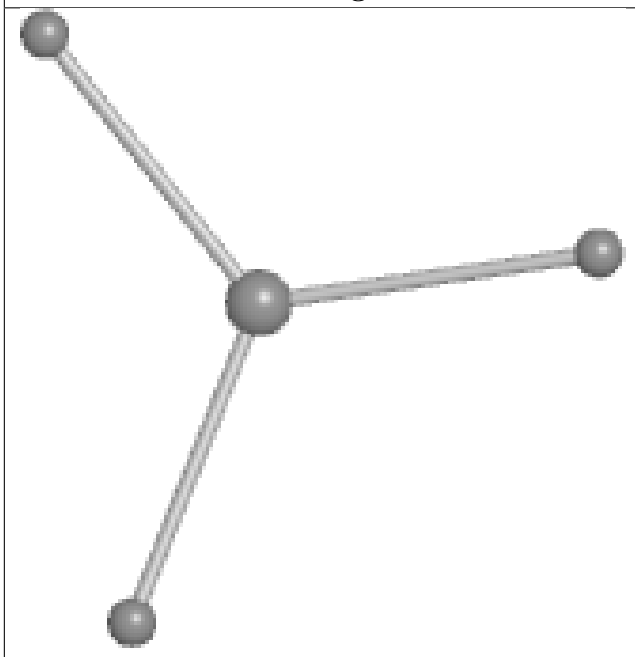
Ligand AF3 a 402



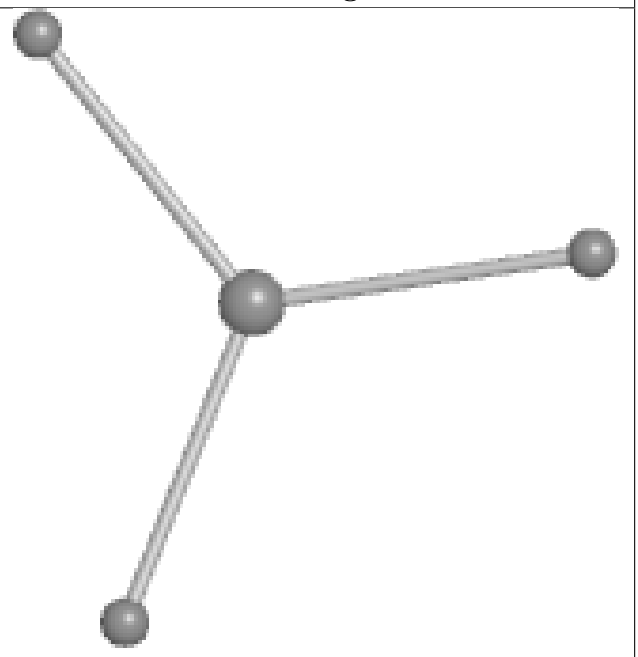
Bond lengths



Bond angles

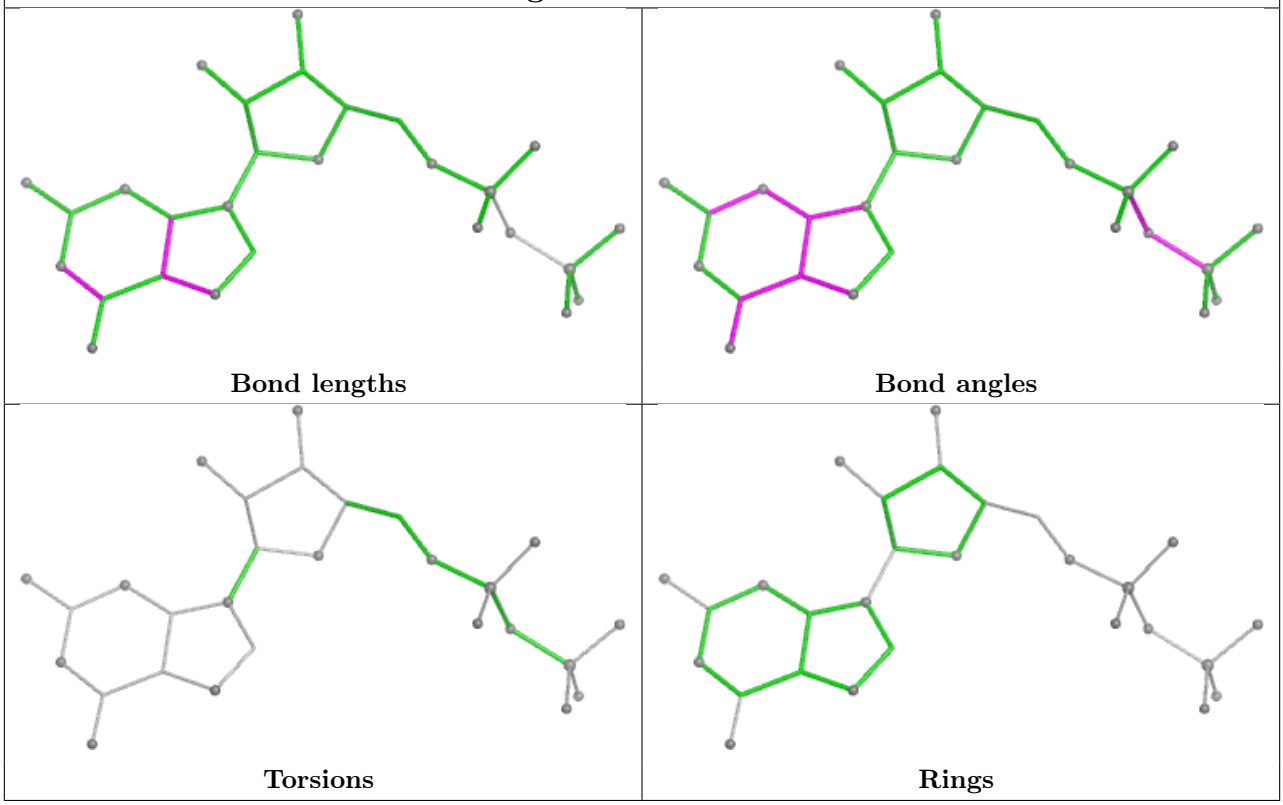


Torsions

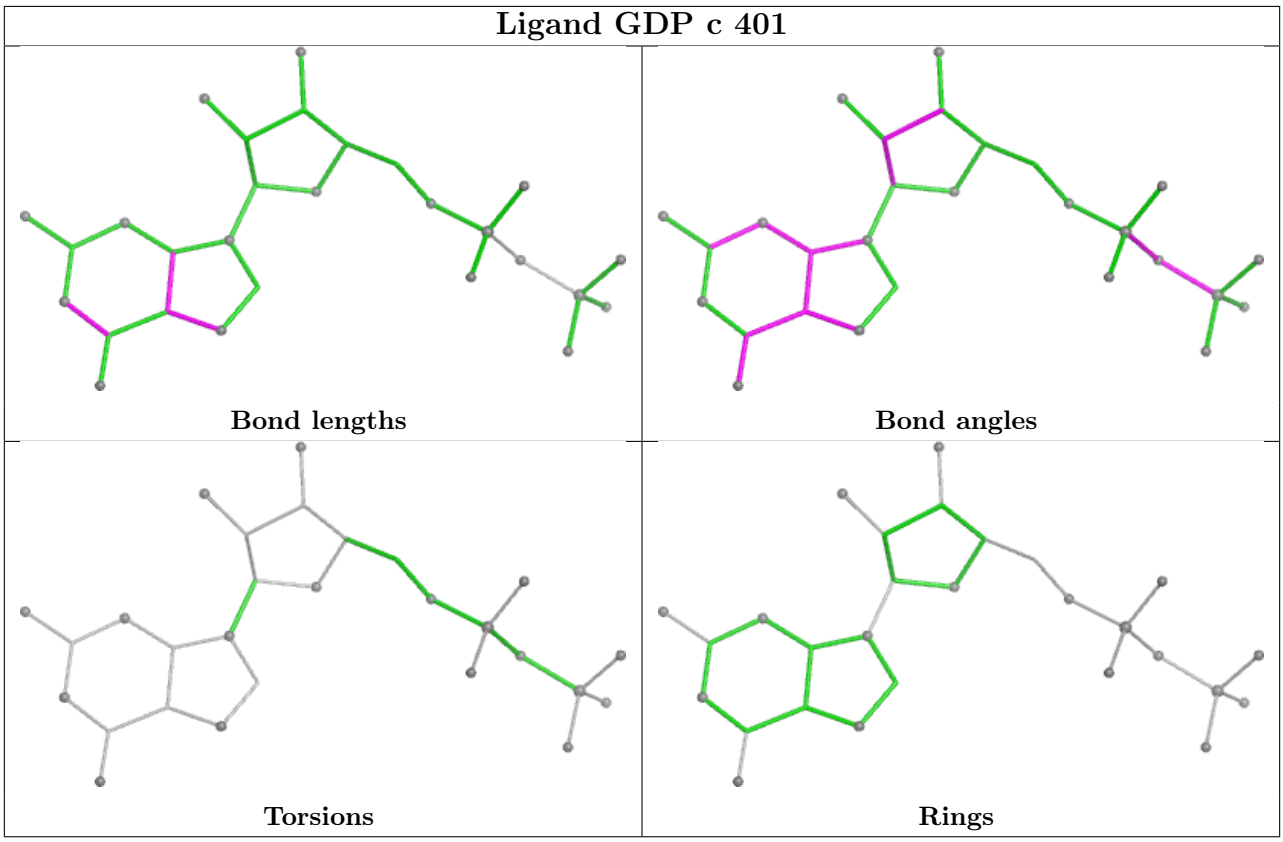


Rings

Ligand GDP a 403



Ligand GDP c 401



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.

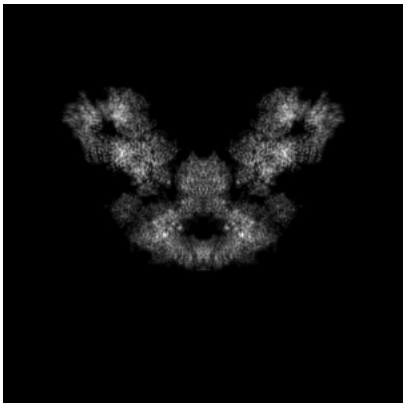
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-51887. These allow visual inspection of the internal detail of the map and identification of artifacts.

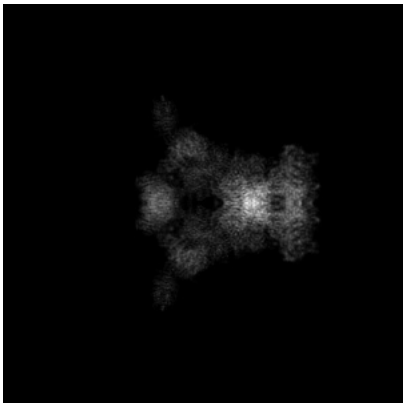
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

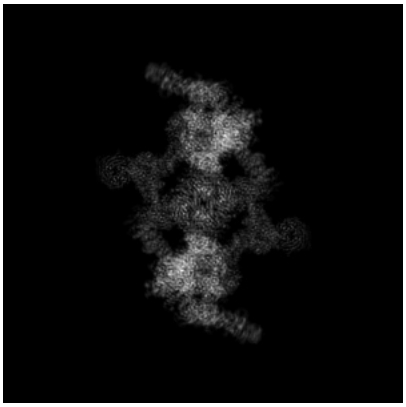
6.1.1 Primary map



X



Y



Z

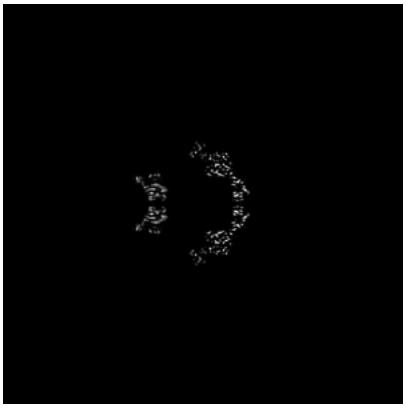
The images above show the map projected in three orthogonal directions.

6.2 Central slices

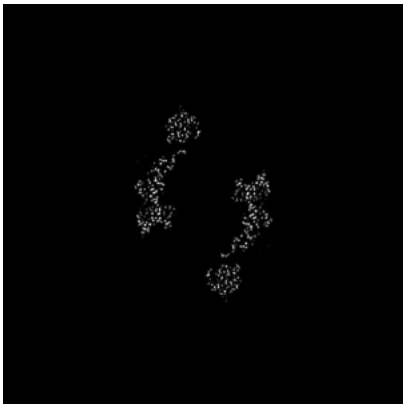
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

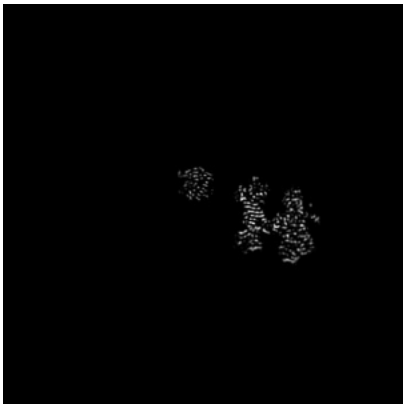
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

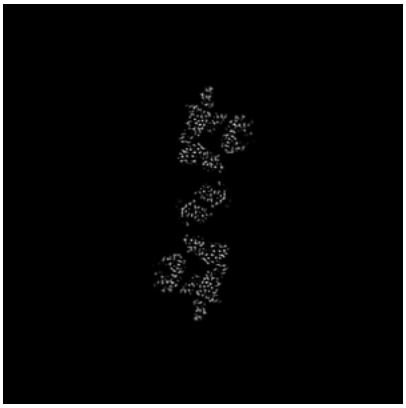
6.3.1 Primary map



X Index: 241



Y Index: 151

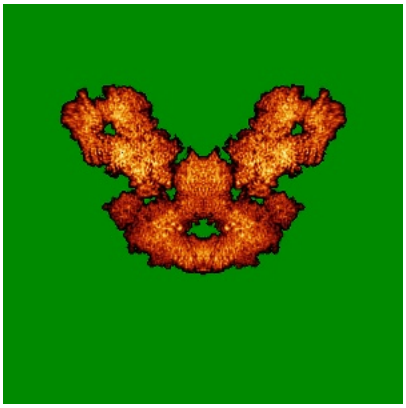


Z Index: 310

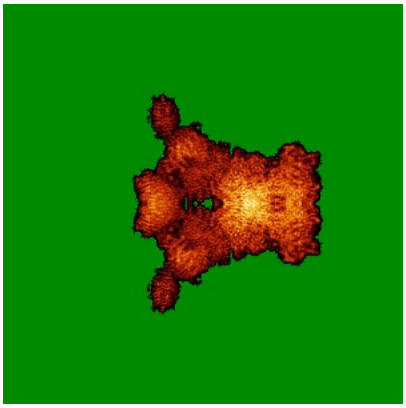
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

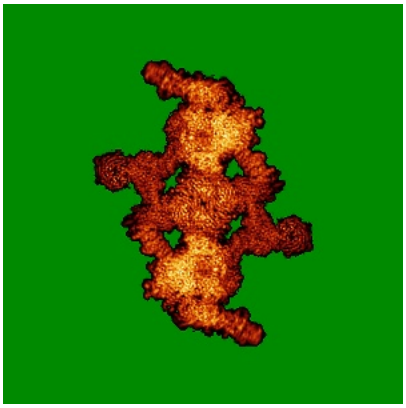
6.4.1 Primary map



X



Y

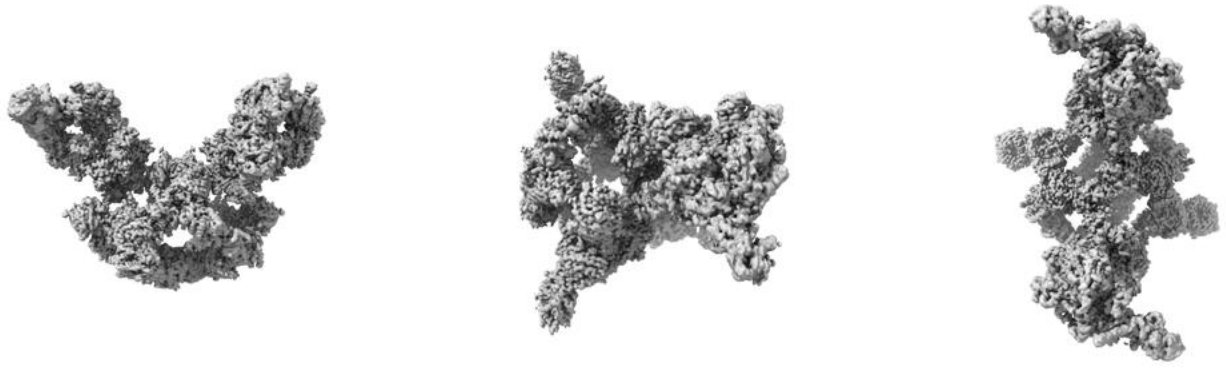


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.0426. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

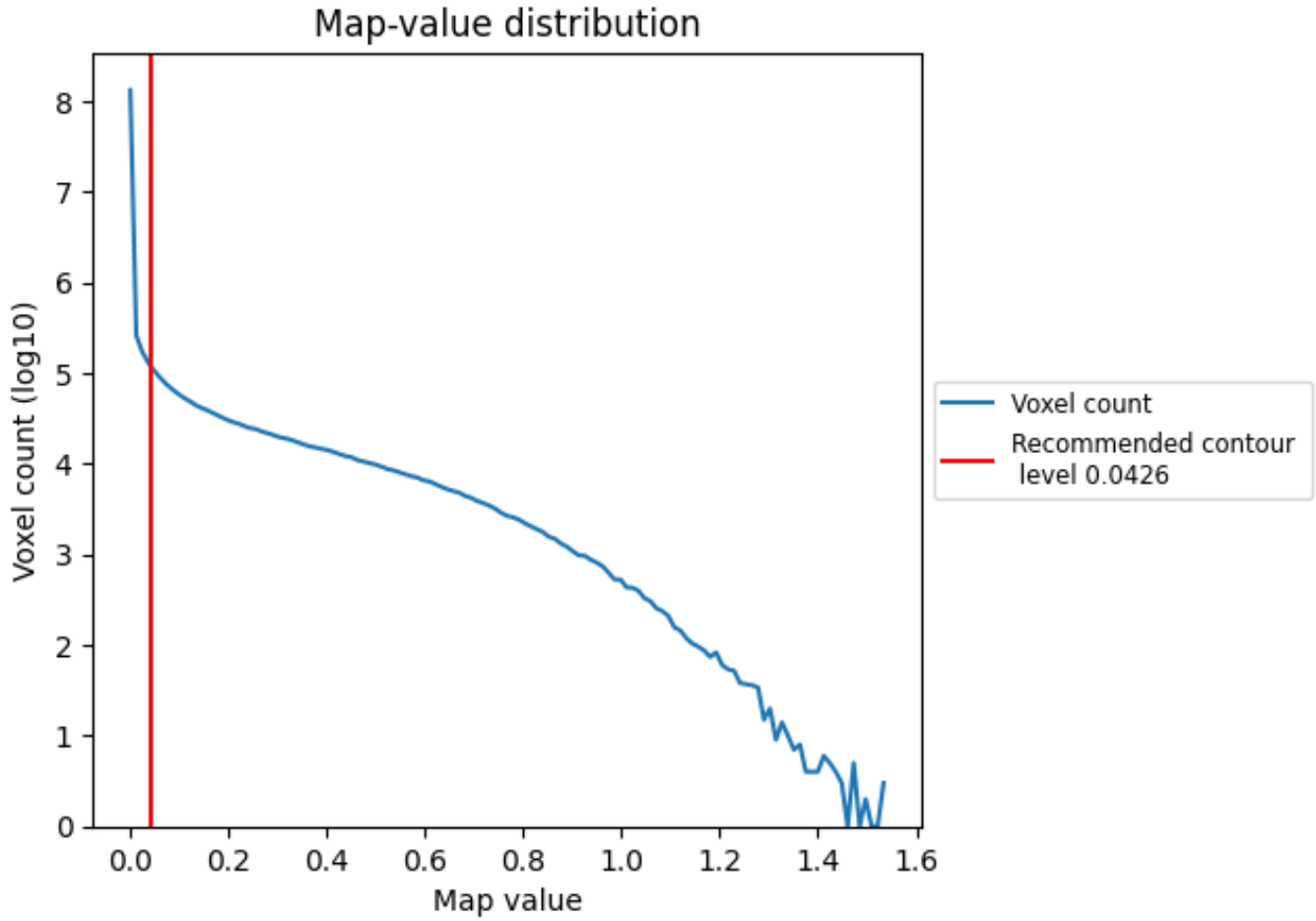
6.6 Mask visualisation (i)

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

7 Map analysis

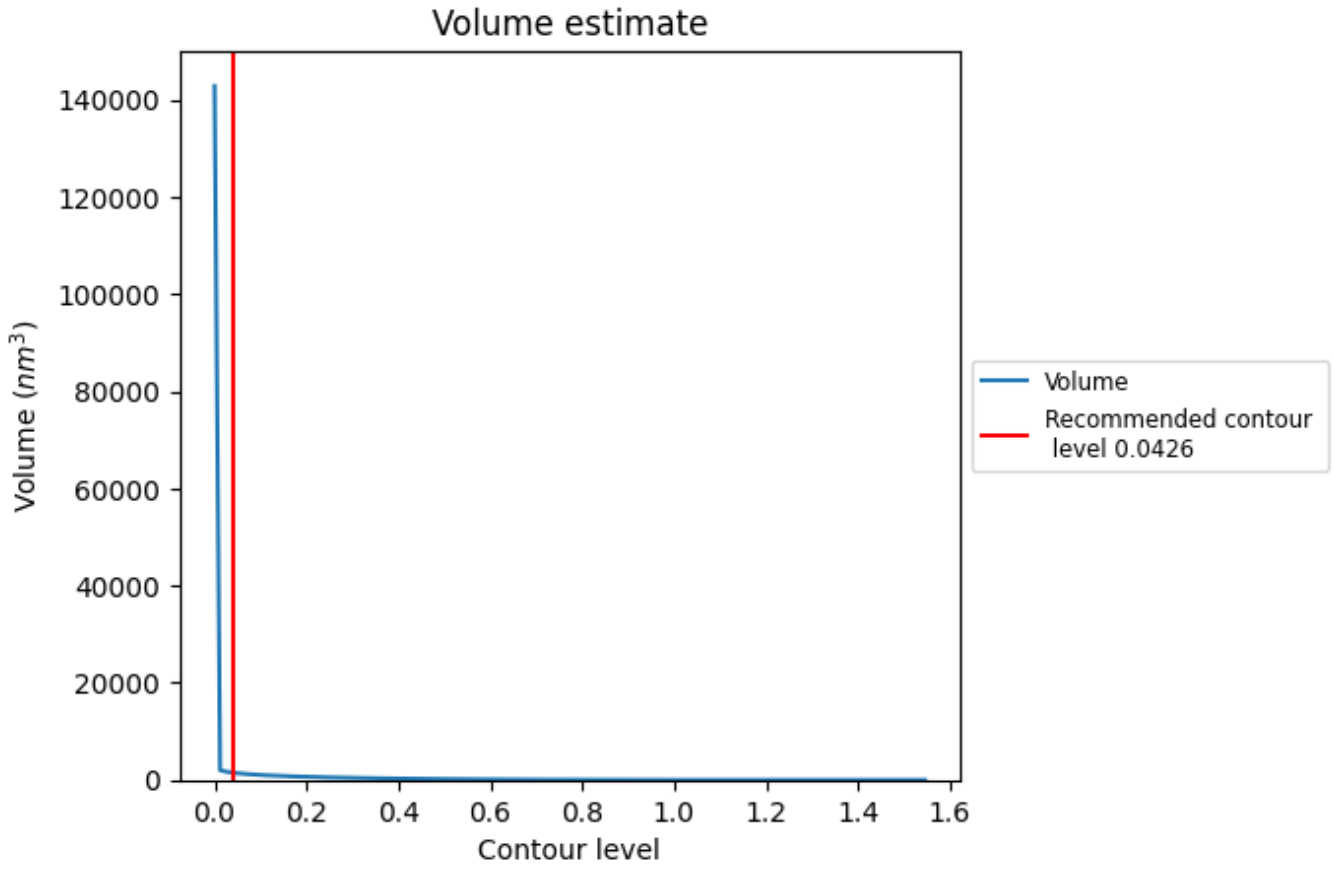
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

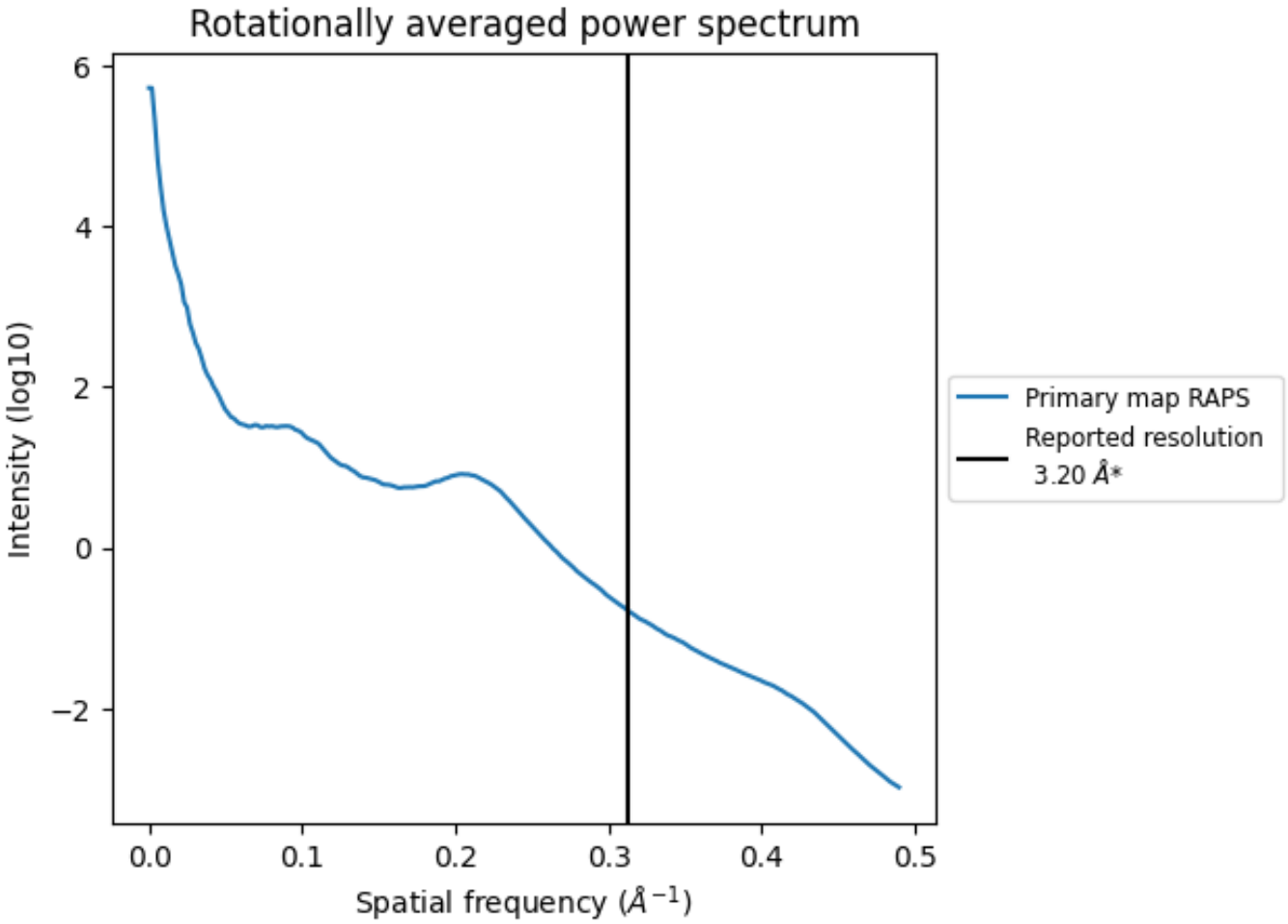
7.2 Volume estimate (i)



The volume at the recommended contour level is 1468 nm^3; this corresponds to an approximate mass of 1326 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)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

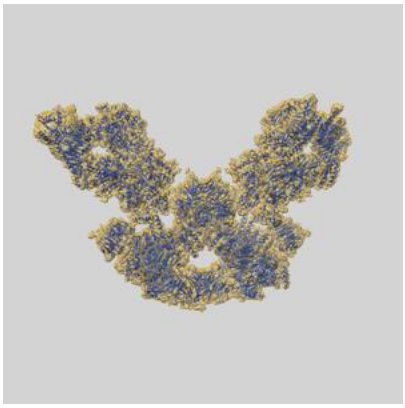
8 Fourier-Shell correlation (i)

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

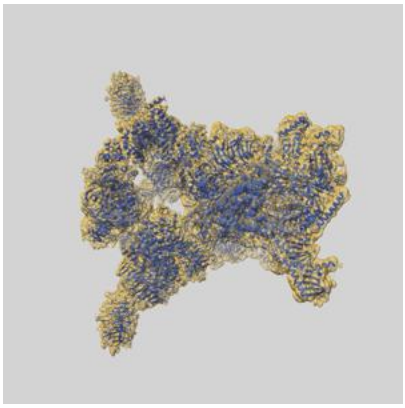
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-51887 and PDB model 9H5K. Per-residue inclusion information can be found in section 3 on page 10.

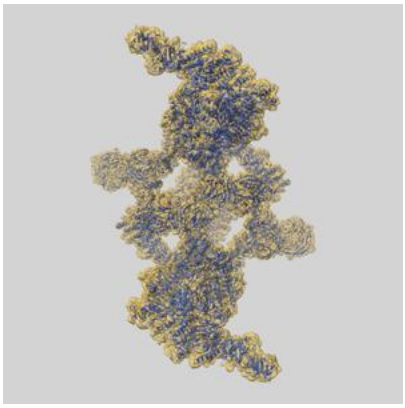
9.1 Map-model overlay



X



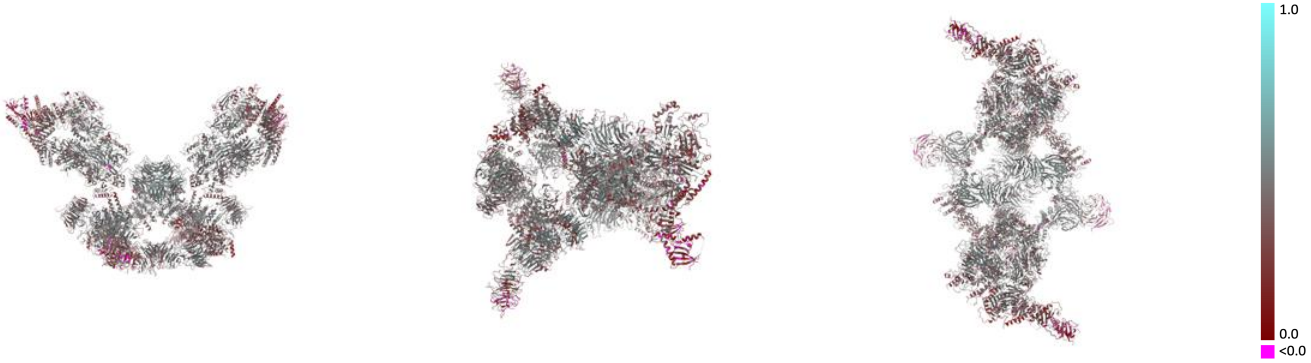
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0426 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.

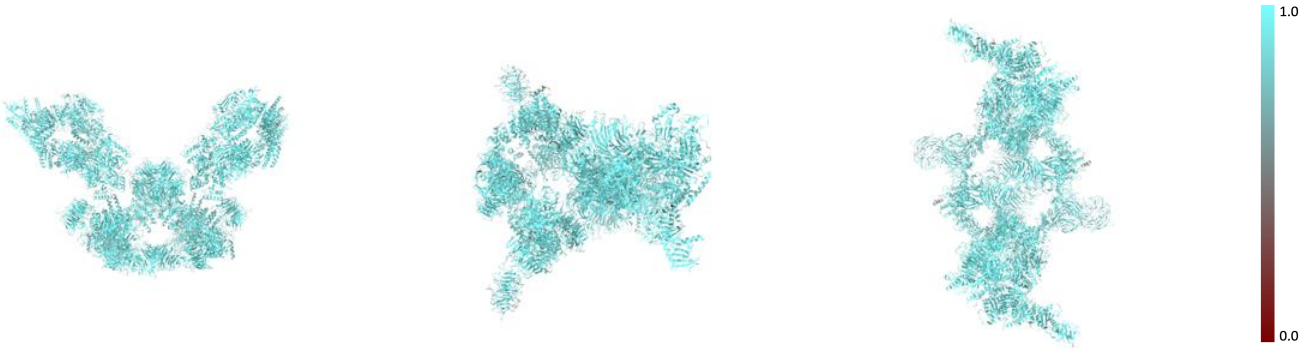
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

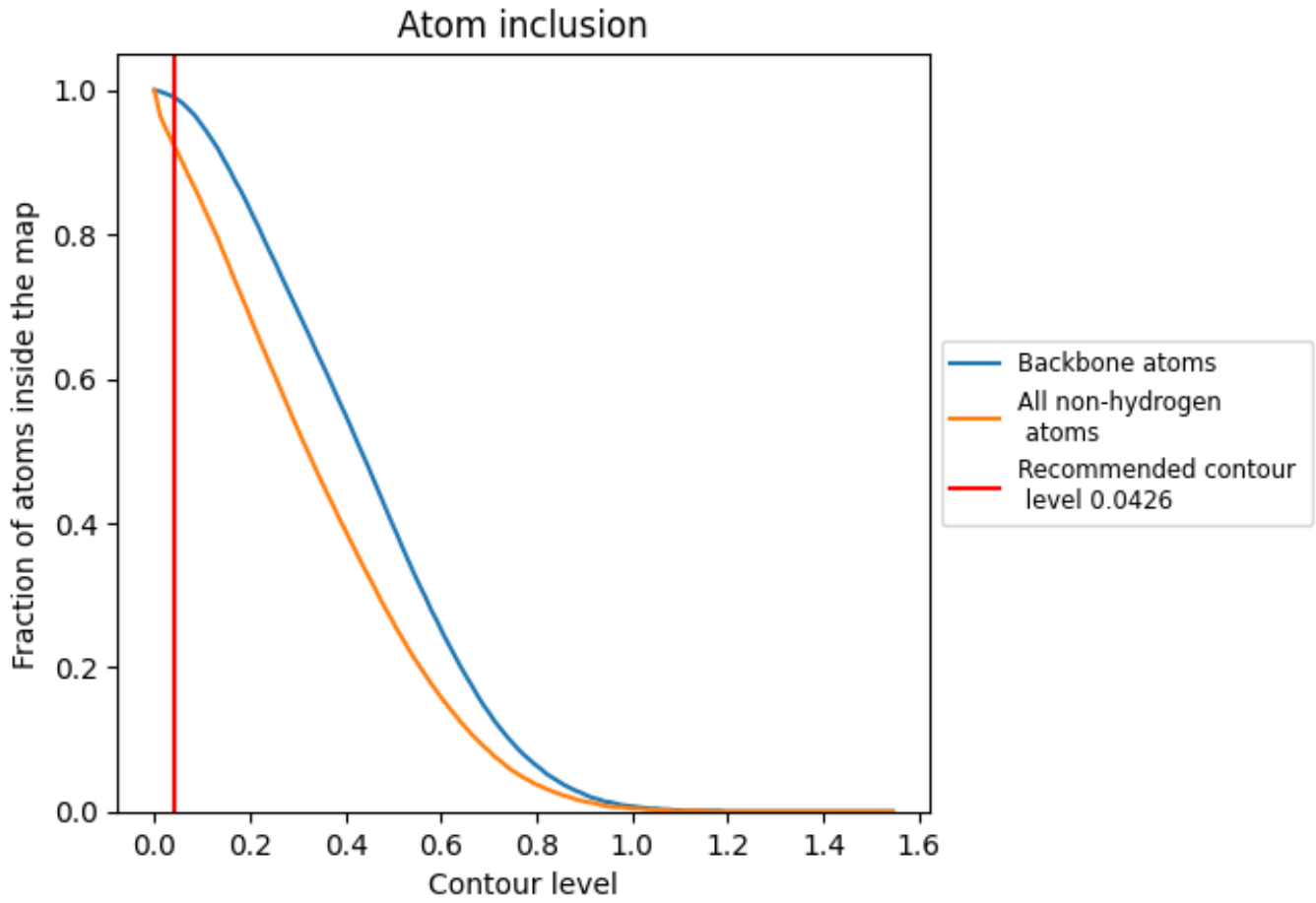
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0426).

9.4 Atom inclusion (i)



At the recommended contour level, 99% of all backbone atoms, 92% 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 (0.0426) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9210	0.4060
A	0.8540	0.3440
B	0.9270	0.4270
C	0.9360	0.4310
D	0.9170	0.4800
E	0.9090	0.4360
F	0.9140	0.4460
G	0.9260	0.3900
H	0.9080	0.4060
I	0.8510	0.3510
J	0.9260	0.4270
K	0.9370	0.4310
L	0.9150	0.4770
M	0.9100	0.4410
N	0.9090	0.4420
O	0.9220	0.3920
P	0.9040	0.4120
R	0.8920	0.2130
S	0.8970	0.2100
T	0.9700	0.4690
U	0.9020	0.1710
W	0.9040	0.1680
X	0.9360	0.4080
Y	0.8650	0.2350
Z	0.8650	0.2330
a	0.9390	0.4120
b	0.9390	0.4120
c	0.8950	0.3380
d	0.8970	0.3370
g	0.9700	0.4680
h	0.9460	0.4290
i	0.9470	0.4300
j	0.9370	0.4070

