wwPDB EM Validation Summary Report (i)

Aug 7, 2023 – 02:54 PM EDT

PDB ID	:	7LSY
EMDB ID	:	EMD-23509
Title	:	NHEJ Short-range synaptic complex
Authors	:	He, Y.; Chen, S.
Deposited on	:	2021-02-18
Resolution	:	8.40 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 (i) 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 (i)) were used in the production of this report:

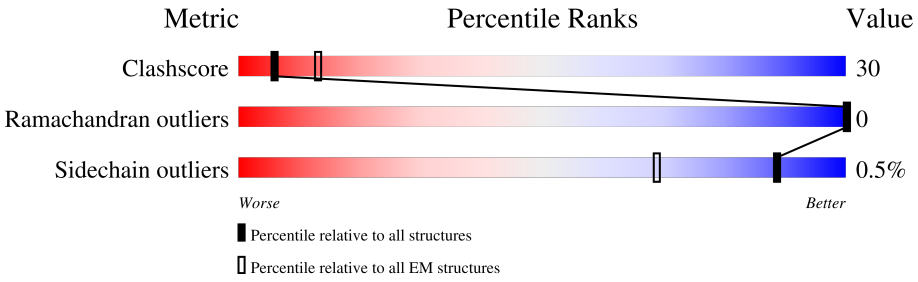
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 8.40 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	A	600	21% 44% 39% 17%
1	J	600	31% 46% 37% 17%
2	B	732	28% 42% 28% 30%
2	K	732	28% 42% 28% 30%
3	D	26	15% 73% 8% ·
4	E	14	93% 7%
5	F	336	7% 29% 31% 40%
5	G	336	10% 24% 32% · 42%

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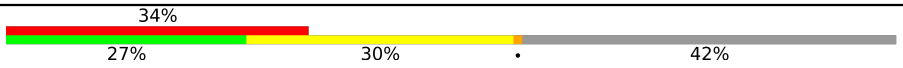
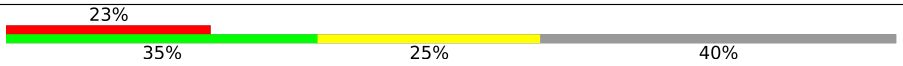
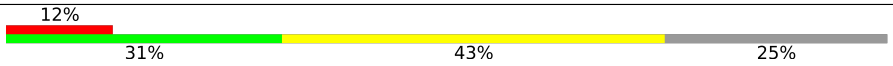
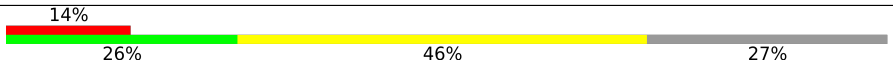
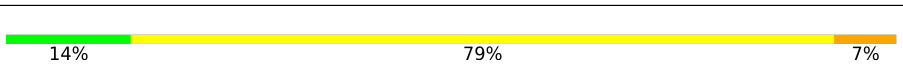
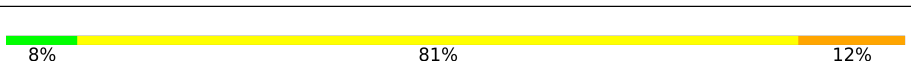
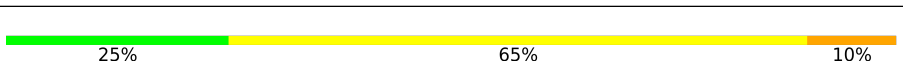
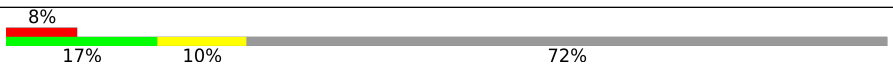
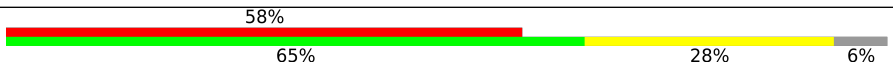
Mol	Chain	Length	Quality of chain
5	O	336	
5	P	336	
6	H	299	
6	I	299	
7	M	14	
8	N	26	
9	V	20	
10	X	911	
10	Y	911	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 37034 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 X-ray repair cross-complementing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	497	Total	C	N	O	S	0	0
			4021	2577	680	746	18		
1	J	497	Total	C	N	O	S	0	0
			4021	2577	680	746	18		

- Molecule 2 is a protein called X-ray repair cross-complementing protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	511	Total	C	N	O	S	0	0
			4099	2622	686	768	23		
2	K	511	Total	C	N	O	S	0	0
			4099	2622	686	768	23		

- Molecule 3 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	26	Total	C	N	O	P	0	0
			529	255	90	158	26		

- Molecule 4 is a DNA chain called DNA (5'-D(P*GP*TP*TP*CP*TP*TP*AP*GP*TP*AP *TP*AP*TP*A)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	14	Total	C	N	O	P	0	0
			287	139	47	87	14		

- Molecule 5 is a protein called DNA repair protein XRCC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		
5	G	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	195	Total	C	N	O	S	0	0
			1595	1012	272	304	7		
5	P	201	Total	C	N	O	S	0	0
			1628	1031	278	312	7		

- Molecule 6 is a protein called Non-homologous end-joining factor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	223	Total	C	N	O	S	0	0
			1779	1140	298	326	15		
6	I	218	Total	C	N	O	S	0	0
			1737	1111	290	321	15		

- Molecule 7 is a DNA chain called DNA (5'-D(P*TP*AP*TP*AP*TP*AP*CP*TP*AP*AP *GP*AP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	14	Total	C	N	O	P	0	0
			287	138	54	81	14		

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	26	Total	C	N	O	P	0	0
			530	257	82	165	26		

- Molecule 9 is a DNA chain called DNA (5'-D(P*CP*AP*AP*TP*GP*AP*AP*AP*CP*GP *GP*AP*AP*CP*AP*GP*TP*CP*AP*G)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
9	V	20	Total	C	N	O	P	0	0
			415	196	86	113	20		

- Molecule 10 is a protein called DNA ligase 4.

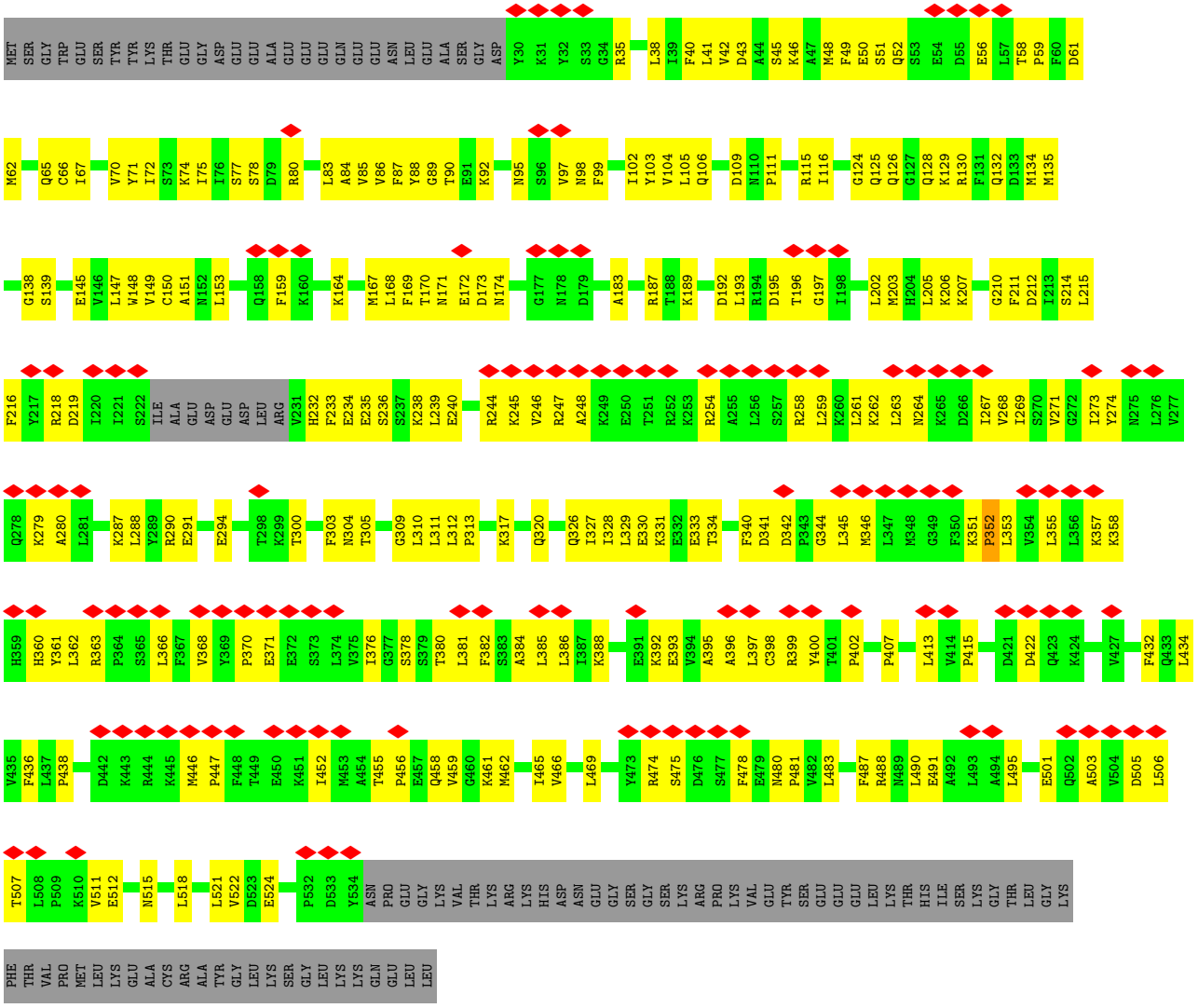
Mol	Chain	Residues	Atoms					AltConf	Trace
10	X	254	Total	C	N	O	S	0	0
			2064	1314	348	389	13		
10	Y	855	Total	C	N	O	S	2	0
			6720	4297	1139	1238	46		

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.

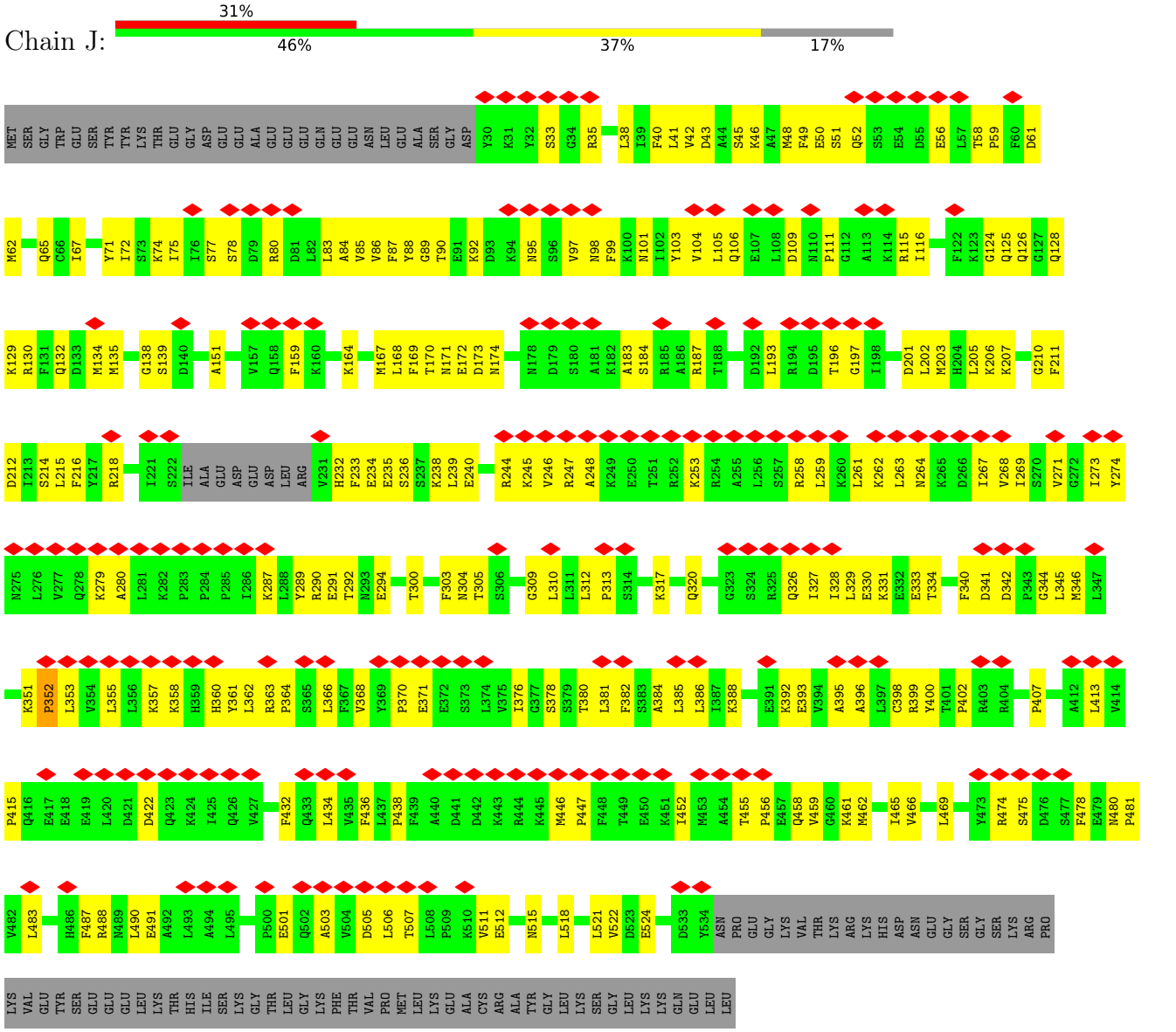
• Molecule 1: X-ray repair cross-complementing protein 6

Chain A:



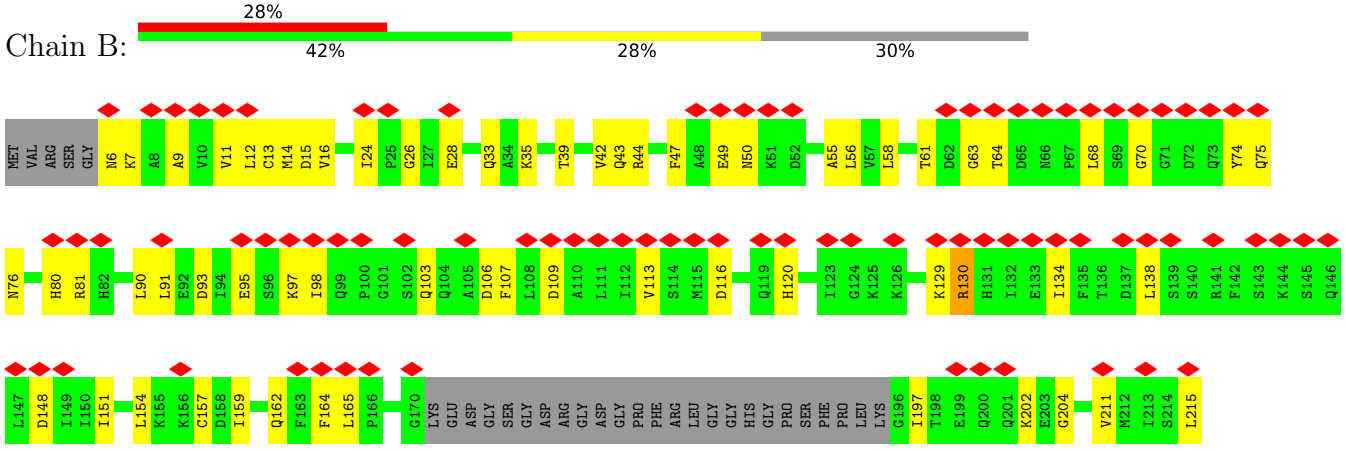
• Molecule 1: X-ray repair cross-complementing protein 6

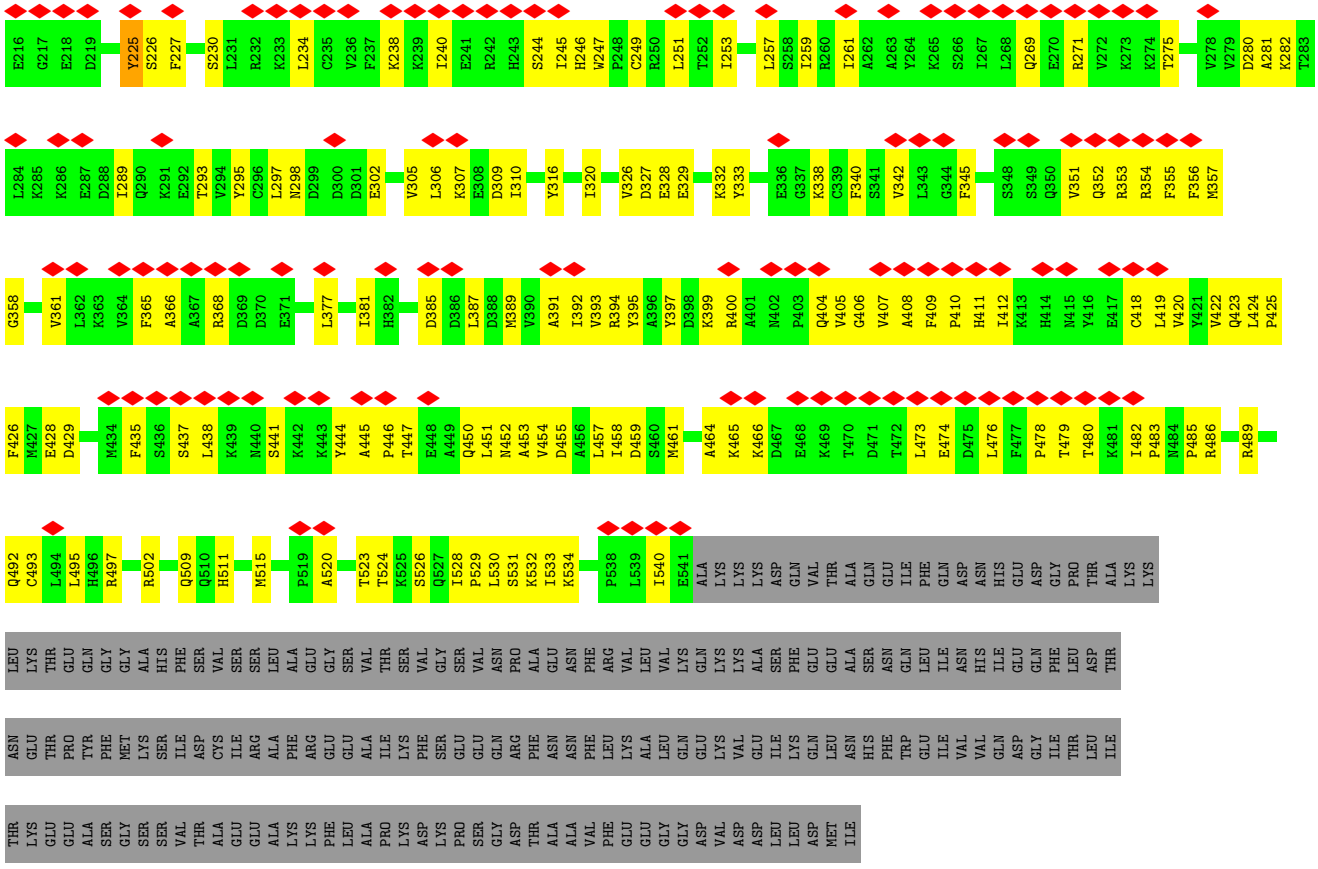
Chain J:



• Molecule 2: X-ray repair cross-complementing protein 5

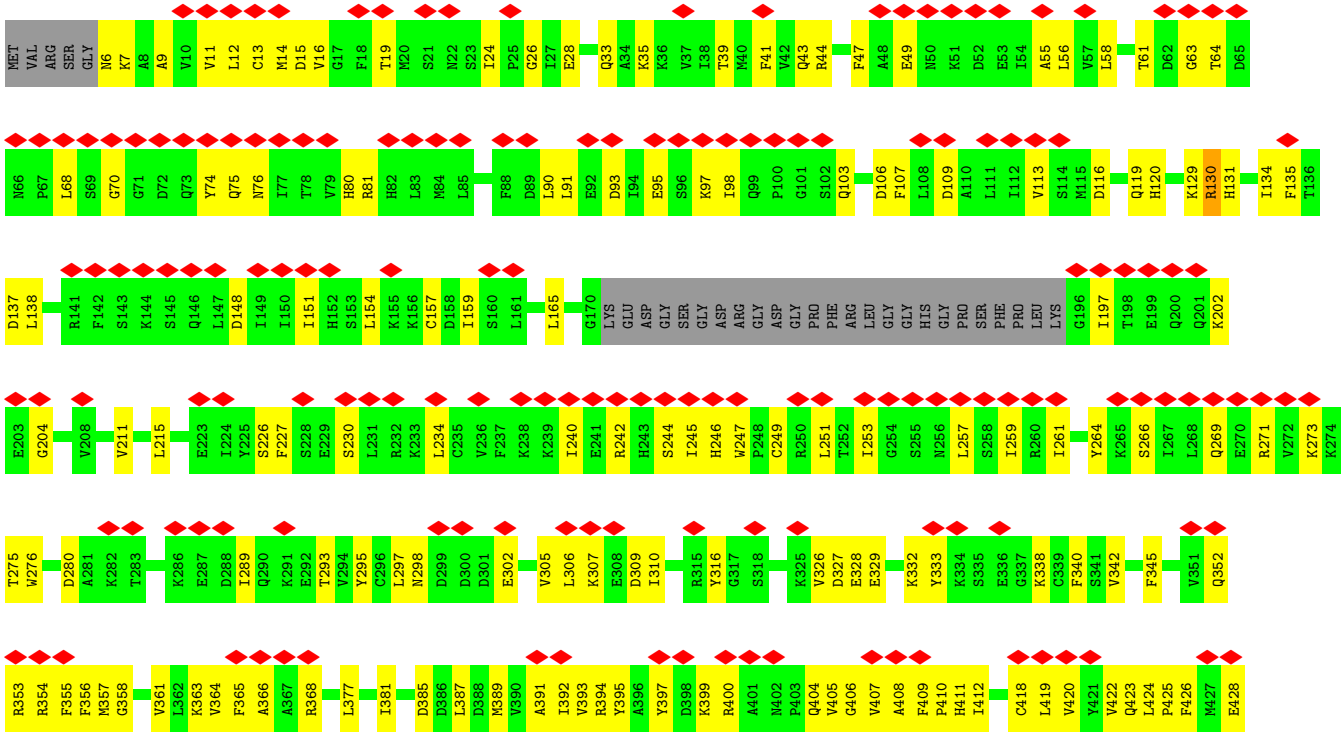
Chain B:

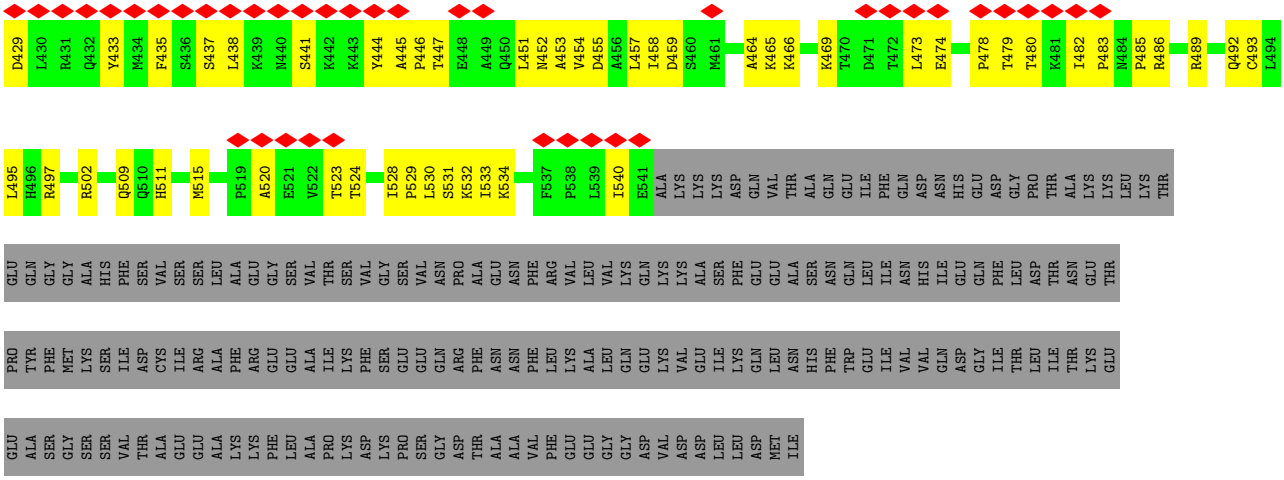




• Molecule 2: X-ray repair cross-complementing protein 5

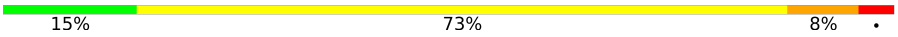
Chain K:

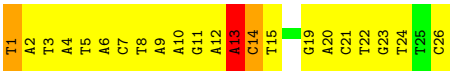




• Molecule 3: DNA (26-MER)

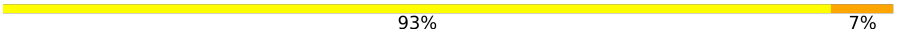
Chain D:

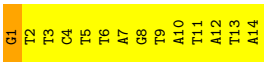




• Molecule 4: DNA (5'-D(P*GP*TP*TP*CP*TP*TP*AP*GP*TP*AP*TP*AP*TP*A)-3')

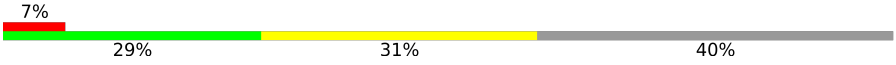
Chain E:

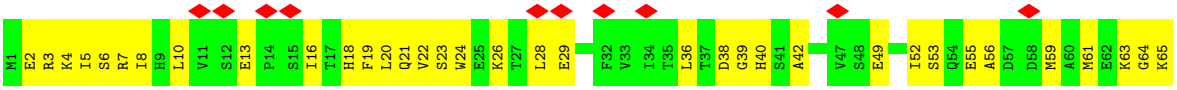


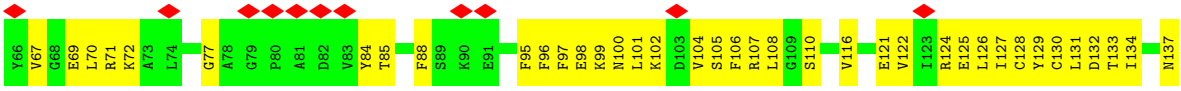


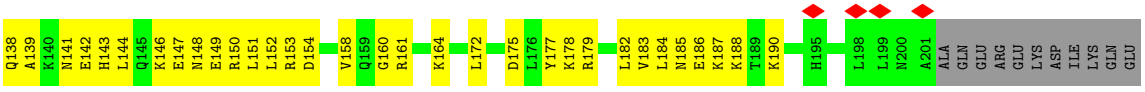
• Molecule 5: DNA repair protein XRCC4

Chain F:



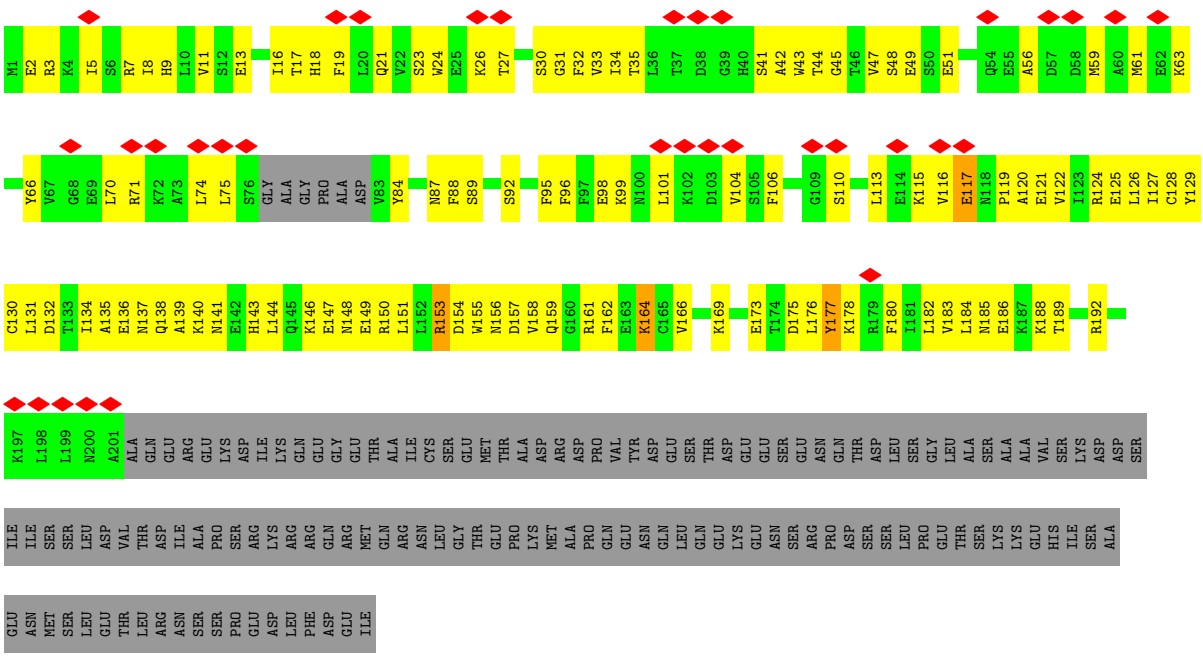






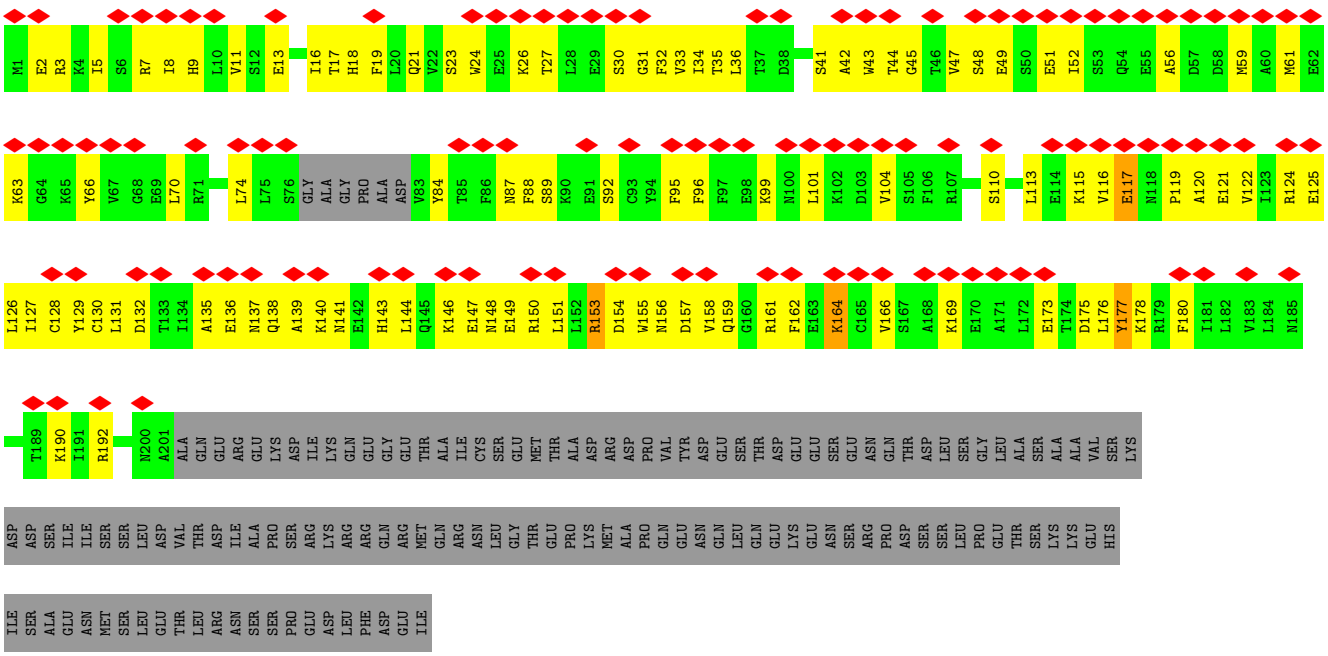
• Molecule 5: DNA repair protein XRCC4

Chain G:



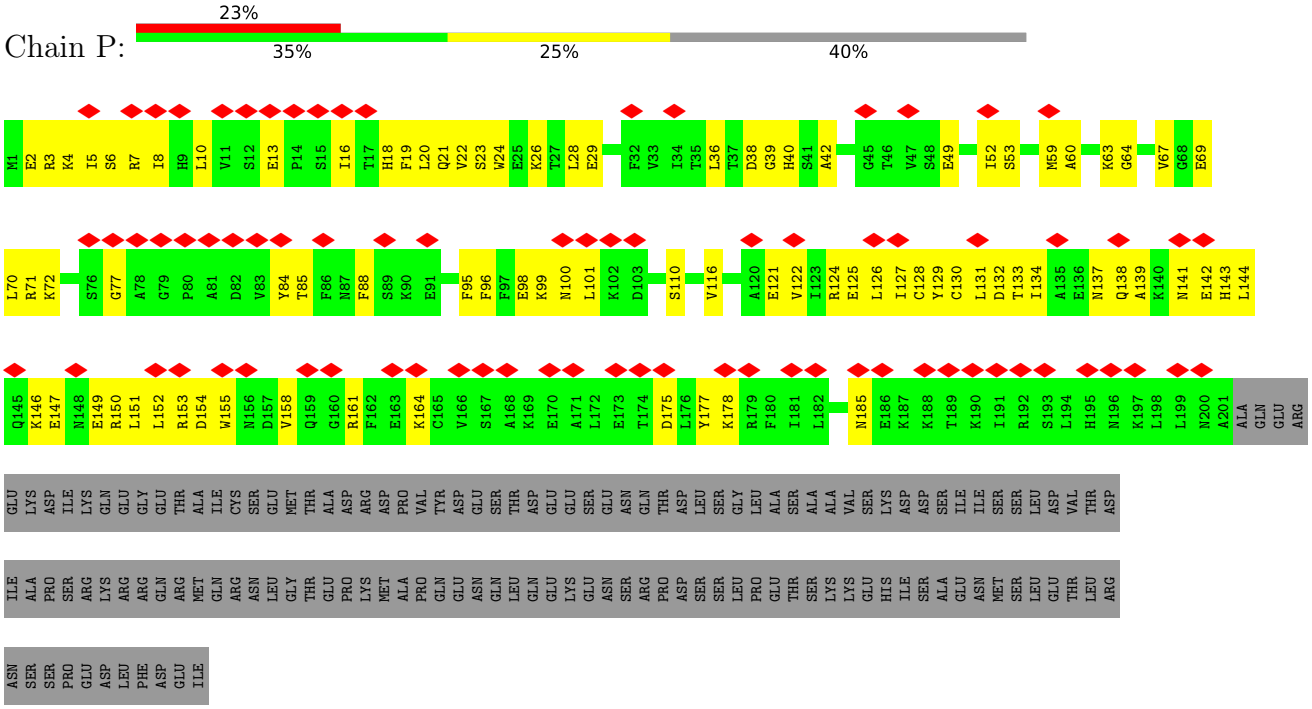
• Molecule 5: DNA repair protein XRCC4

Chain O:



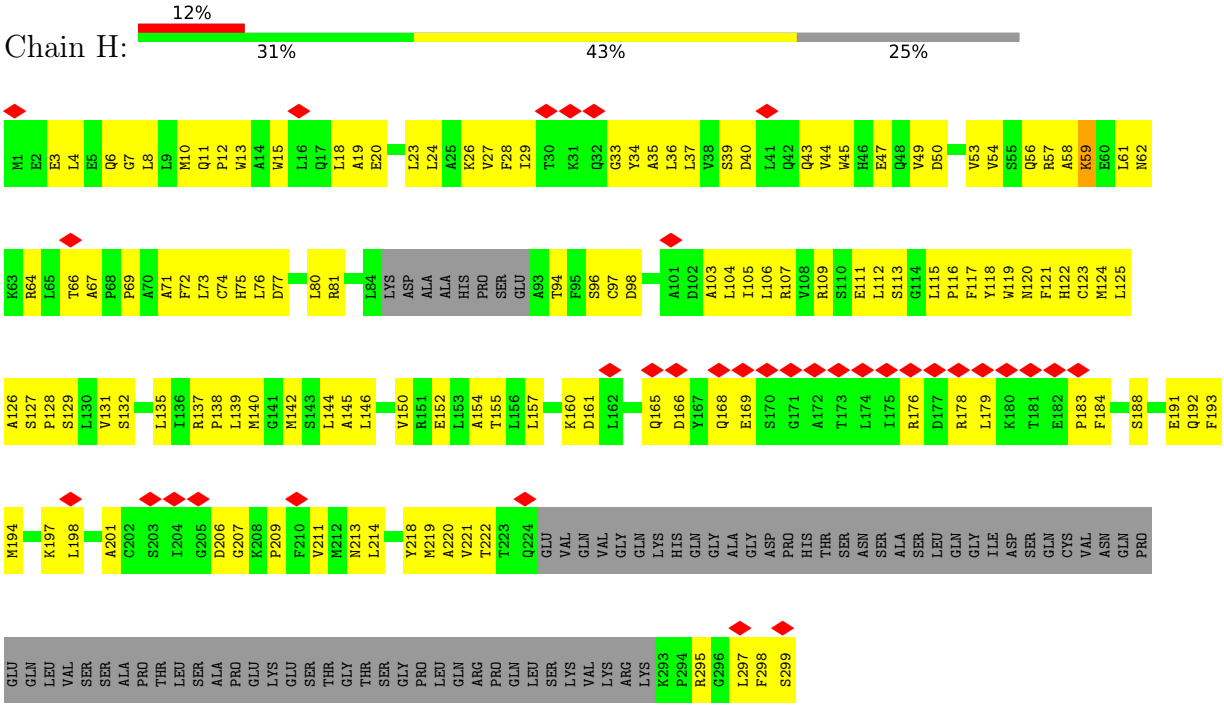
• Molecule 5: DNA repair protein XRCC4

Chain P:



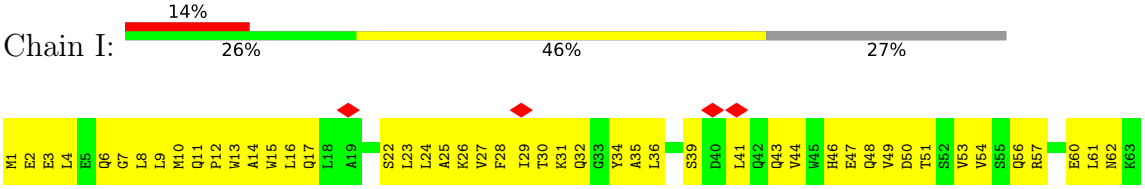
• Molecule 6: Non-homologous end-joining factor 1

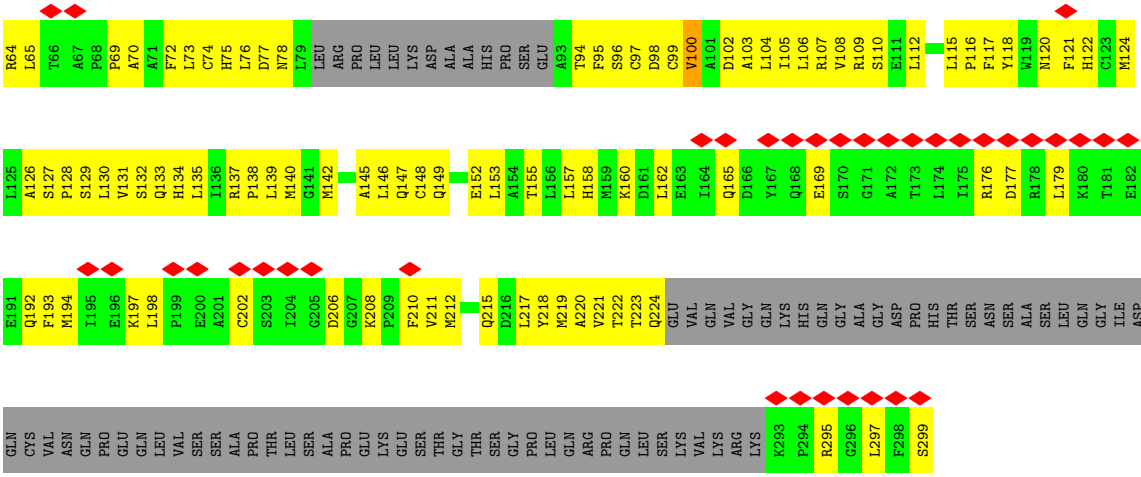
Chain H:



• Molecule 6: Non-homologous end-joining factor 1

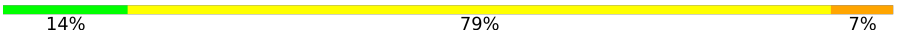
Chain I:

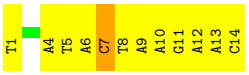




• Molecule 7: DNA (5'-D(P*TP*AP*TP*AP*TP*AP*CP*TP*AP*AP*GP*AP*AP*C)-3')

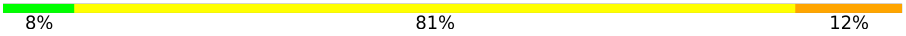
Chain M:

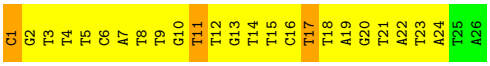




• Molecule 8: DNA (26-MER)

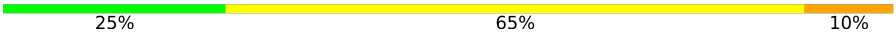
Chain N:

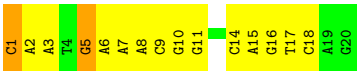




• Molecule 9: DNA (5'-D(P*CP*AP*AP*TP*GP*AP*AP*AP*CP*GP*GP*AP*AP*CP*AP*GP*TP*CP*AP*G)-3')

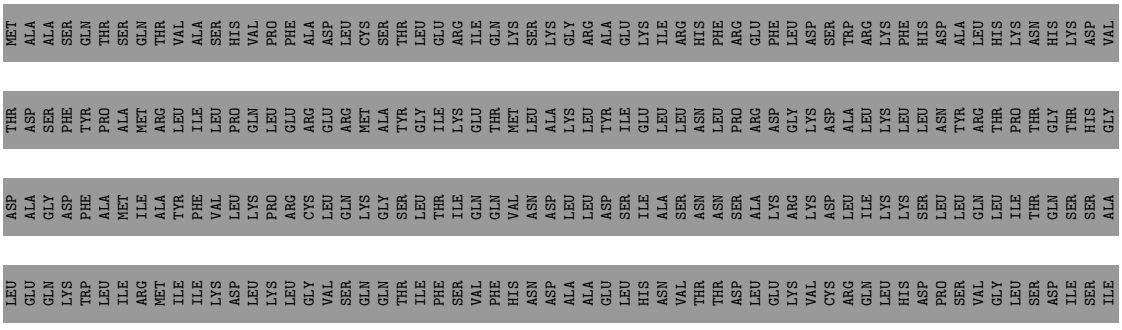
Chain V:

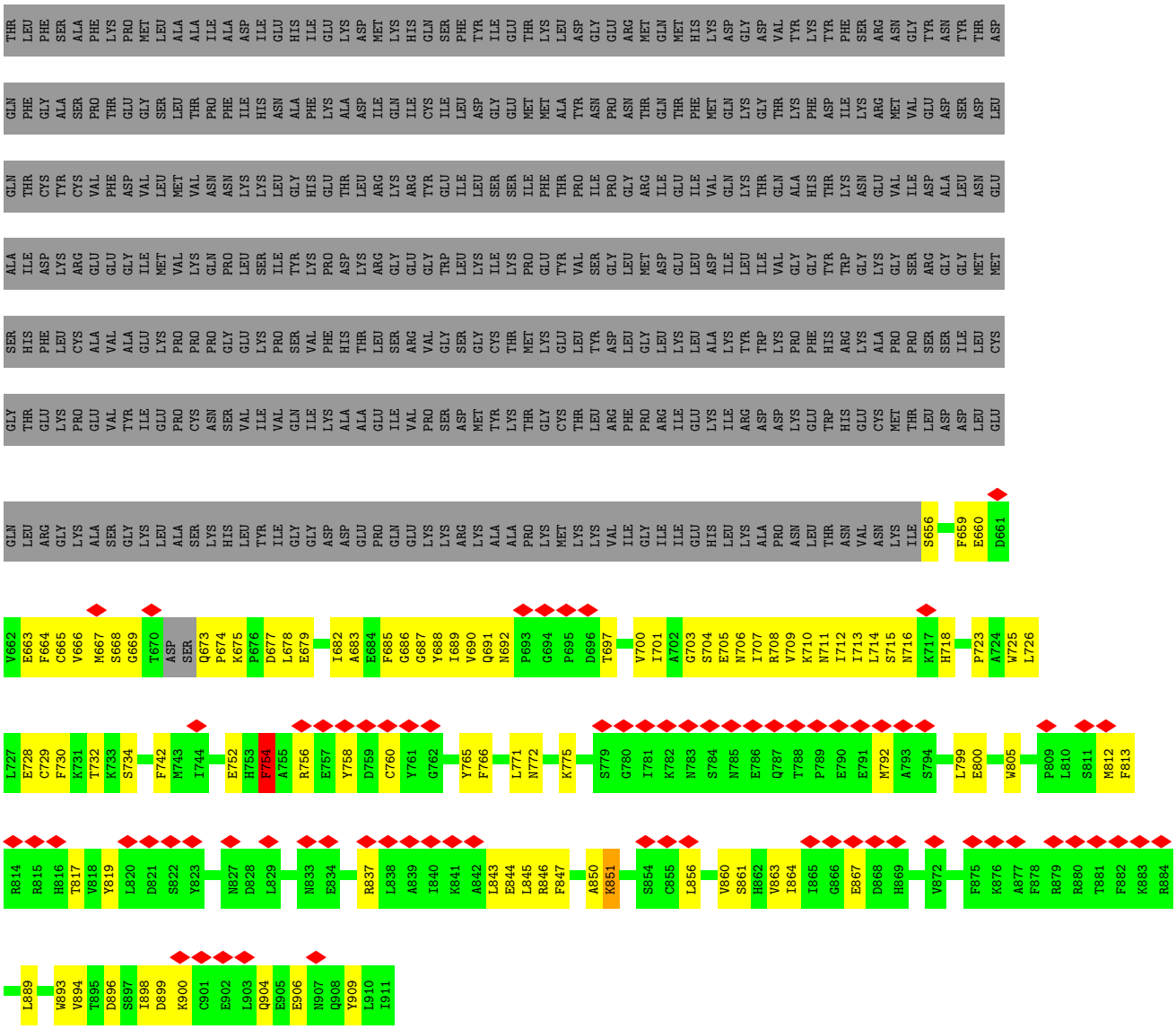




• Molecule 10: DNA ligase 4

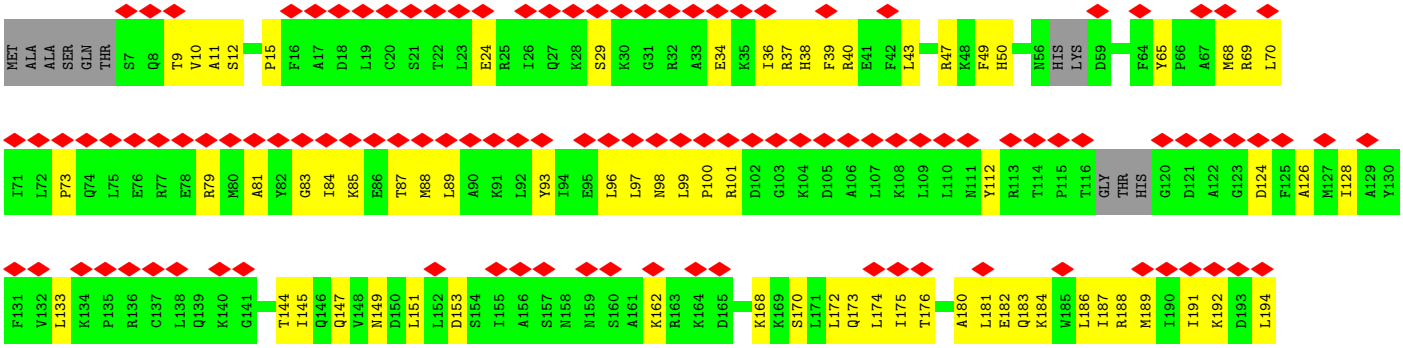
Chain X:

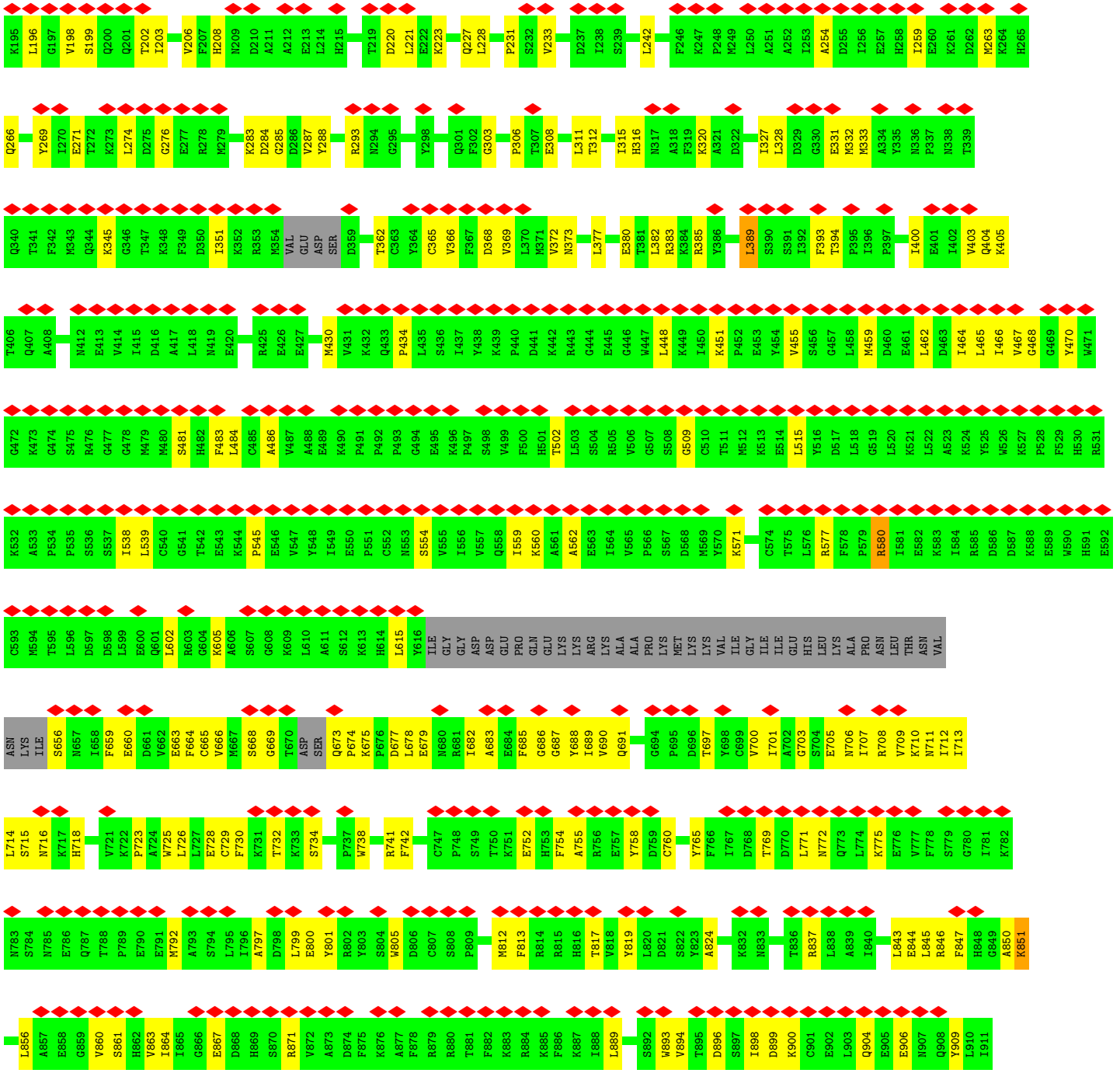




• Molecule 10: DNA ligase 4

Chain Y:




K195 L196 G197 V198 S199 Q200 Q201 T202 I203 V206 F207 H208 N209 D210 A211 A212 E213 L214 H215 T219 D220 L221 E222 K223 Q227 L228 P231 S232 V233 D237 I238 S239 L242 F246 K247 P248 M249 L250 A251 A252 I253 A254 D255 I256 E257 H258 I259 E260 K261 D262 M263 K264 H265
Q266 Y269 I270 E271 T272 K273 L274 D275 G276 E277 R278 M279 K283 D284 G285 D286 V287 Y288 R293 N294 G295 Y298 Q301 F302 G303 P306 T307 E308 L311 T312 I315 H316 N317 A318 F319 K320 A321 D322 I327 L328 D329 G330 E331 M332 M333 A334 Y335 N336 P337 N338 T339
Q340 T341 F342 M343 Q344 K345 G346 T347 K348 F349 D350 I351 K352 R353 M354 VAL GLU ASP SER D359 T362 G363 Y364 C365 V366 F367 D368 V369 L370 M371 V372 N373 L377 E380 T381 L382 R383 K384 R385 Y386 L389 S390 S391 I392 F393 T394 P395 I396 P397 I400 E401 I402 V403 Q404 K405
T406 Q407 A408 N412 E413 V414 I415 D416 A417 L418 N419 E420 R425 E426 E427 M430 V431 K432 Q433 P434 L435 S436 I437 Y438 K439 P440 D441 K442 R443 G444 E445 G446 W447 L448 K449 I450 K451 P452 E453 Y454 V455 S456 G457 L458 M459 D460 E461 L462 D463 I464 L465 I466 V467 G468 G469 Y470 W471
G472 K473 G474 S475 R476 G477 G478 M479 M480 S481 H482 F483 L484 C485 A486 V487 A488 E489 K490 P491 P492 P493 G494 E495 K496 P497 S498 V499 F500 H501 T502 L503 S504 R505 V506 G507 S508 G509 C510 T511 M512 K513 E514 L515 Y516 D517 L518 G519 L520 K521 L522 A523 K524 Y525 W526 K527 P528 F529 H530 R531
K532 A533 P534 P535 S536 S537 I538 L539 C540 G541 T542 E543 K544 P545 E546 V547 Y548 I549 E550 P551 C552 N553 S554 V555 I556 V557 Q558 I559 K560 A561 A562 E563 I564 V565 P566 S567 D568 N569 Y570 K571 C574 T575 L576 R577 F578 P579 R580 I581 E582 K583 I584 R585 D586 D587 K588 E589 W590 H591 E592
C593 M594 T595 L596 D597 D598 L599 E600 Q601 L602 R603 G604 K605 A606 S607 G608 K609 L610 A611 S612 K613 H614 L615 Y616 ILE GLY GLY ASP ASP GLU PRO GLN GLU LYS LYS ARG LYS ALA ALA PRO LYS MET LYS LYS VAL ILE GLY ILE ILE GLU HIS LEU LYS ALA PRO ASN LEU THR ASN VAL
ASN LYS ILE S656 N657 I658 F659 E660 D661 V662 E663 F664 C665 V666 M667 S668 G669 T670 ASP SER Q673 P674 K675 P676 D677 L678 E679 N680 R681 I682 A683 E684 F685 G686 G687 Y688 I689 V690 Q691 G694 P695 D696 T697 Y698 C699 V700 I701 A702 G703 S704 E705 N706 I707 R708 V709 K710 N711 I712 I713
L714 S715 N716 K717 H718 V721 K722 P723 A724 W725 L726 L727 E728 C729 F730 K731 T732 K733 S734 P737 W738 R741 F742 C747 P748 S749 T750 K751 E752 H753 F754 A755 R756 E757 Y758 D759 C760 Y765 F766 I767 D768 T769 D770 L771 N772 Q773 L774 K775 E776 V777 F778 S779 G780 I781 K782
N783 S784 N785 E786 Q787 T788 P789 E790 E791 M792 A793 S794 L795 I796 A797 D798 L799 E800 Y801 R802 Y803 S804 W805 D806 C807 S808 P809 M812 F813 R814 R815 H816 T817 V818 Y819 L820 D821 S822 Y823 A824 K832 N833 T836 R837 L838 A839 I840 L843 E844 L845 R846 F847 H848 G849 A850 K851
L856 A857 E858 G859 V860 S861 H862 V863 I864 I865 G866 E867 D868 H869 S870 R871 V872 A873 D874 F875 K876 A877 F878 R879 R880 T881 F882 K883 R884 K885 F886 K887 I888 L889 S892 W893 V894 T895 D896 S897 I898 D899 K900 C901 E902 L903 Q904 E905 E906 N907 Q908 Y909 L910 I911

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175866	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 ($e^-/Å^2$)	46	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	30000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	318.72, 318.72, 318.72	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.66, 1.66, 1.66	Depositor

5 Model quality

5.1 Standard geometry

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	0.38	0/4101	0.66	5/5523 (0.1%)
1	J	0.36	0/4101	0.64	4/5523 (0.1%)
2	B	0.32	0/4180	0.53	0/5640
2	K	0.31	0/4180	0.51	0/5640
3	D	1.38	3/591 (0.5%)	1.42	13/909 (1.4%)
4	E	1.59	0/320	1.31	1/492 (0.2%)
5	F	0.40	0/1657	0.58	0/2228
5	G	0.39	0/1622	0.59	1/2178 (0.0%)
5	O	0.42	0/1622	0.64	1/2178 (0.0%)
5	P	0.45	0/1657	0.66	0/2228
6	H	0.40	0/1814	0.57	0/2454
6	I	0.46	0/1771	0.63	1/2395 (0.0%)
7	M	1.46	1/322 (0.3%)	1.21	1/494 (0.2%)
8	N	1.18	0/590	1.22	3/909 (0.3%)
9	V	1.07	0/468	1.04	2/720 (0.3%)
10	X	0.45	0/2112	0.74	3/2851 (0.1%)
10	Y	0.35	0/6863	0.59	2/9271 (0.0%)
All	All	0.49	4/37971 (0.0%)	0.67	37/51633 (0.1%)

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	B	0	1
3	D	0	1
5	G	0	2
5	O	0	2
6	I	0	1
10	X	0	1
10	Y	0	1
All	All	0	9

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	13	DA	C5-C4	-6.02	1.34	1.38
3	D	13	DA	N9-C4	-5.89	1.34	1.37
3	D	13	DA	C6-N6	-5.16	1.29	1.33
7	M	7	DC	C1'-N1	-5.04	1.40	1.47

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	134	ILE	CA-CB-CG1	9.65	129.33	111.00
3	D	3	DT	O4'-C1'-N1	-9.38	101.44	108.00
1	A	352	PRO	CA-N-CD	-9.23	98.57	111.50
1	J	352	PRO	CA-N-CD	-9.14	98.70	111.50
3	D	13	DA	C4-C5-C6	-8.56	112.72	117.00

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	225	TYR	Sidechain
3	D	13	DA	Sidechain
5	G	117	GLU	Peptide
5	G	177	TYR	Peptide
6	I	100	VAL	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4021	0	4100	229	0
1	J	4021	0	4100	217	0
2	B	4099	0	4139	183	0
2	K	4099	0	4139	200	0
3	D	529	0	297	90	0
4	E	287	0	162	73	0
5	F	1628	0	1620	169	0
5	G	1595	0	1592	140	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	O	1595	0	1592	136	0
5	P	1628	0	1620	117	0
6	H	1779	0	1797	208	0
6	I	1737	0	1744	216	0
7	M	287	0	159	59	0
8	N	530	0	301	79	0
9	V	415	0	223	46	0
10	X	2064	0	2012	117	0
10	Y	6720	0	6571	263	0
All	All	37034	0	36168	2138	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 30.

The worst 5 of 2138 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)
6:H:220:ALA:HB1	6:I:194:MET:HE1	1.16	1.15
6:I:116:PRO:HG2	5:P:60:ALA:O	1.55	1.02
2:K:245:ILE:HD11	7:M:6:DA:O3'	1.58	1.02
5:F:102:LYS:HE2	6:H:71:ALA:O	1.59	1.01
6:H:297:LEU:HD12	2:K:41:PHE:CE1	1.95	1.01

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	493/600 (82%)	457 (93%)	36 (7%)	0	100	100
1	J	493/600 (82%)	455 (92%)	38 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	507/732 (69%)	456 (90%)	51 (10%)	0	100	100
2	K	507/732 (69%)	456 (90%)	51 (10%)	0	100	100
5	F	199/336 (59%)	196 (98%)	3 (2%)	0	100	100
5	G	191/336 (57%)	181 (95%)	10 (5%)	0	100	100
5	O	191/336 (57%)	182 (95%)	9 (5%)	0	100	100
5	P	199/336 (59%)	195 (98%)	4 (2%)	0	100	100
6	H	217/299 (73%)	204 (94%)	13 (6%)	0	100	100
6	I	212/299 (71%)	195 (92%)	17 (8%)	0	100	100
10	X	250/911 (27%)	220 (88%)	30 (12%)	0	100	100
10	Y	844/911 (93%)	794 (94%)	50 (6%)	0	100	100
All	All	4303/6428 (67%)	3991 (93%)	312 (7%)	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	A	452/540 (84%)	452 (100%)	0	100	100
1	J	452/540 (84%)	452 (100%)	0	100	100
2	B	463/649 (71%)	461 (100%)	2 (0%)	91	94
2	K	463/649 (71%)	461 (100%)	2 (0%)	91	94
5	F	180/303 (59%)	180 (100%)	0	100	100
5	G	178/303 (59%)	175 (98%)	3 (2%)	60	78
5	O	178/303 (59%)	175 (98%)	3 (2%)	60	78
5	P	180/303 (59%)	180 (100%)	0	100	100
6	H	198/262 (76%)	197 (100%)	1 (0%)	88	93
6	I	193/262 (74%)	193 (100%)	0	100	100
10	X	230/808 (28%)	227 (99%)	3 (1%)	69	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	Y	710/808 (88%)	706 (99%)	4 (1%)	86 92
All	All	3877/5730 (68%)	3859 (100%)	18 (0%)	89 93

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	Y	580	ARG
10	Y	851	LYS
10	Y	754	PHE
5	O	153	ARG
10	X	851	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 26 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	326	GLN
2	K	119	GLN
10	Y	266	GLN
2	K	103	GLN
5	O	21	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.

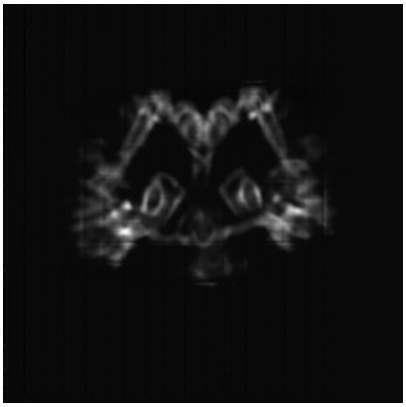
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23509. These allow visual inspection of the internal detail of the map and identification of artifacts.

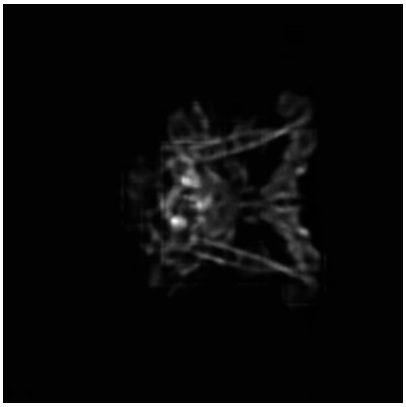
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

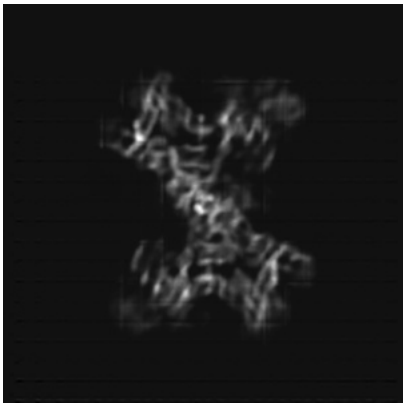
6.1.1 Primary map



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: 96

Y Index: 96

Z Index: 96

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: 87

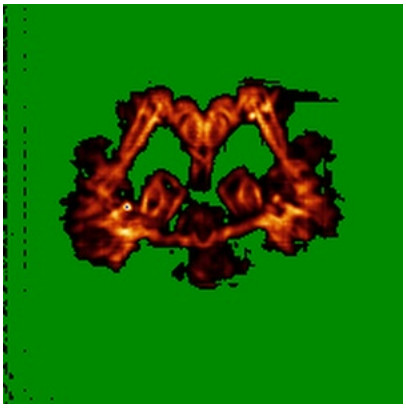
Y Index: 59

Z Index: 82

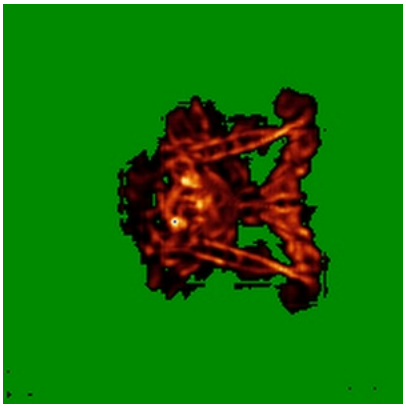
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



X



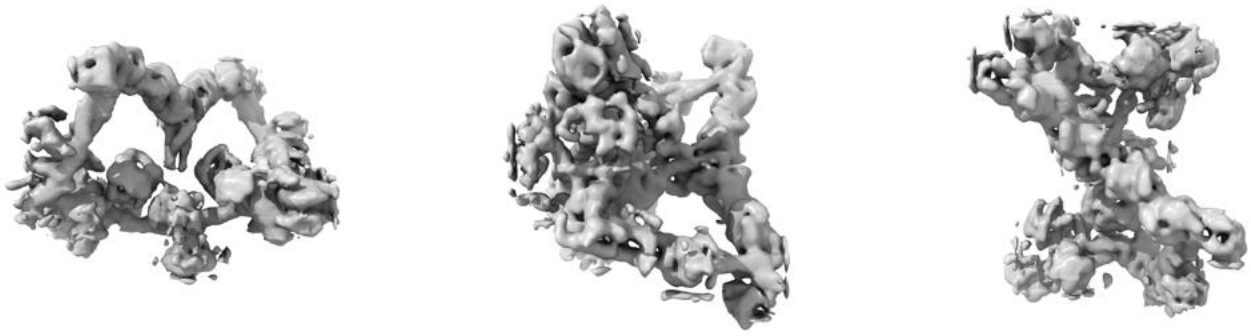
Y

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

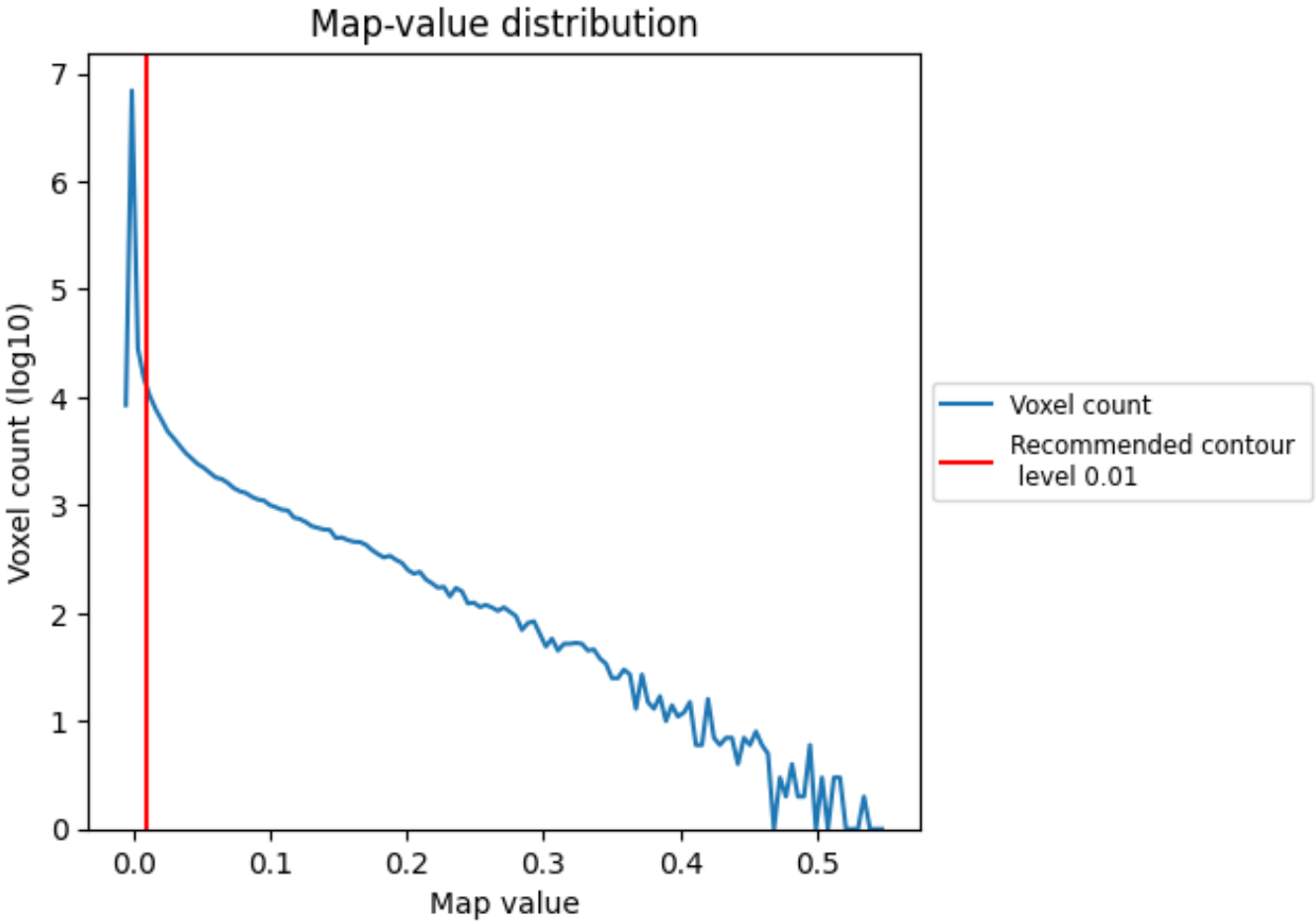
6.6 Mask visualisation (i)

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

7 Map analysis

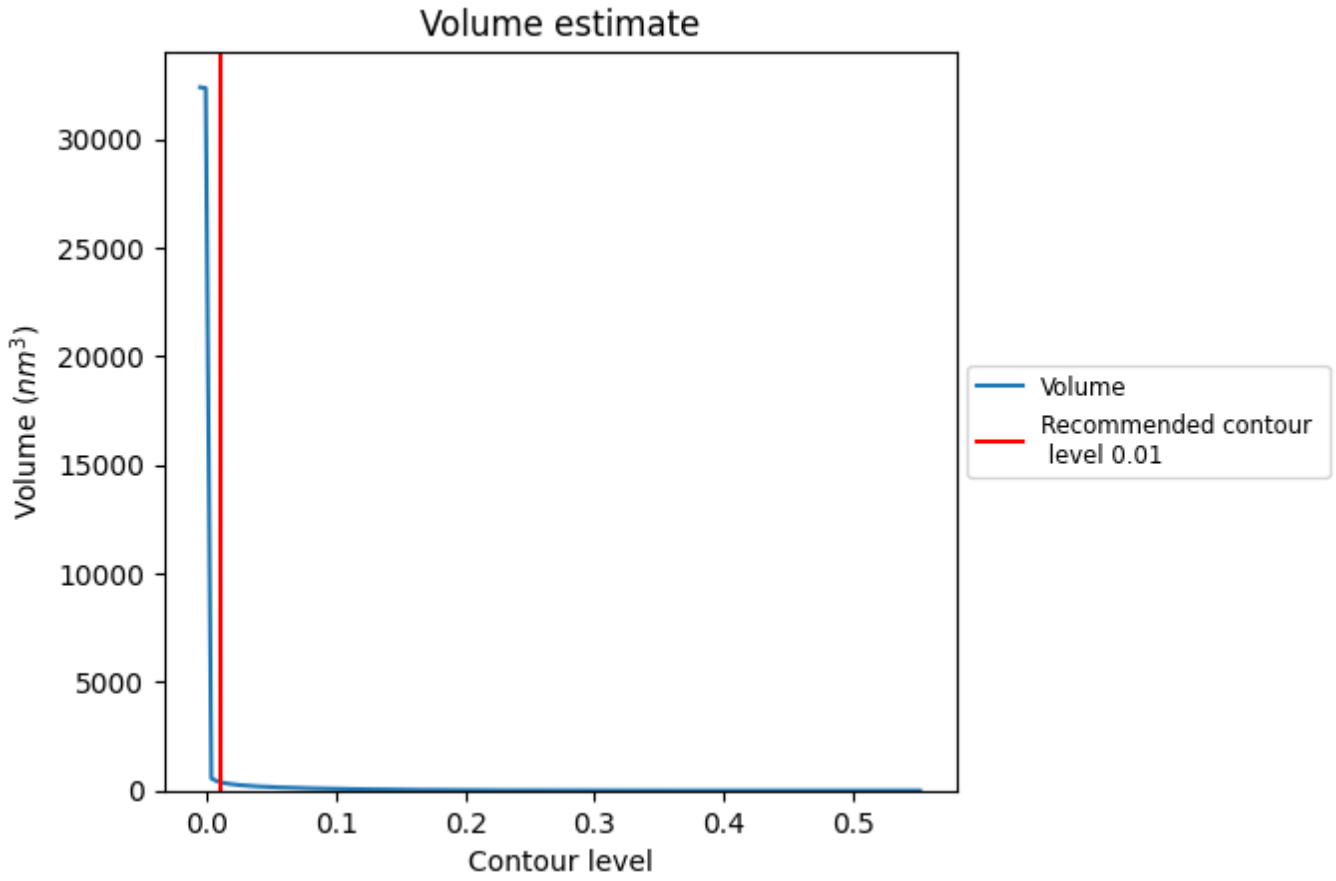
This section contains the results of statistical analysis of the map.

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.

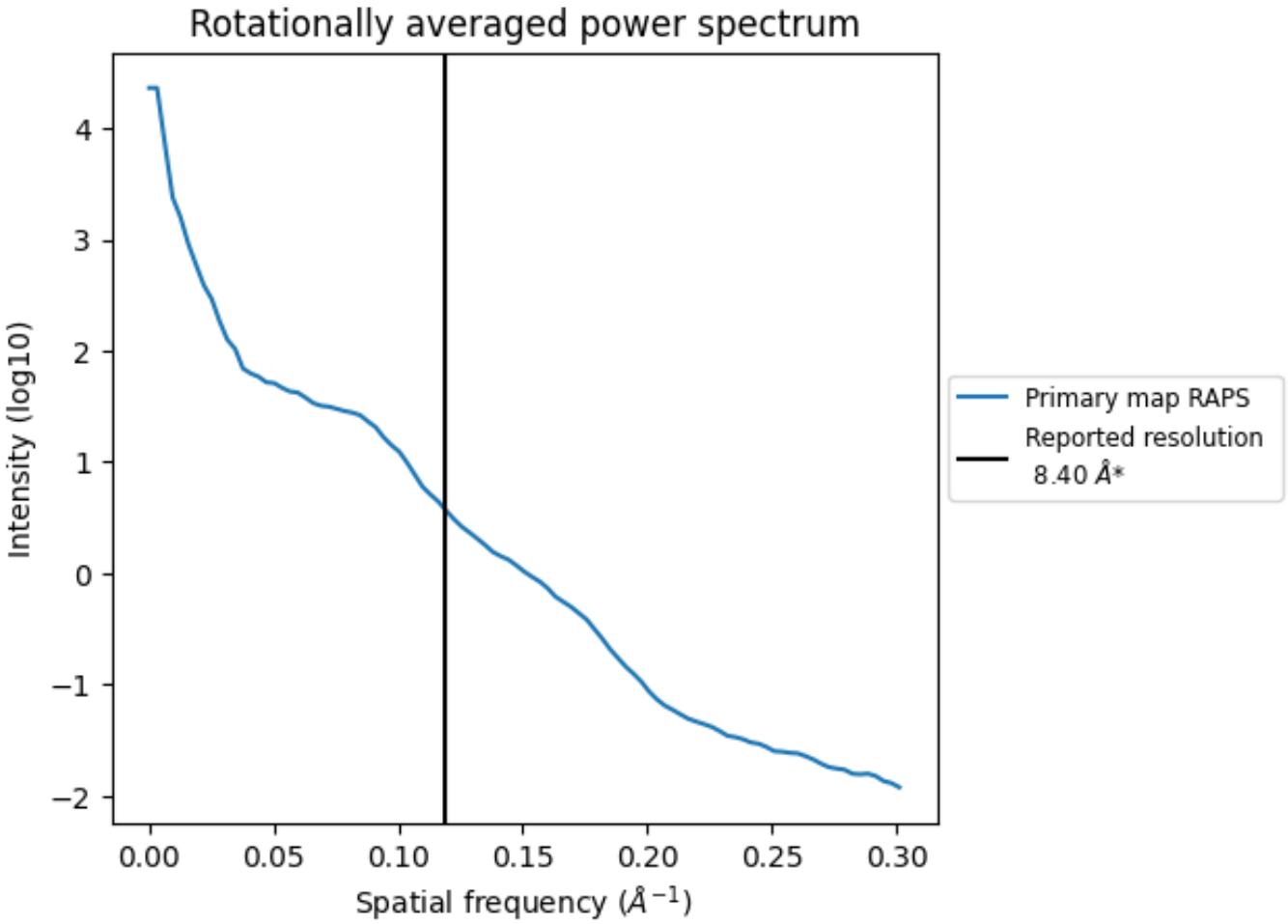
7.2 Volume estimate (i)



The volume at the recommended contour level is 395 nm^3; this corresponds to an approximate mass of 357 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 0.119 Å^{-1}

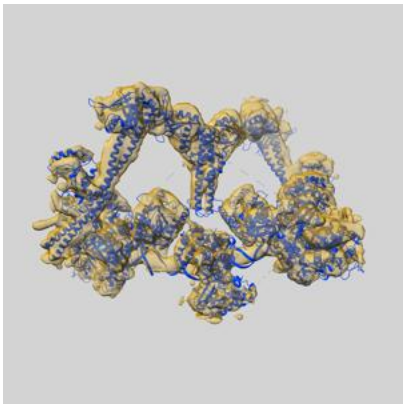
8 Fourier-Shell correlation

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

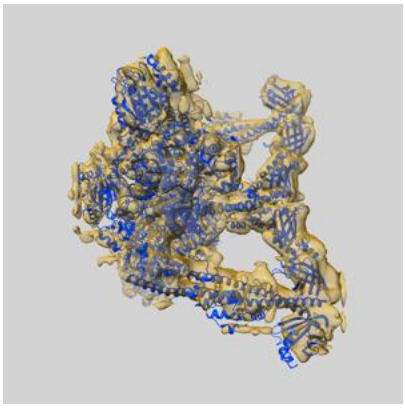
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23509 and PDB model 7LSY. Per-residue inclusion information can be found in section 3 on page 6.

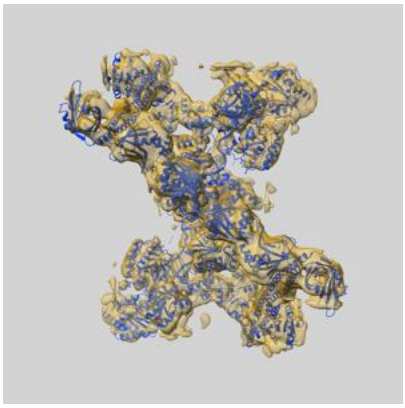
9.1 Map-model overlay



X



Y



Z

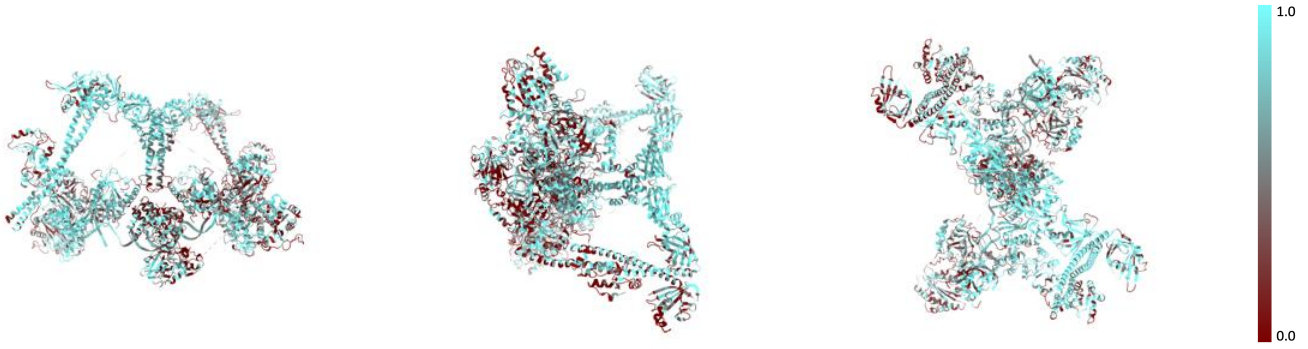
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

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.

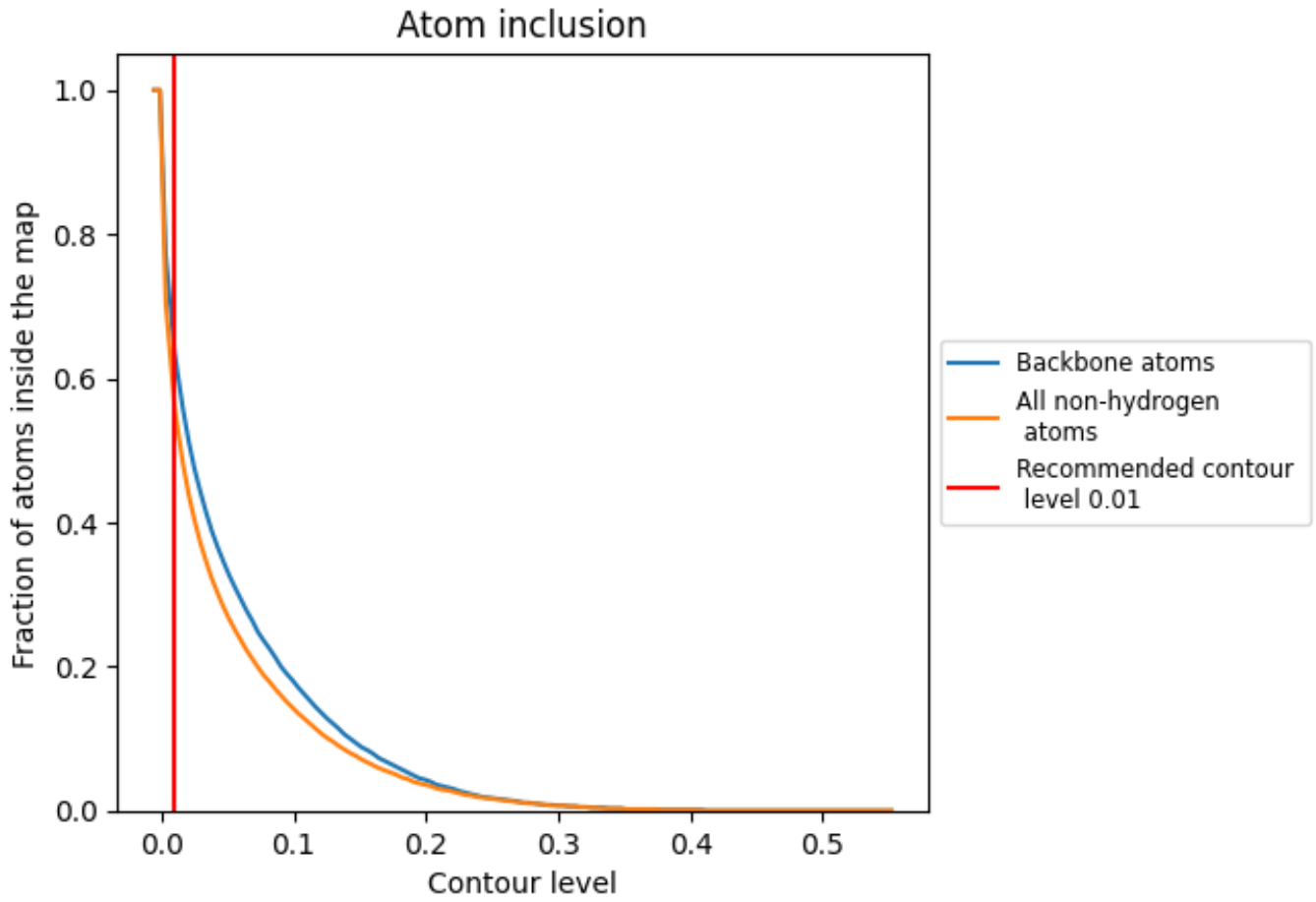
9.3 Atom inclusion mapped to coordinate model



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 64% of all backbone atoms, 56% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5610	0.0150
A	0.6100	0.0210
B	0.5180	0.0080
D	0.8150	0.1600
E	0.8950	0.1760
F	0.8020	0.0770
G	0.7490	0.0530
H	0.7460	0.0680
I	0.7340	0.0740
J	0.5260	0.0040
K	0.5130	-0.0040
M	0.7110	0.0860
N	0.7910	0.1000
O	0.3840	-0.0600
P	0.5570	-0.0500
V	0.7280	0.1000
X	0.6440	0.0350
Y	0.3570	-0.0240