



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 02:54 PM EST

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 ⓘ 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.dev43
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) : 2.31.2

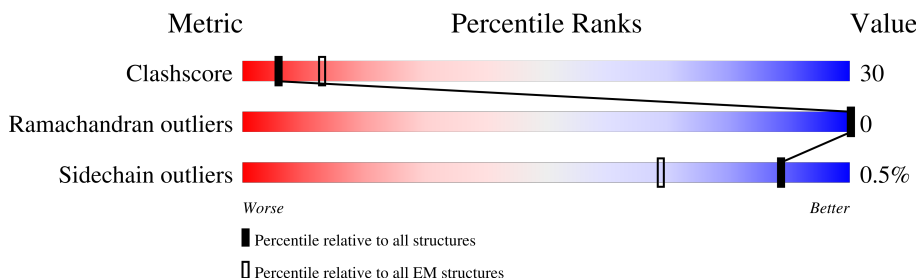
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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 $\leq 5\%$. 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	600	
1	J	600	
2	B	732	
2	K	732	
3	D	26	
4	E	14	
5	F	336	
5	G	336	

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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 [i](#)

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		

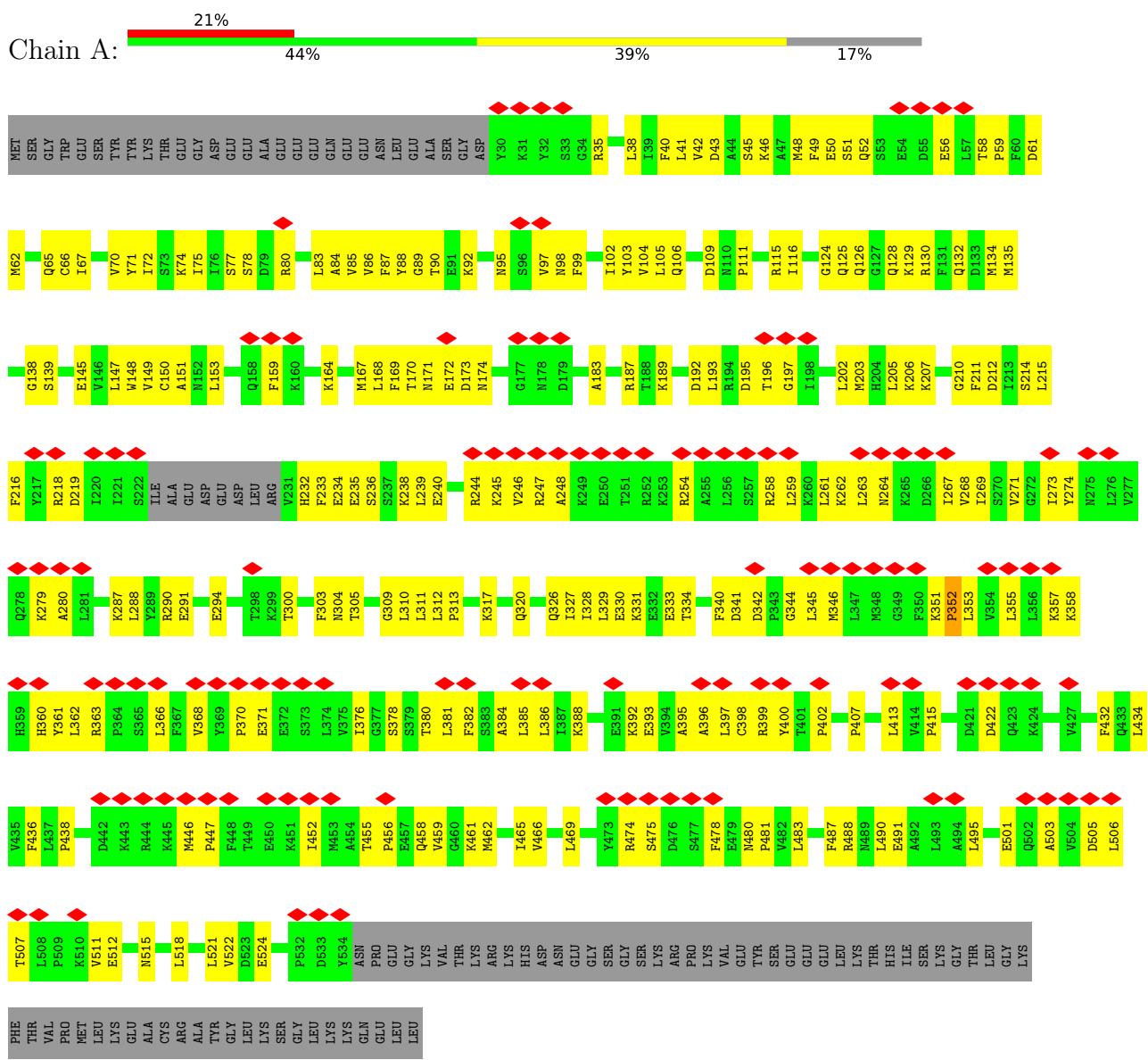
- Molecule 10 is a protein called DNA ligase 4.

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		

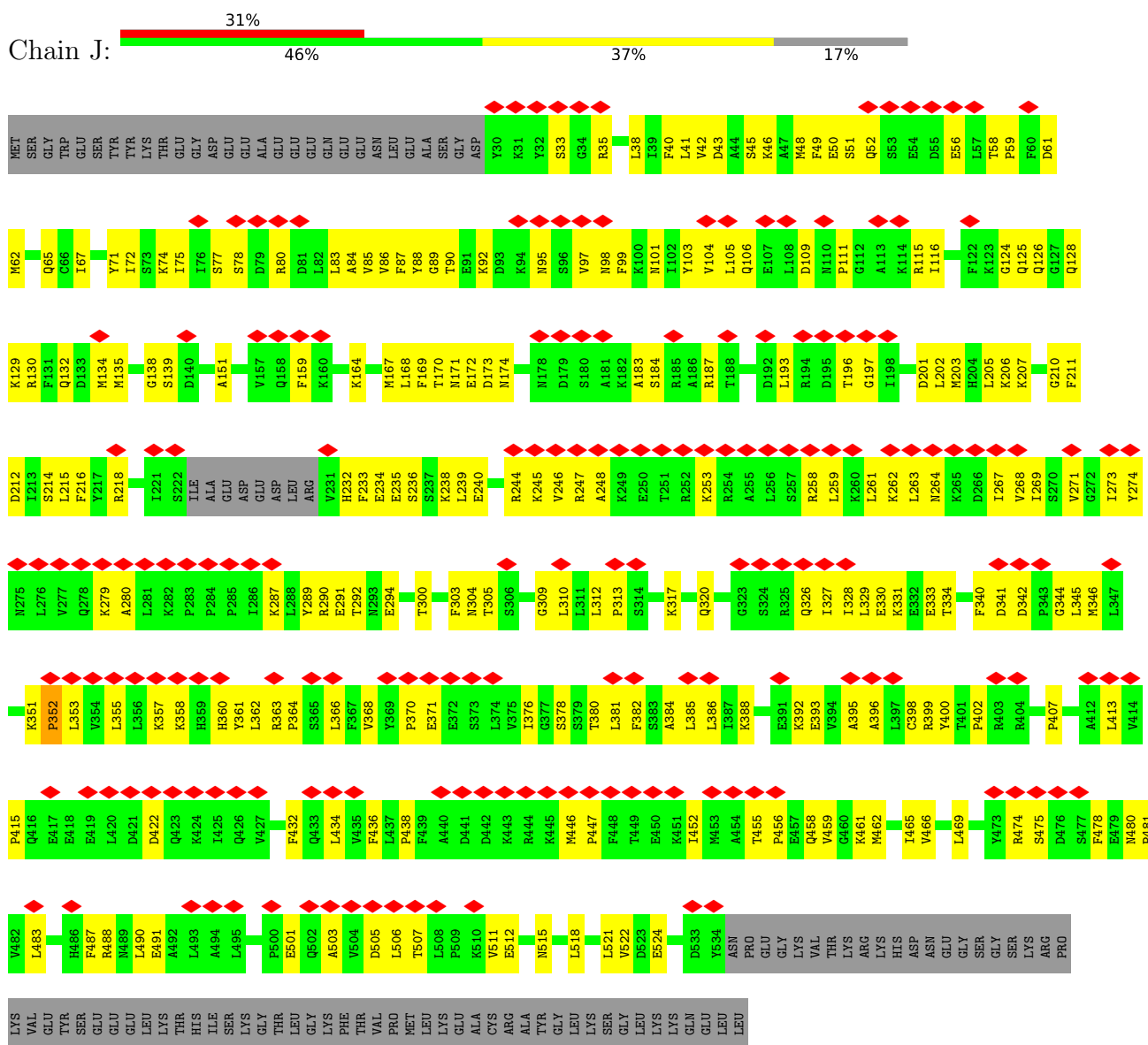
3 Residue-property plots

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.

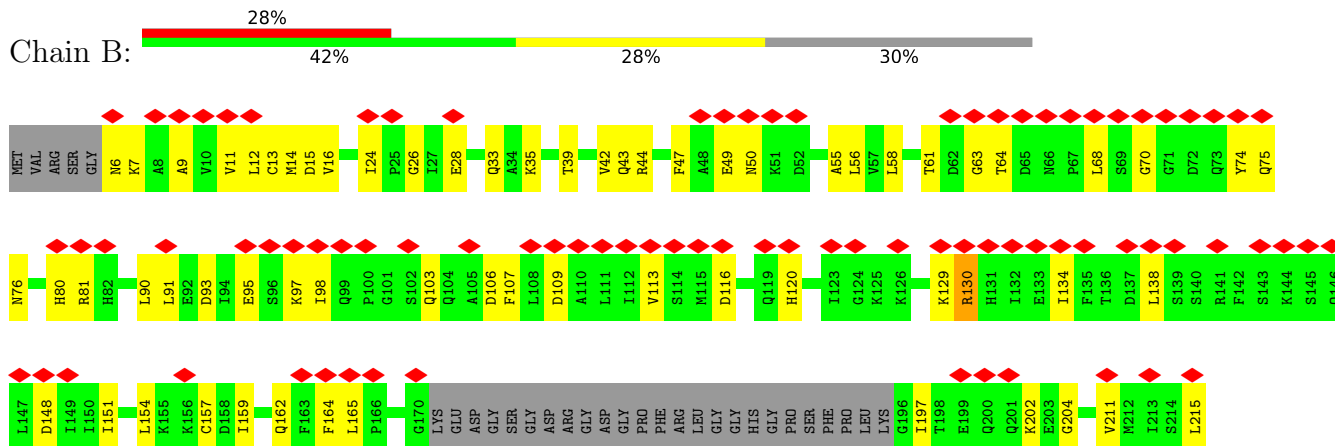
- Molecule 1: X-ray repair cross-complementing protein 6

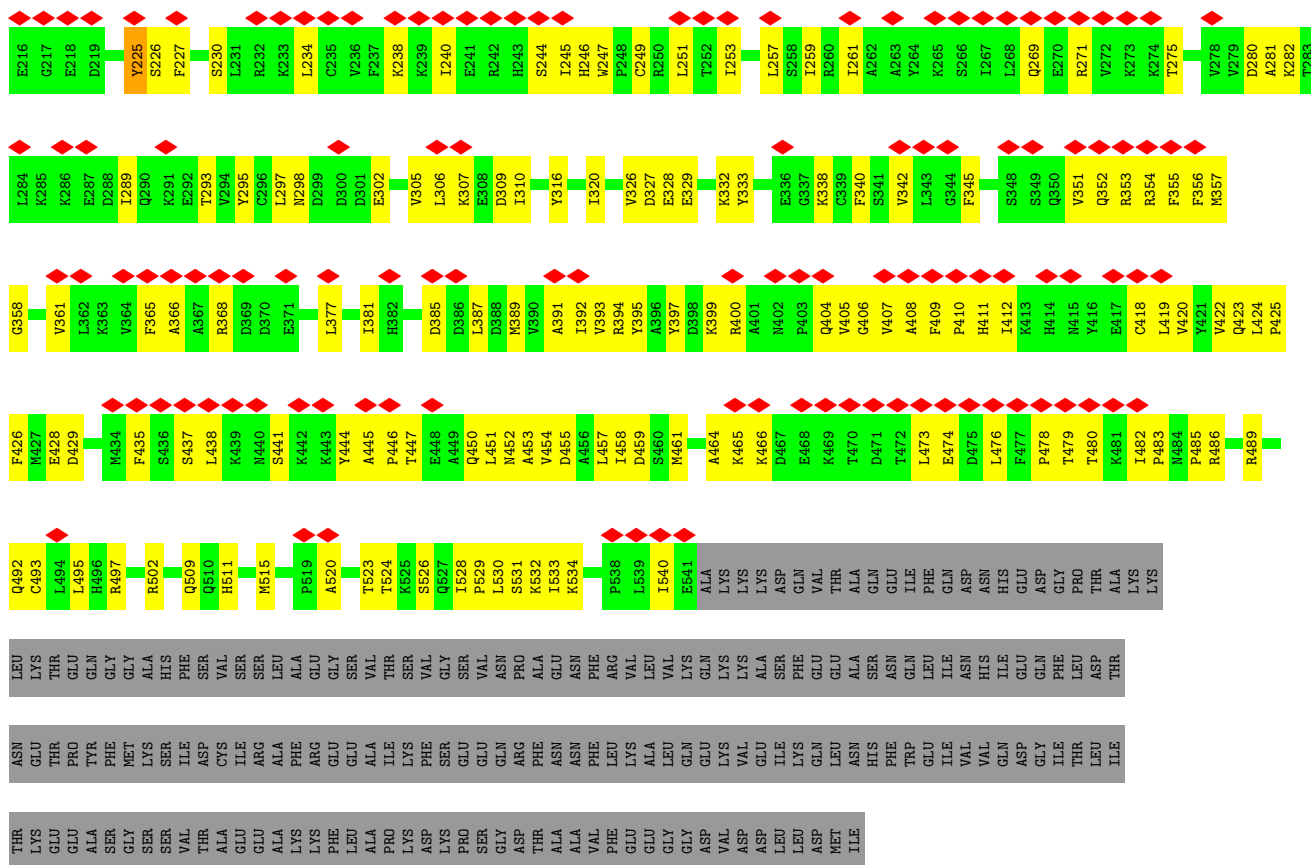


- Molecule 1: X-ray repair cross-complementing protein 6




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

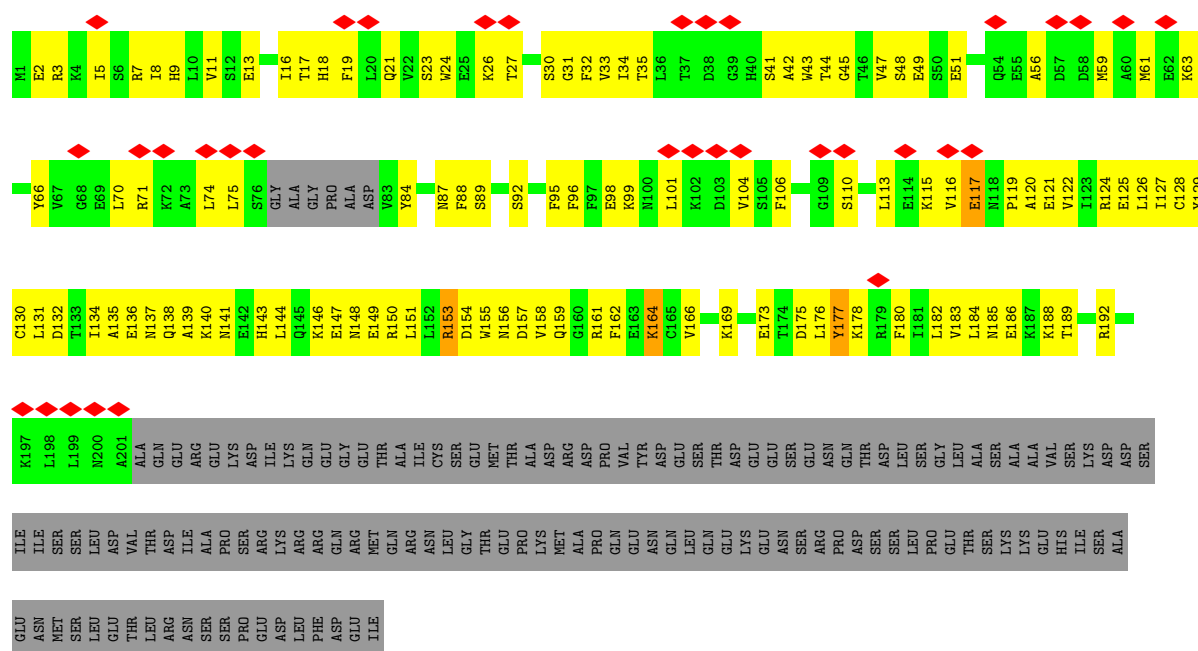





PHE
ASP
GLU
ILE

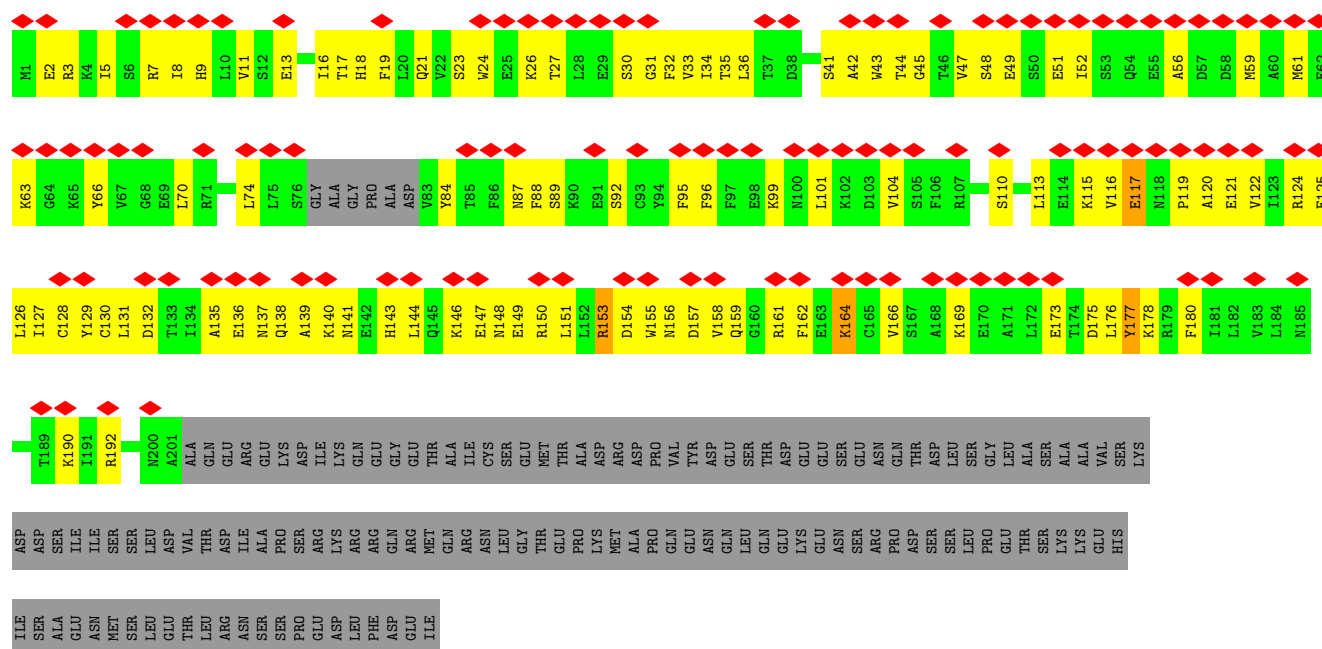
• Molecule 5: DNA repair protein XRCC4

Chain G: 

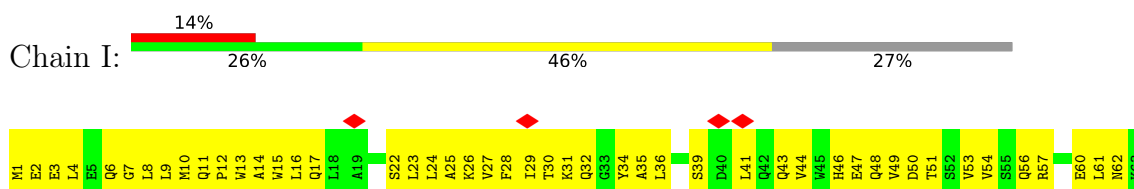
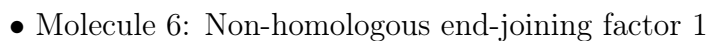


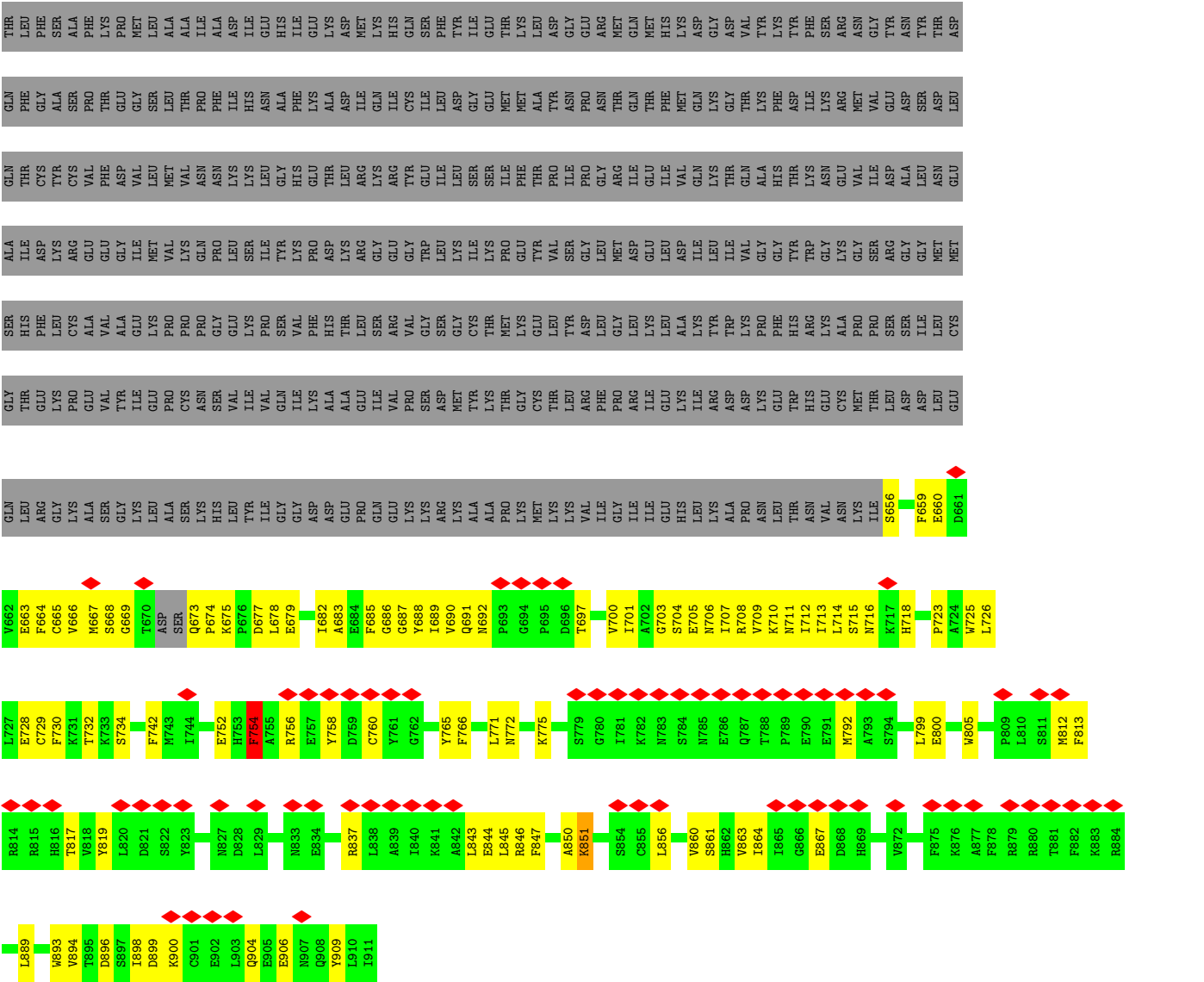
• Molecule 5: DNA repair protein XRCC4

Chain O: 

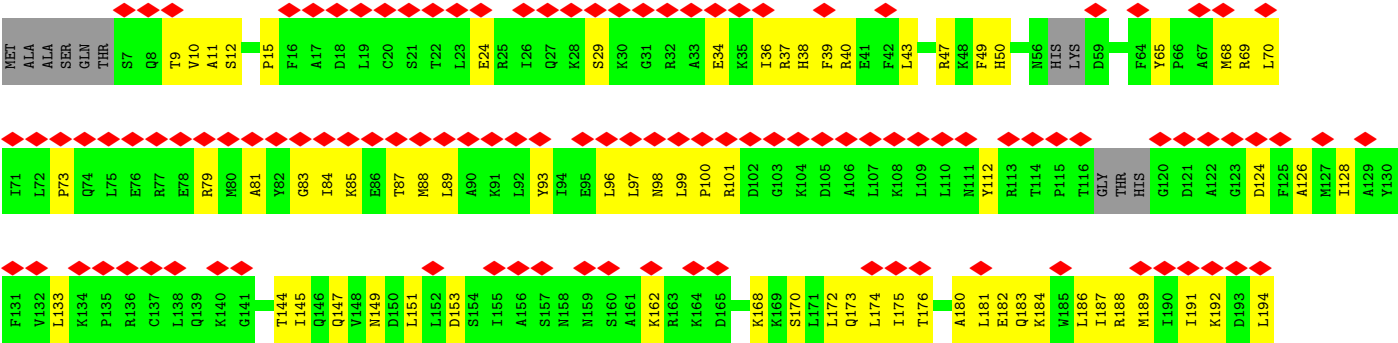


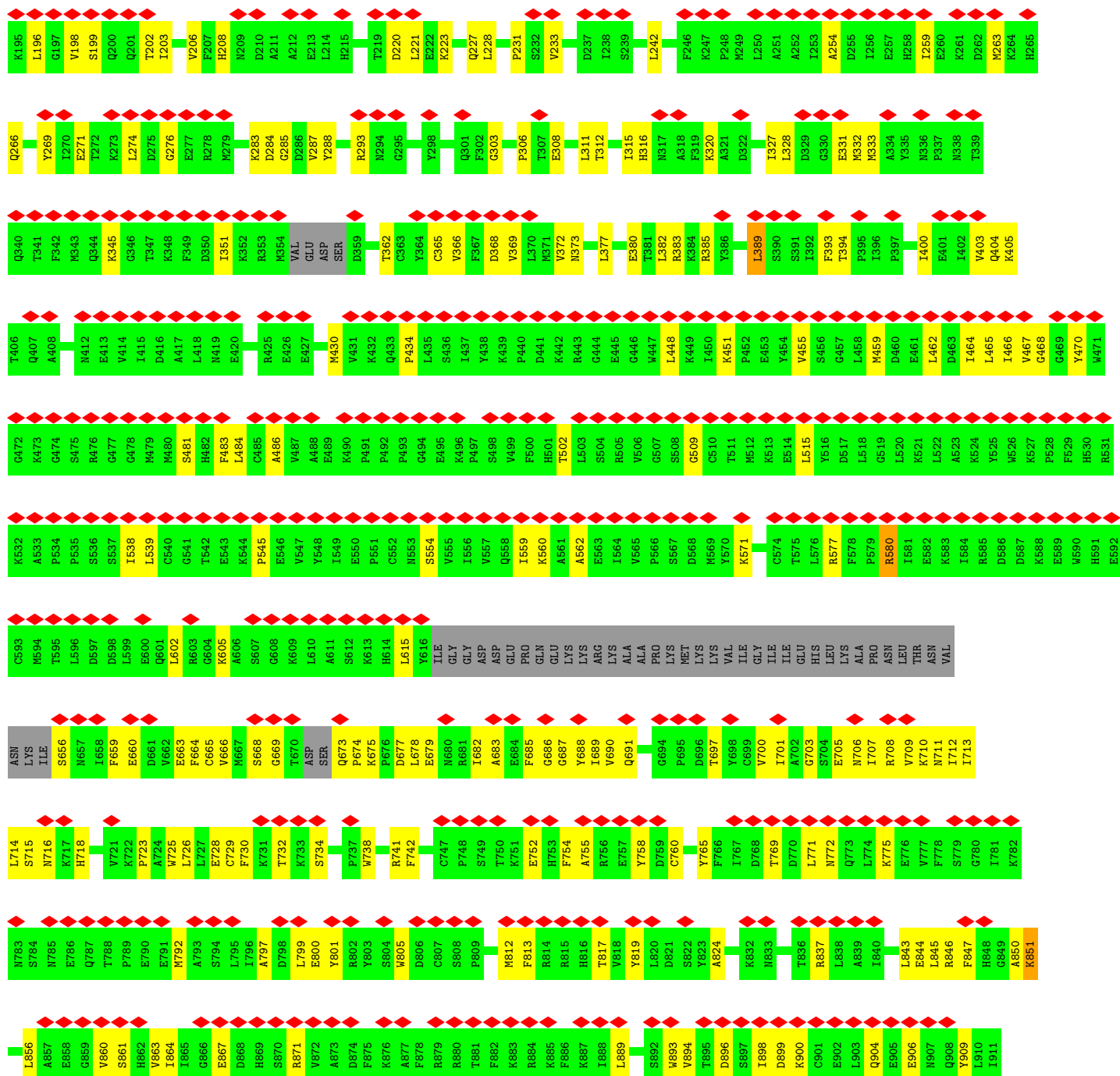
• Molecule 5: DNA repair protein XRCC4





● Molecule 10: DNA ligase 4





4 Experimental information

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 ($e^-/\text{\AA}^2$)	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 (\AA)	318.72, 318.72, 318.72	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	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(°)	Ideal(°)
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 ⓘ

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.

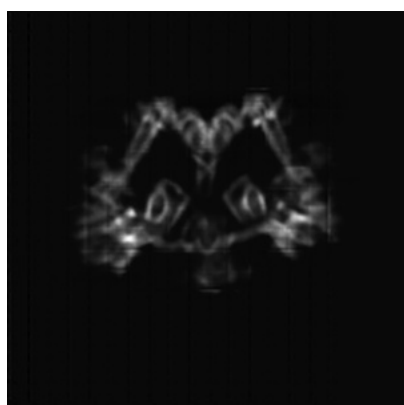
6 Map visualisation [i](#)

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.

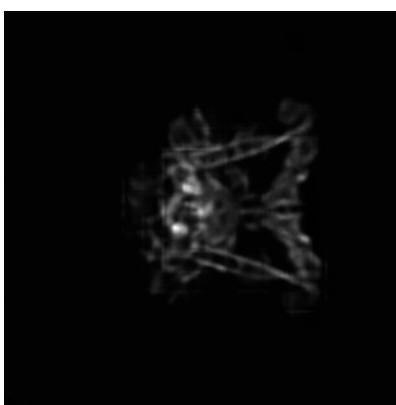
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

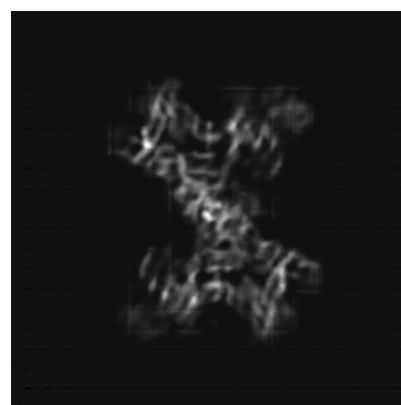
6.1.1 Primary map



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: 96



Y Index: 96

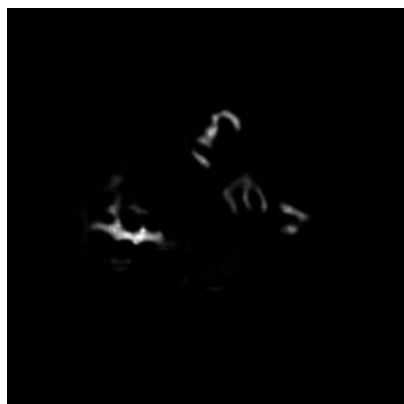


Z Index: 96

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

6.3 Largest variance slices [i](#)

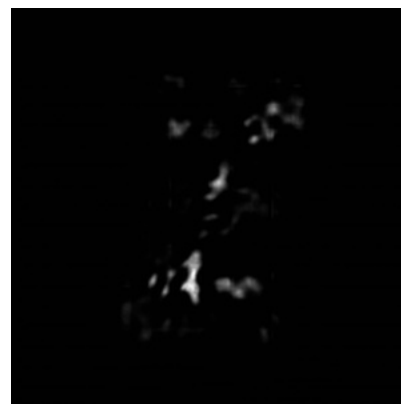
6.3.1 Primary map



X Index: 87



Y Index: 59



Z Index: 82

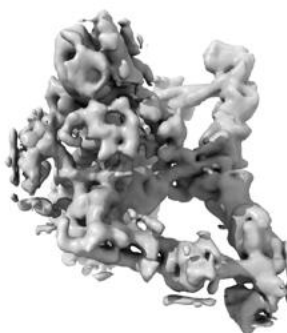
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

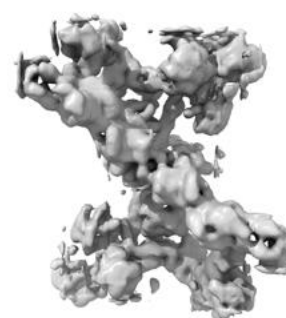
6.4.1 Primary map



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.

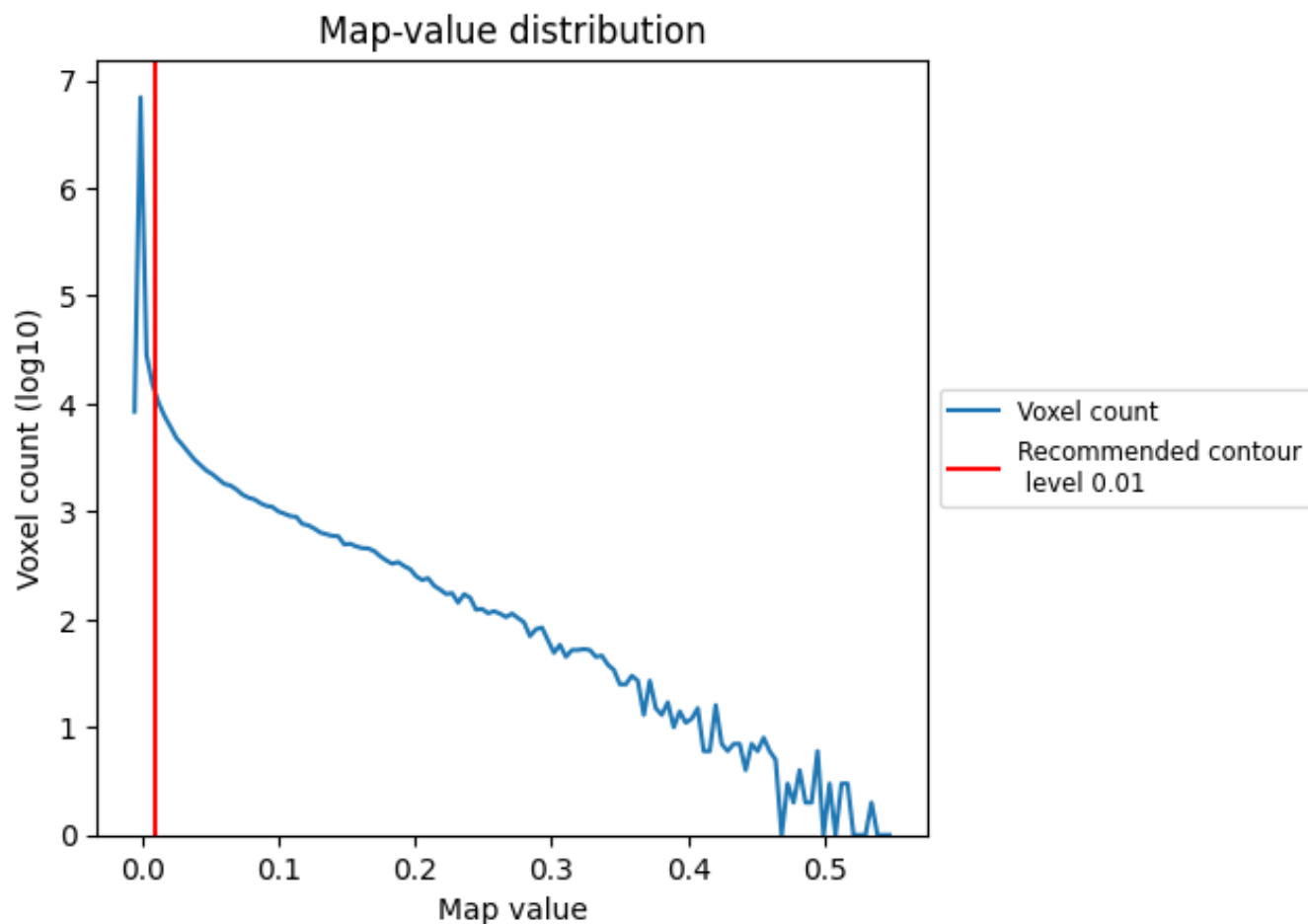
6.5 Mask visualisation

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

7 Map analysis [i](#)

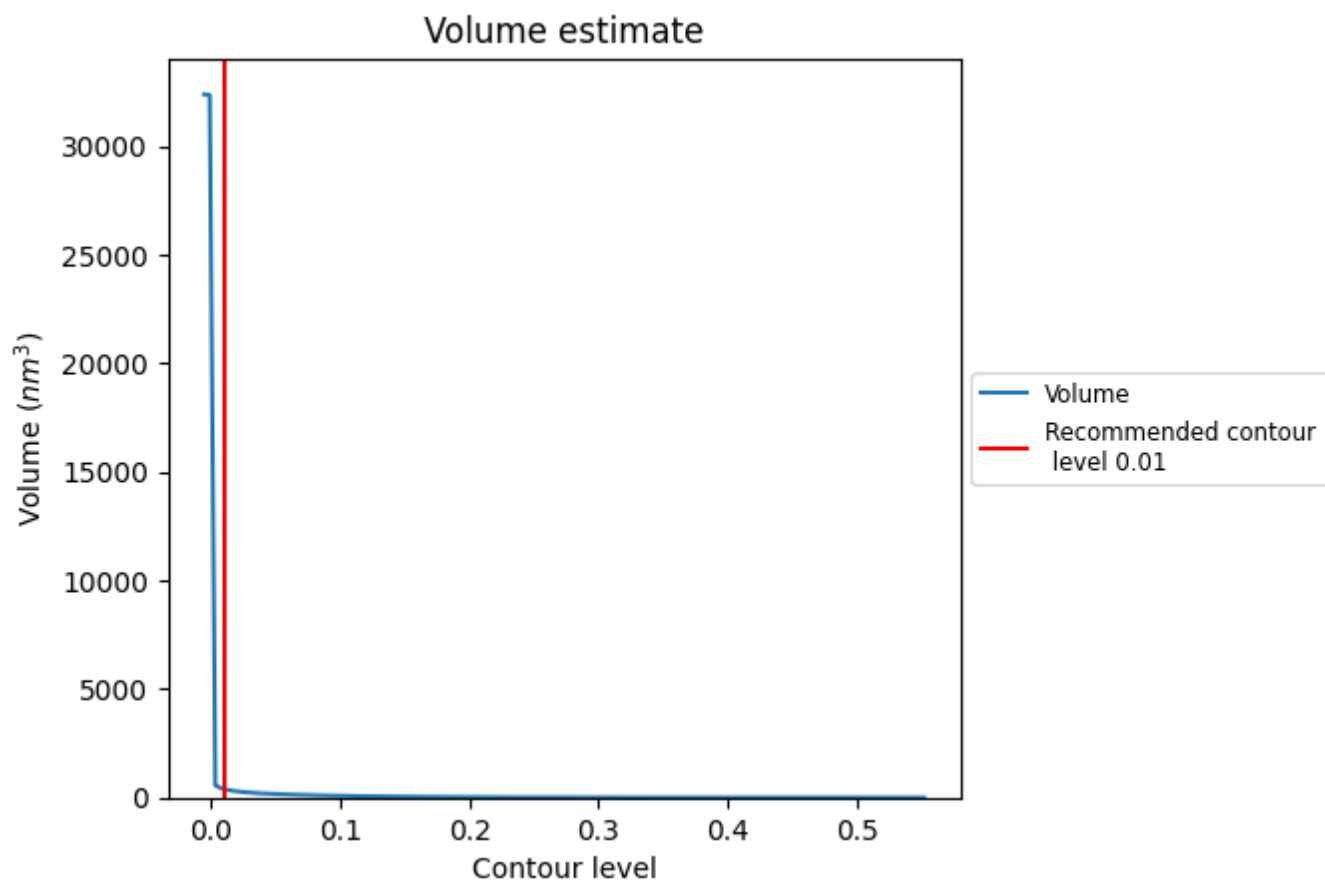
This section contains the results of statistical analysis of the map.

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.

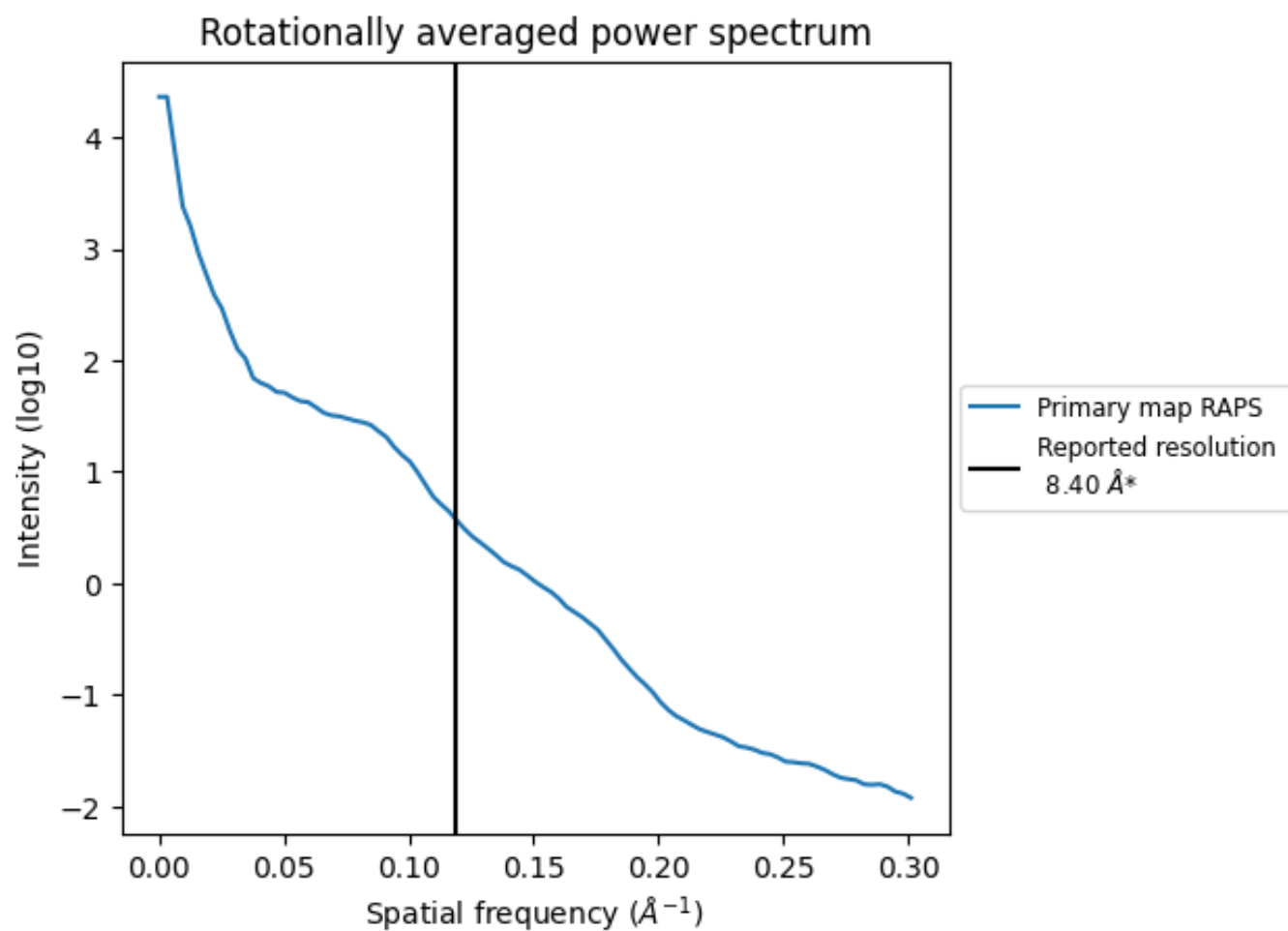
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.119 Å⁻¹

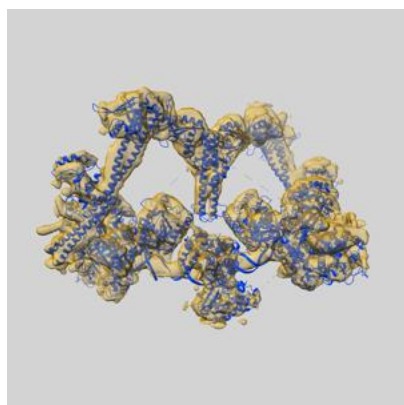
8 Fourier-Shell correlation

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

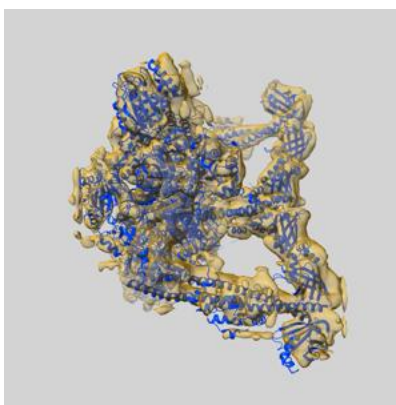
9 Map-model fit [i](#)

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](#).

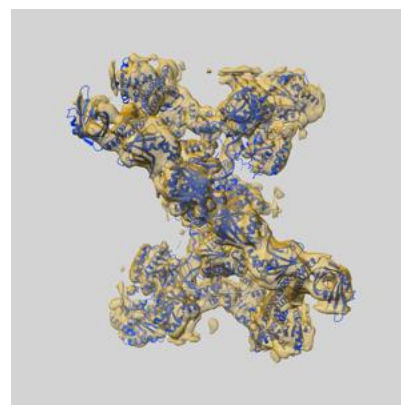
9.1 Map-model overlay [i](#)



X



Y



Z

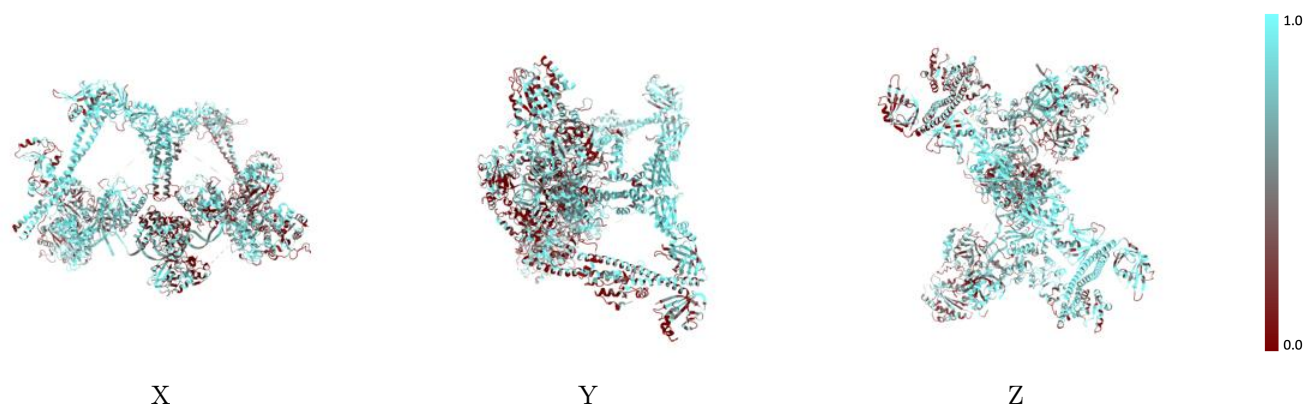
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



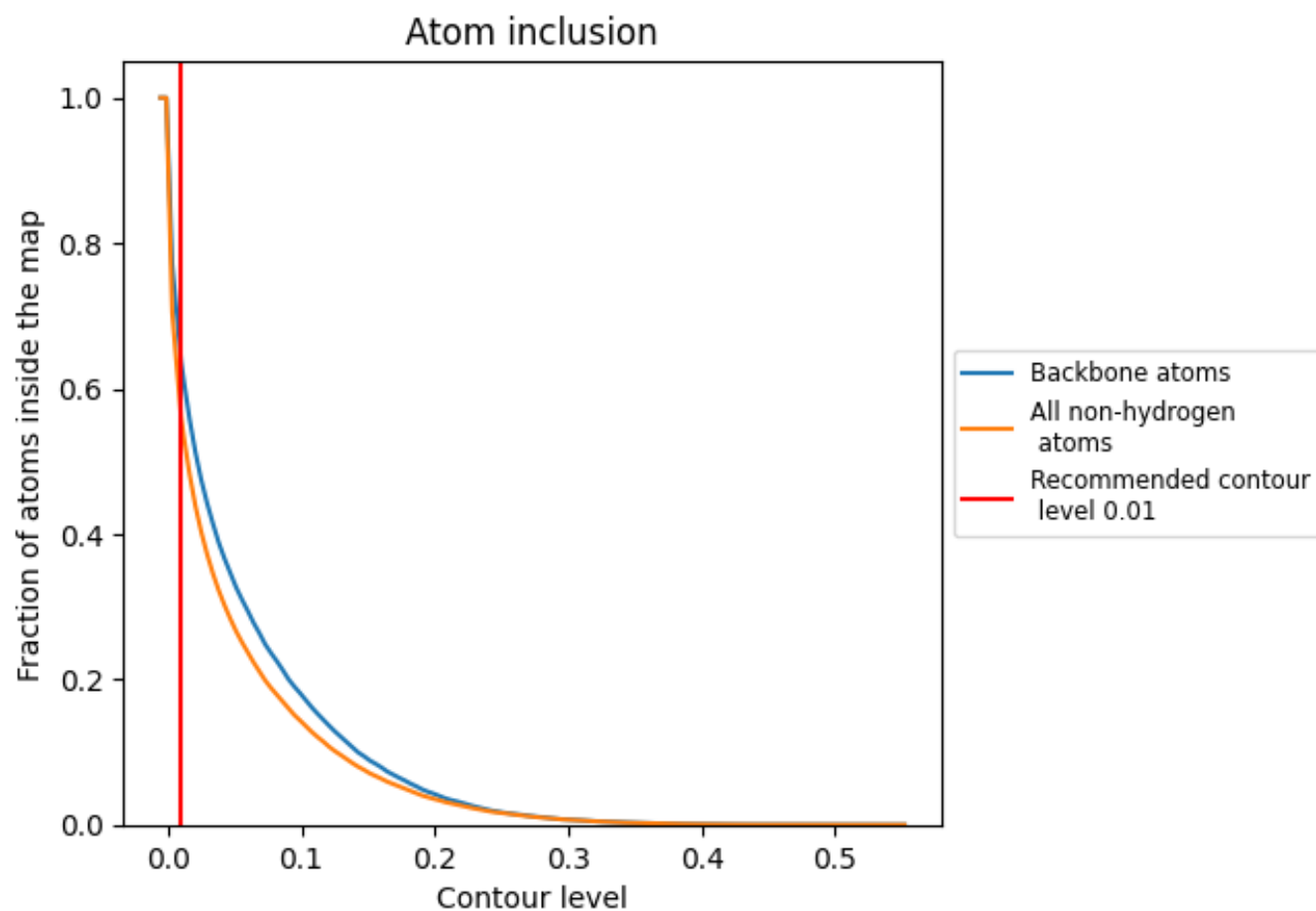
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).





































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	 0.5607	 0.0150
A	 0.6101	 0.0210
B	 0.5178	 0.0080
D	 0.8147	 0.1600
E	 0.8955	 0.1760
F	 0.8025	 0.0770
G	 0.7492	 0.0530
H	 0.7459	 0.0680
I	 0.7335	 0.0740
J	 0.5265	 0.0040
K	 0.5126	 -0.0040
M	 0.7108	 0.0860
N	 0.7906	 0.1000
O	 0.3842	 -0.0600
P	 0.5569	 -0.0500
V	 0.7277	 0.1000
X	 0.6438	 0.0350
Y	 0.3567	 -0.0240

