wwPDB EM Validation Summary Report (i)

Dec 16, 2024 – 05:37 PM EST

PDB ID	:	7K04
EMDB ID	:	EMD-22588
Title	:	Structure of TFIIH/Rad4-Rad23-Rad33/DNA in DNA opening
Authors	:	van Eeuwen, T.; Min, J.H.; Murakami, K.
Deposited on	:	2020-09-03
Resolution	:	9.25 Å(reported)
Based on initial model	:	6CFI

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:

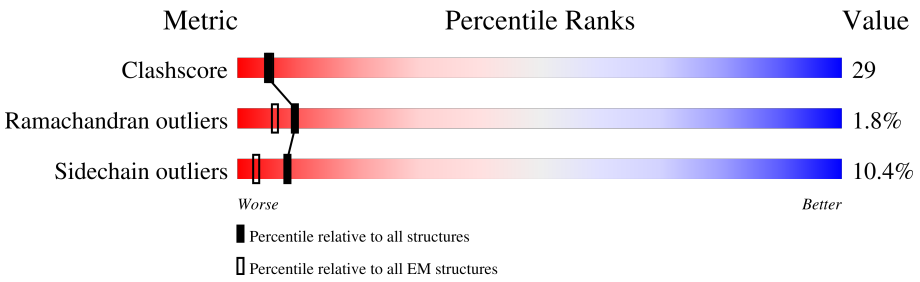
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 9.25 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	E	177	17% 13% 5% 65%
2	2	513	56% 29% 5% 10%
3	0	778	41% 49% 8%
4	1	642	16% 39% 31% 5% 24%
5	4	338	43% 33% 7% 16%
6	6	461	43% 28% 6% 24%
7	Y	27	15% 22% 48% 22% 7%
8	W	29	10% 45% 38% 17%

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Mol	Chain	Length	Quality of chain
9	A	754	34% 58% 11% 31%
10	7	843	46% 27% 24%
11	5	72	50% 40% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	SF4	0	801	-	-	X	-

2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 32727 atoms, of which 4782 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 DNA repair protein RAD33.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	E	62	476	301	77	92	6	0	0

- Molecule 2 is a protein called General transcription and DNA repair factor IIH subunit TFB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	460	3011	1856	562	584	9	0	0

- Molecule 3 is a protein called DNA repair helicase RAD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	0	754	6108	3891	1032	1147	38	0	0

- Molecule 4 is a protein called General transcription and DNA repair factor IIH subunit TFB1.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
4	1	487	4240	2123	884	605	616	12	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
1	1	PRO	-	insertion	UNP P32776

- Molecule 5 is a protein called General transcription and DNA repair factor IIH subunit TFB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	284	2041	1310	343	376	12	0	0

- Molecule 6 is a protein called General transcription and DNA repair factor IIH subunit SSL1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	6	351	2526	1589	454	456	27	0	0

- Molecule 7 is a DNA chain called Damaged DNA strand.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
7	Y	25	717	256	183	92	160	26	0	0

- Molecule 8 is a DNA chain called Undamaged DNA strand.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	P		
8	W	29	758	282	170	111	167	28	0	0

- Molecule 9 is a protein called DNA repair protein RAD4.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
9	A	524	7859	2747	3545	774	766	27	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	223	GLU	VAL	conflict	UNP P14736
A	427	ARG	GLN	conflict	UNP P14736

- Molecule 10 is a protein called DNA repair helicase RAD25.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	7	638	4478	2739	832	883	24	0	0

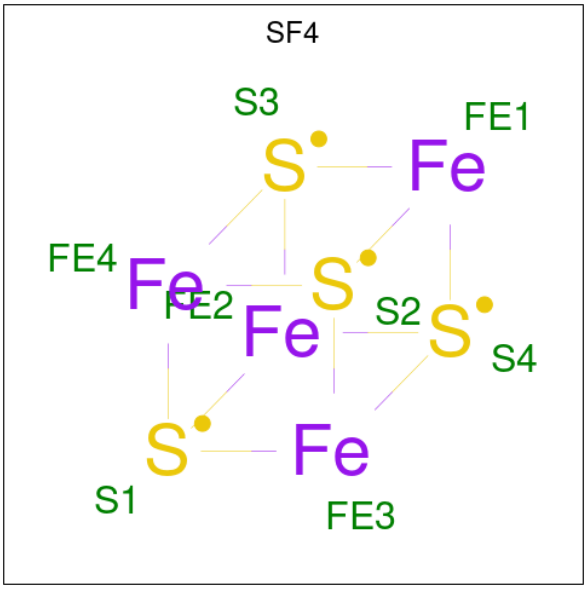
- Molecule 11 is a protein called RNA polymerase II transcription factor B subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	5	66	498	314	89	93	2	0	0

- Molecule 12 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
12	E	2	2	2	0

- Molecule 13 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
13	0	1	8	4	4	0

- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

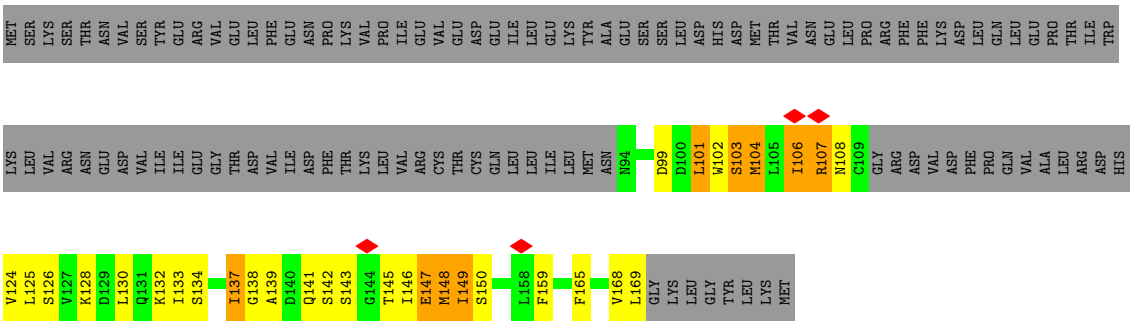
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
14	4	1	1	1	0
			Total	Zn	
14	6	4	4	4	0

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.

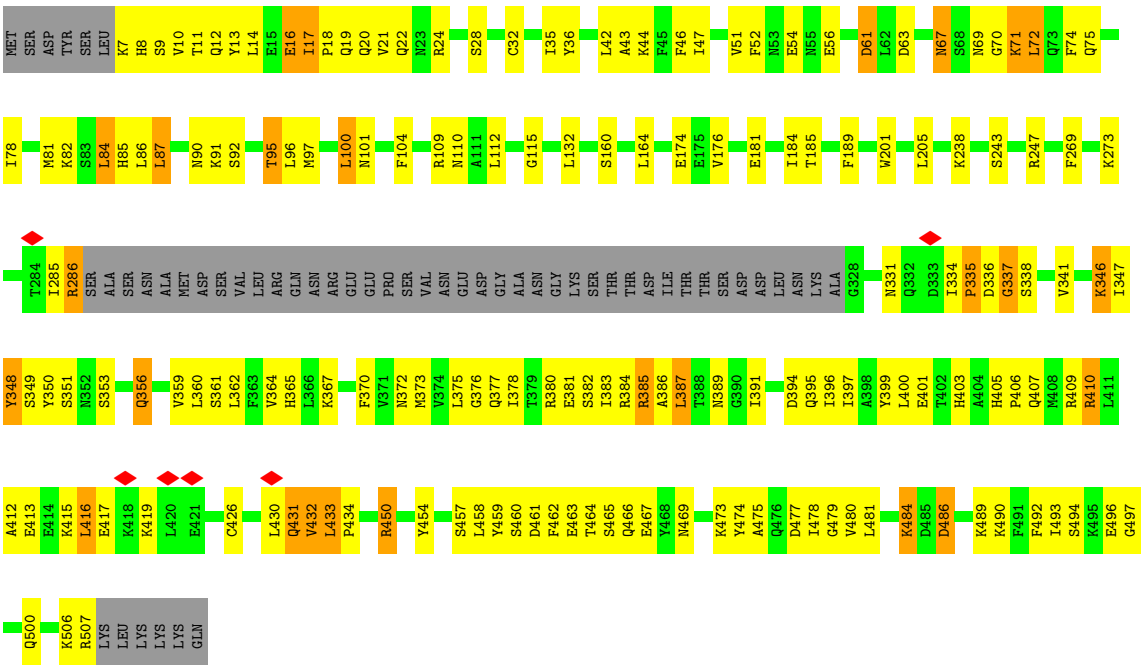
- Molecule 1: DNA repair protein RAD33

Chain E:



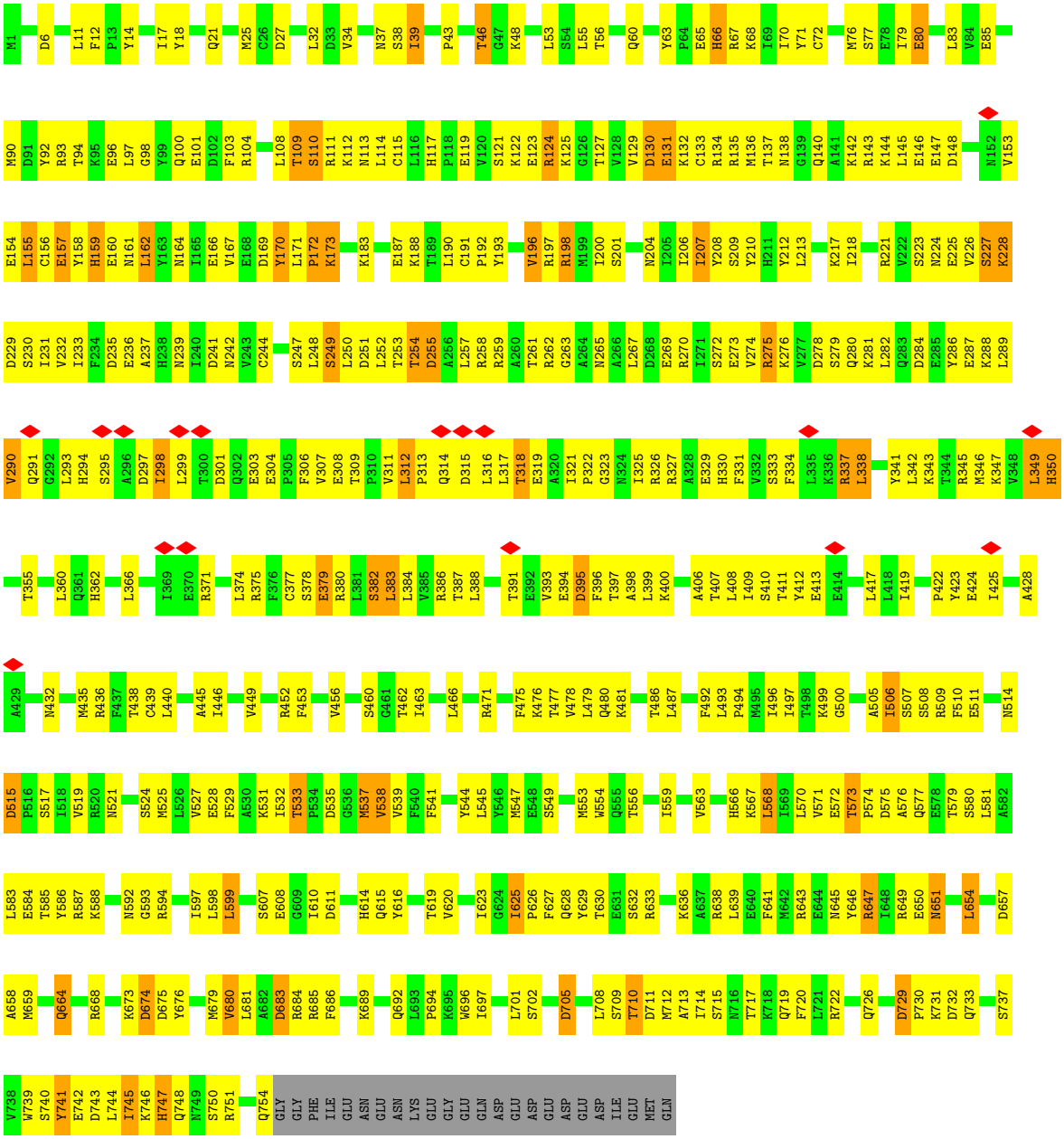
- Molecule 2: General transcription and DNA repair factor IIH subunit TFB2

Chain 2:



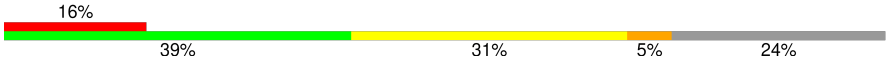
• Molecule 3: DNA repair helicase RAD3

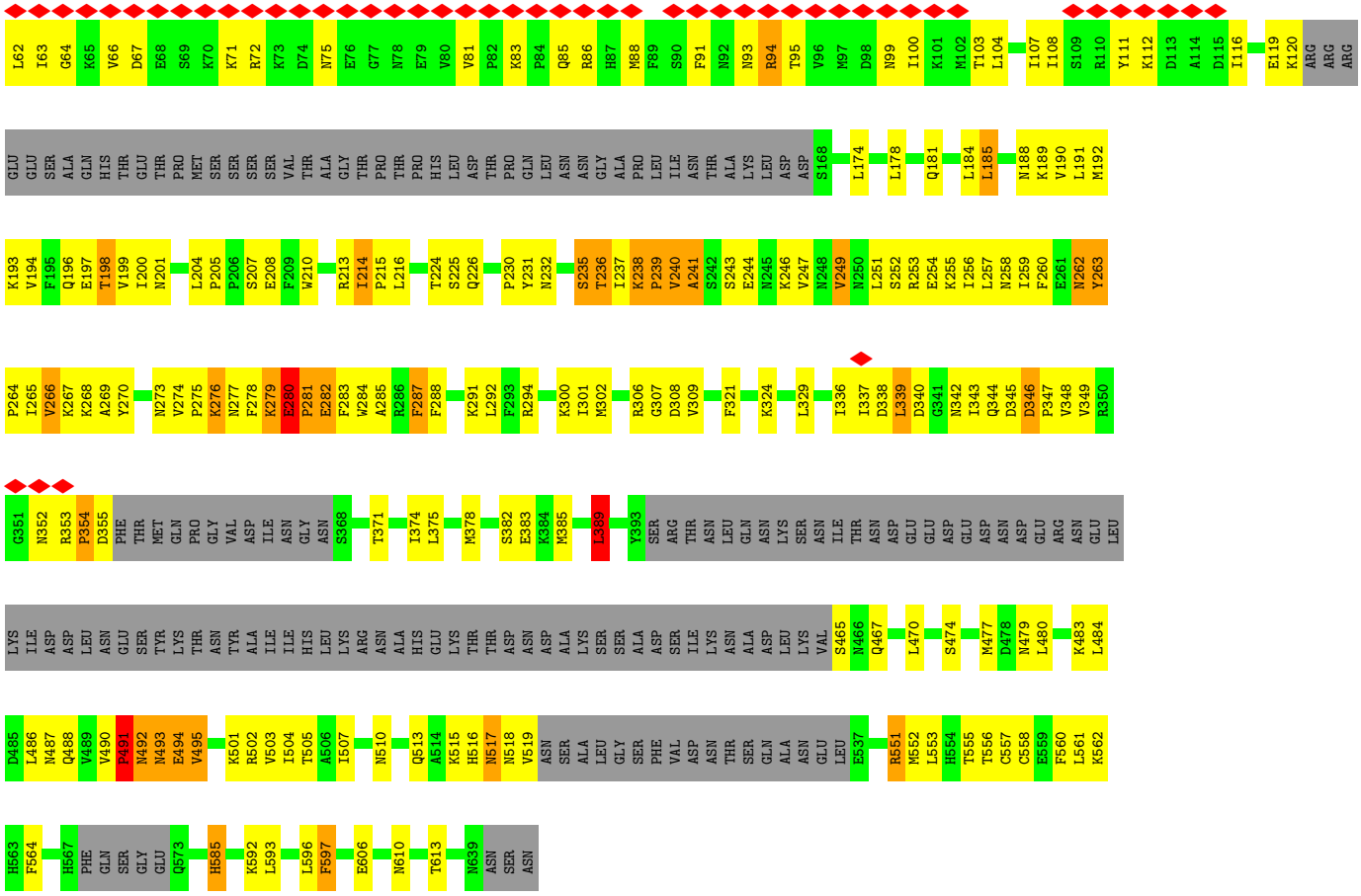
Chain 0:



• Molecule 4: General transcription and DNA repair factor IIH subunit TFB1

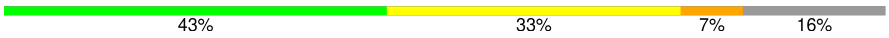
Chain 1:

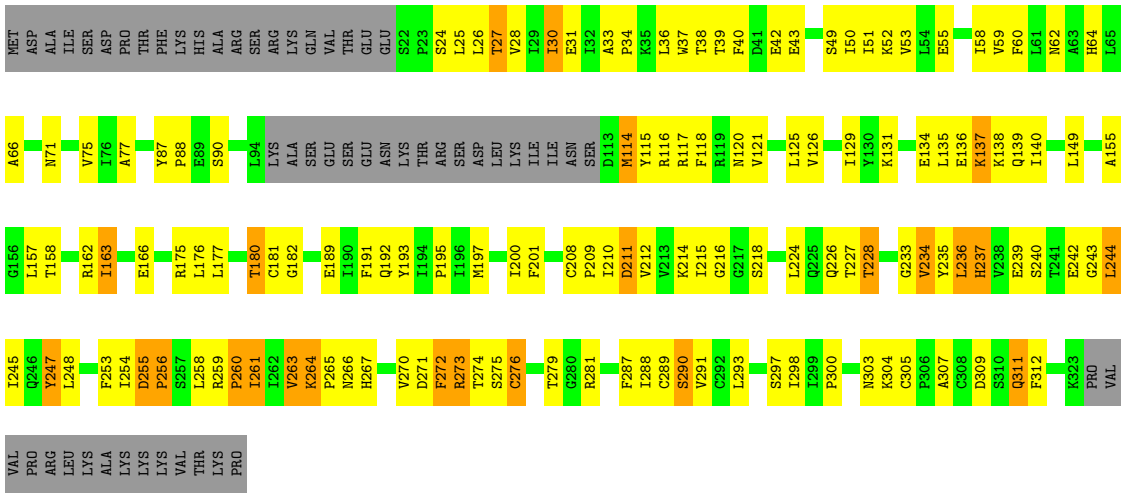




• Molecule 5: General transcription and DNA repair factor IIH subunit TFB4

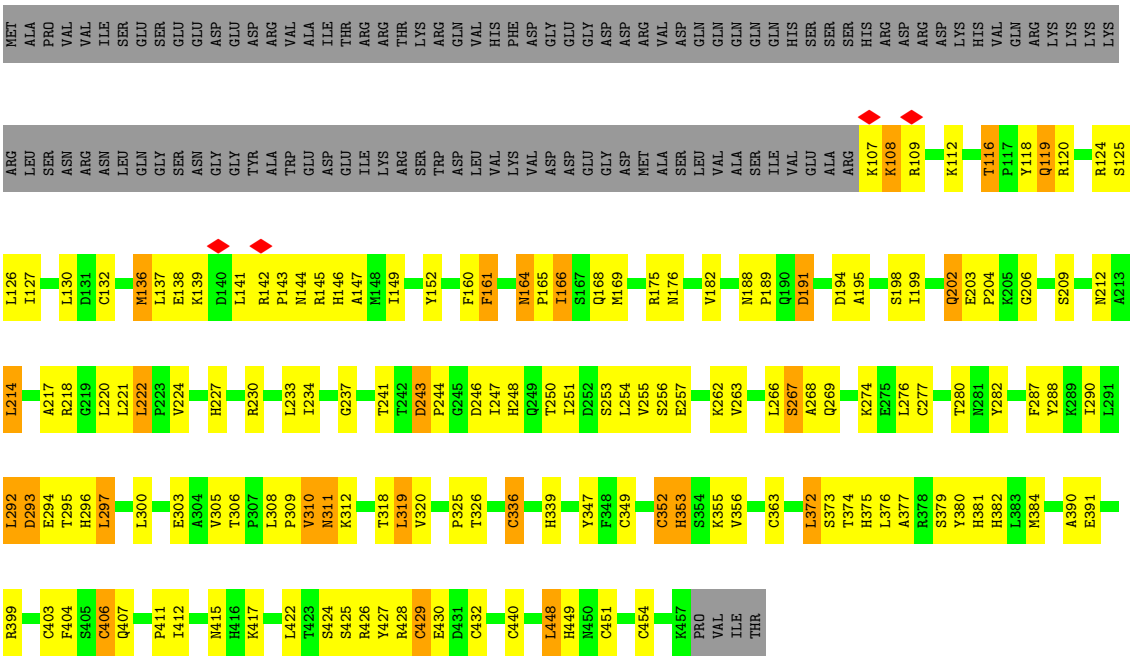
Chain 4:





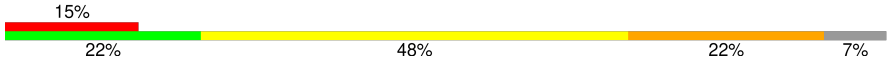
• Molecule 6: General transcription and DNA repair factor IIH subunit SSL1

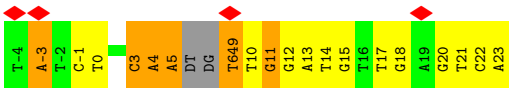
Chain 6:



- Molecule 7: Damaged DNA strand

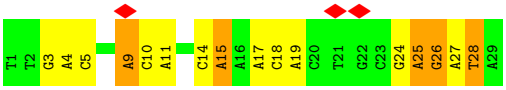
Chain Y:





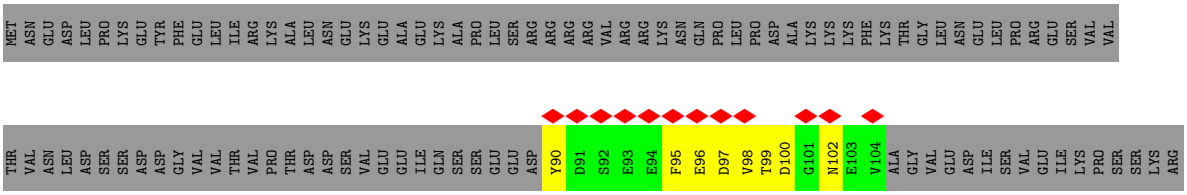
- Molecule 8: Undamaged DNA strand

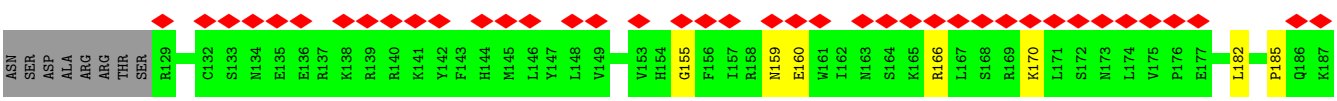
Chain W:

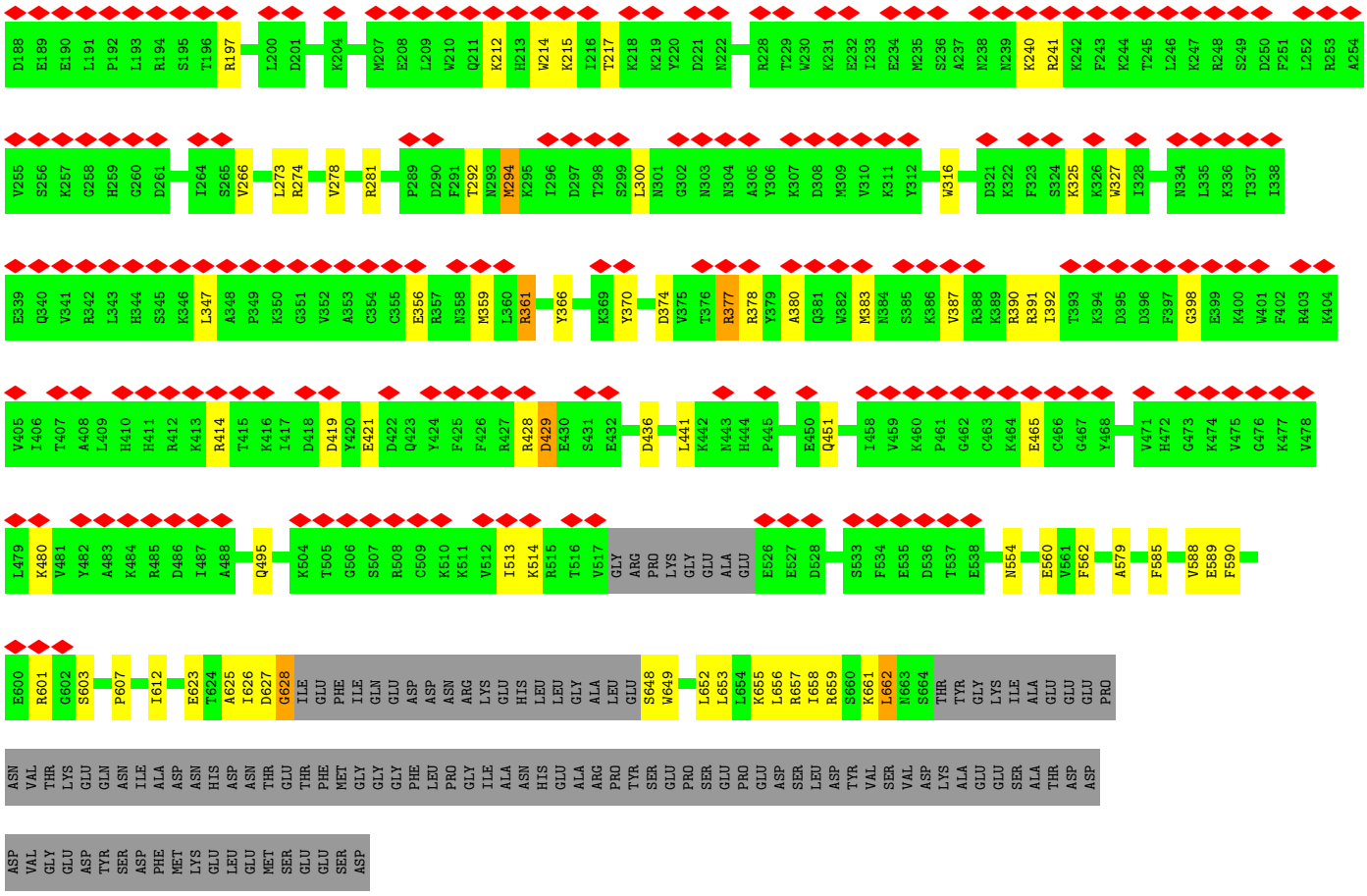


- Molecule 9: DNA repair protein RAD4

Chain A:

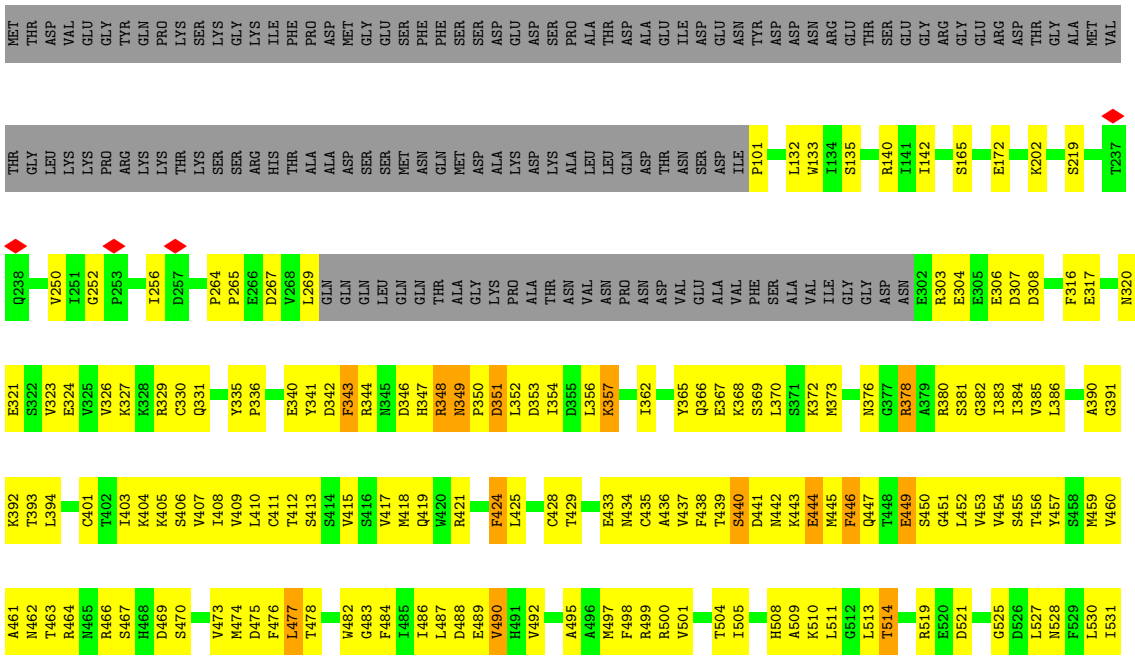


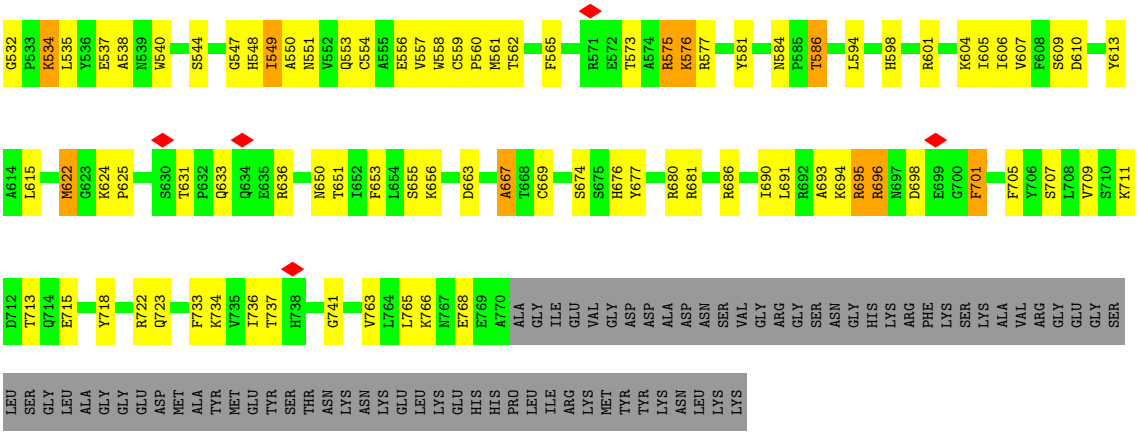




- Molecule 10: DNA repair helicase RAD25

Chain 7:





- Molecule 11: RNA polymerase II transcription factor B subunit 5

Chain 5:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	73146	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.007	Depositor
Minimum map value	0.000	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.00167	Depositor
Map size (Å)	324.0, 324.0, 324.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: T64, CA, SF4, ZN

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	E	0.38	0/479	0.81	2/644 (0.3%)
2	2	0.28	0/3057	0.47	0/4071
3	0	0.54	0/6226	0.54	0/8407
4	1	0.37	0/3400	0.51	2/4618 (0.0%)
5	4	0.52	0/2072	0.57	0/2819
6	6	0.54	0/2571	0.57	1/3494 (0.0%)
7	Y	1.01	3/552 (0.5%)	1.33	4/848 (0.5%)
8	W	0.92	1/660 (0.2%)	1.51	8/1015 (0.8%)
9	A	0.33	0/4404	0.56	2/5919 (0.0%)
10	7	0.34	0/4552	0.58	3/6078 (0.0%)
11	5	0.23	0/502	0.47	0/677
All	All	0.46	4/28475 (0.0%)	0.62	22/38590 (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
7	Y	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	W	15	DA	O3'-P	9.91	1.73	1.61
7	Y	5	DA	P-O5'	5.70	1.65	1.59
7	Y	3	DC	C1'-N1	-5.35	1.39	1.47
7	Y	3	DC	C3'-O3'	-5.09	1.37	1.44

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	W	28	DT	O5'-P-OP1	-26.89	78.44	110.70
8	W	26	DG	O5'-P-OP1	-14.80	92.38	105.70
9	A	628	GLY	N-CA-C	10.82	140.15	113.10
8	W	28	DT	O5'-P-OP2	10.40	123.18	110.70
8	W	27	DA	OP1-P-O3'	8.39	123.66	105.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	Y	-3	DA	Sidechain

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	E	476	0	487	127	0
2	2	3011	0	2600	182	0
3	0	6108	0	6167	406	0
4	1	3356	884	2945	287	0
5	4	2041	0	1953	151	0
6	6	2526	0	2333	124	0
7	Y	534	183	298	45	0
8	W	588	170	327	21	0
9	A	4314	3545	4388	126	0
10	7	4478	0	3928	268	0
11	5	498	0	506	35	0
12	E	2	0	0	0	0
13	0	8	0	0	2	0
14	4	1	0	0	0	0
14	6	4	0	0	0	0
All	All	27945	4782	25932	1534	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 29.

The worst 5 of 1534 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)
1:E:149:ILE:HG12	9:A:649:TRP:CZ2	1.31	1.65
1:E:149:ILE:HA	9:A:649:TRP:CZ2	1.27	1.65
4:1:270:TYR:CE1	4:1:279:LYS:HE3	1.26	1.62
1:E:149:ILE:CG1	9:A:649:TRP:CH2	1.78	1.60
4:1:279:LYS:HA	4:1:283:PHE:CB	1.27	1.56

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	E	58/177 (33%)	47 (81%)	9 (16%)	2 (3%)	3 21
2	2	456/513 (89%)	380 (83%)	71 (16%)	5 (1%)	12 47
3	0	752/778 (97%)	632 (84%)	118 (16%)	2 (0%)	37 73
4	1	475/642 (74%)	387 (82%)	50 (10%)	38 (8%)	1 9
5	4	280/338 (83%)	210 (75%)	65 (23%)	5 (2%)	7 35
6	6	349/461 (76%)	284 (81%)	59 (17%)	6 (2%)	7 37
9	A	516/754 (68%)	490 (95%)	25 (5%)	1 (0%)	44 78
10	7	634/843 (75%)	562 (89%)	65 (10%)	7 (1%)	12 47
11	5	64/72 (89%)	59 (92%)	5 (8%)	0	100 100
All	All	3584/4578 (78%)	3051 (85%)	467 (13%)	66 (2%)	9 35

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	335	PRO
4	1	230	PRO
4	1	236	THR
4	1	239	PRO
4	1	338	ASP

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	E	56/165 (34%)	50 (89%)	6 (11%)	5	19
2	2	258/468 (55%)	227 (88%)	31 (12%)	4	16
3	0	686/707 (97%)	595 (87%)	91 (13%)	3	13
4	1	277/589 (47%)	243 (88%)	34 (12%)	4	15
5	4	198/300 (66%)	165 (83%)	33 (17%)	2	9
6	6	247/418 (59%)	208 (84%)	39 (16%)	2	10
9	A	474/678 (70%)	459 (97%)	15 (3%)	34	53
10	7	417/737 (57%)	389 (93%)	28 (7%)	13	34
11	5	53/66 (80%)	52 (98%)	1 (2%)	52	69
All	All	2666/4128 (65%)	2388 (90%)	278 (10%)	8	19

5 of 278 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	6	406	CYS
9	A	197	ARG
10	7	445	MET
3	0	515	ASP
3	0	477	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
6	6	227	HIS
6	6	375	HIS
10	7	584	ASN
9	A	154	HIS
3	0	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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	$\#\|Z\| > 2$
7	T64	Y	9	7	41,44,45	4.22	18 (43%)	53,69,72	2.15	17 (32%)

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
7	T64	Y	9	7	-	11/22/76/77	0/3/5/5

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	Y	9	T64	C6T-N1T	11.81	1.58	1.38
7	Y	9	T64	C6-C4T	10.24	1.64	1.51
7	Y	9	T64	C6T-C5T	9.92	1.50	1.34
7	Y	9	T64	C2-N3	8.33	1.52	1.38
7	Y	9	T64	C2-N1	7.98	1.51	1.36

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	9	T64	C6T-N1T-C2T	-6.21	112.68	120.95
7	Y	9	T64	C6-C5-C4	5.20	117.81	109.70
7	Y	9	T64	C5T-C4T-N3T	-4.40	119.82	123.61
7	Y	9	T64	C4-N3-C2	-4.16	120.40	126.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	Y	9	T64	C2T-N3T-C4T	4.15	122.77	119.02

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	Y	9	T64	C5R-O5R-PB-O4P
7	Y	9	T64	C3'-C4'-C5R-O5R
7	Y	9	T64	O4R-C4'-C5R-O5R
7	Y	9	T64	C3R-C4R-C5'-O5'
7	Y	9	T64	C2R-C1R-N1T-C6T

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	Y	9	T64	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 7 are monoatomic - leaving 1 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	$\#\|Z\| > 2$
13	SF4	0	801	3	0,12,12	-	-	-		

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
13	SF4	0	801	3	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	0	801	SF4	2	0

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.

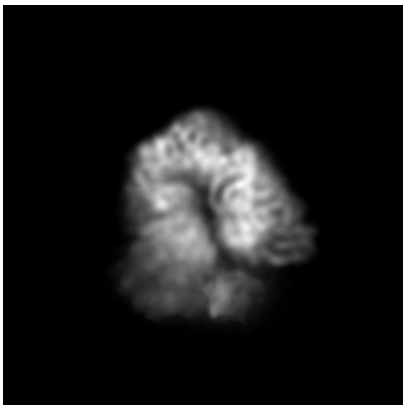
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22588. These allow visual inspection of the internal detail of the map and identification of artifacts.

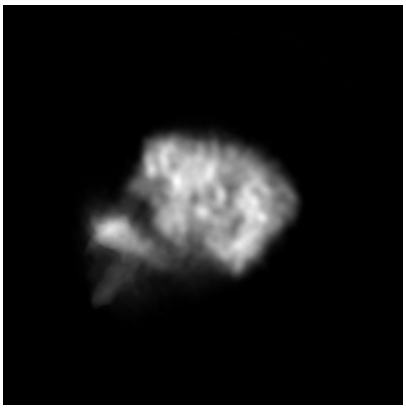
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

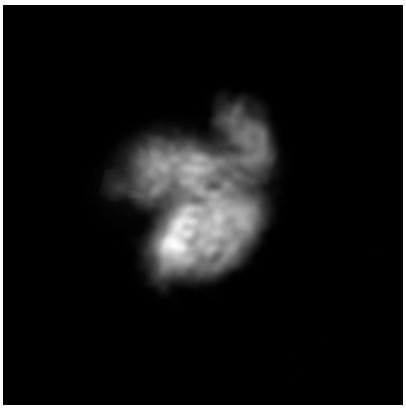
6.1.1 Primary map



X

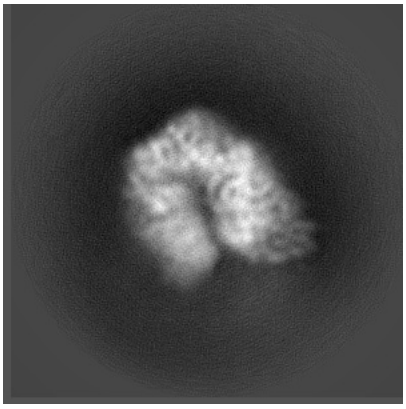


Y

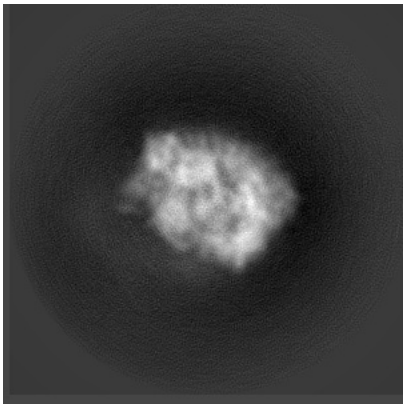


Z

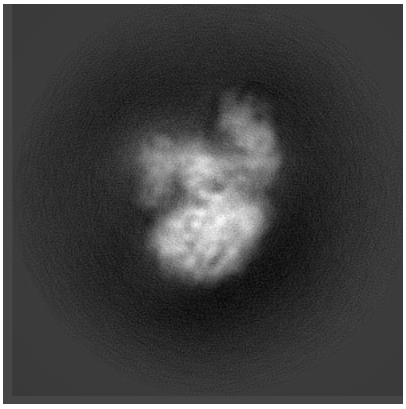
6.1.2 Raw map



X



Y

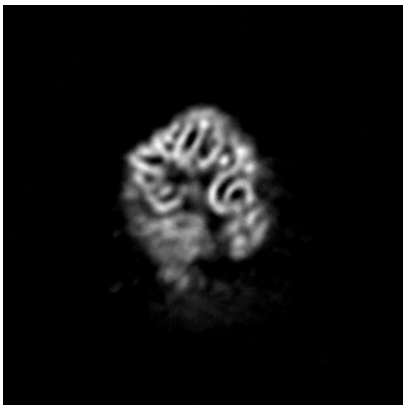


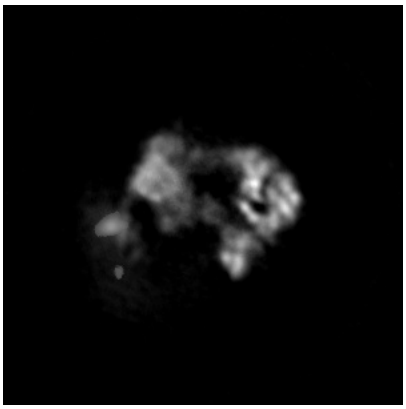
Z

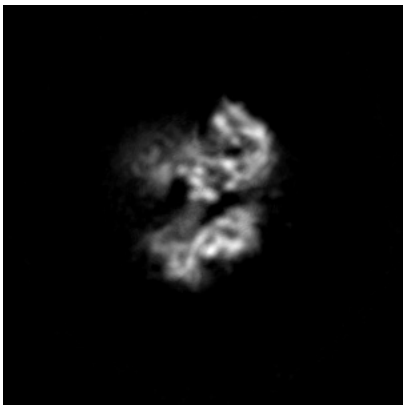
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

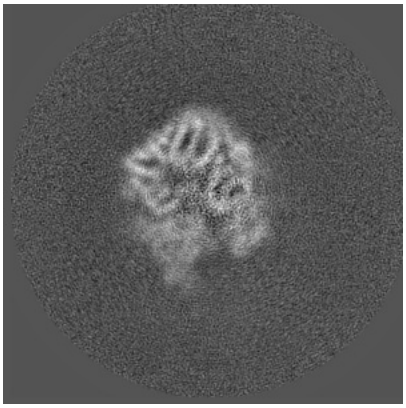
6.2.1 Primary map

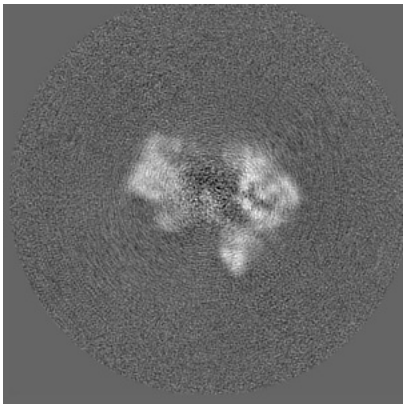

X Index: 150

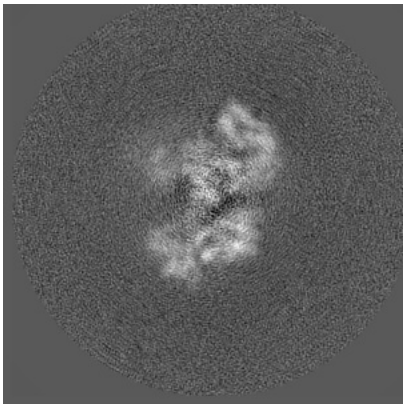

Y Index: 150


Z Index: 150

6.2.2 Raw map


X Index: 150

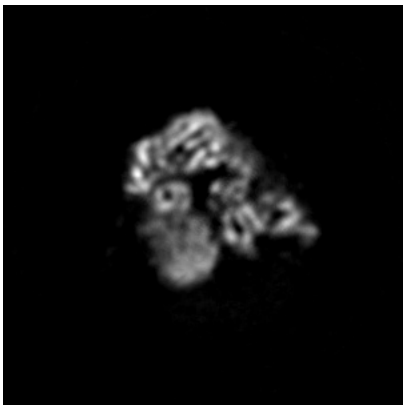

Y Index: 150


Z Index: 150

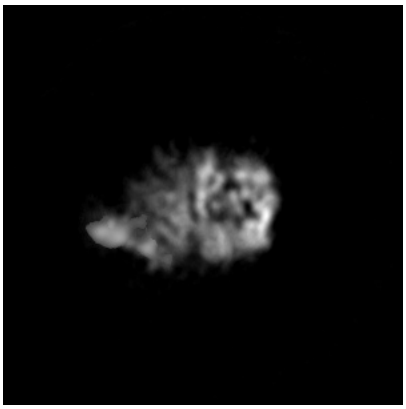
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

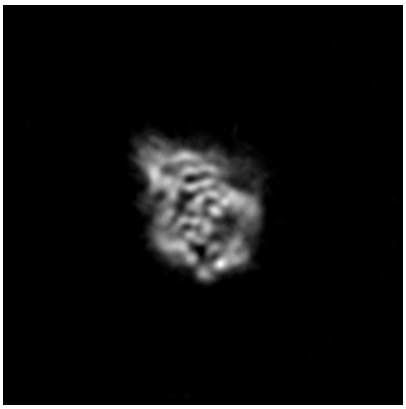
6.3.1 Primary map



X Index: 161

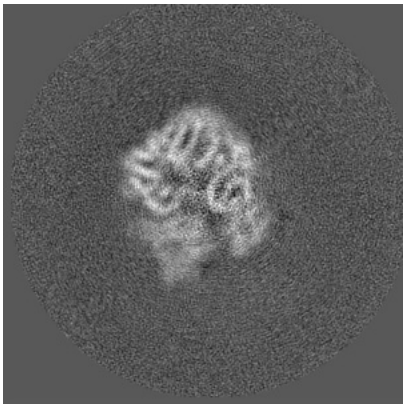


Y Index: 118

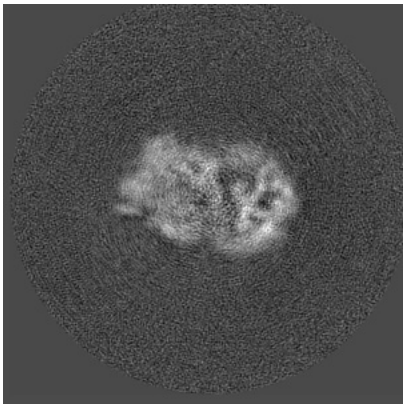


Z Index: 184

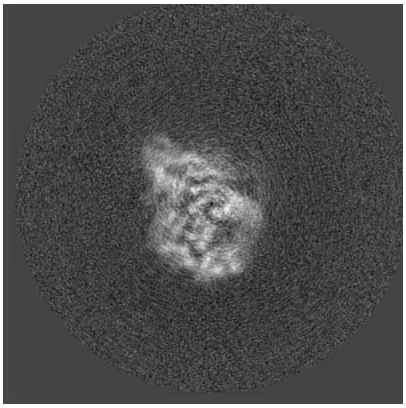
6.3.2 Raw map



X Index: 152



Y Index: 135

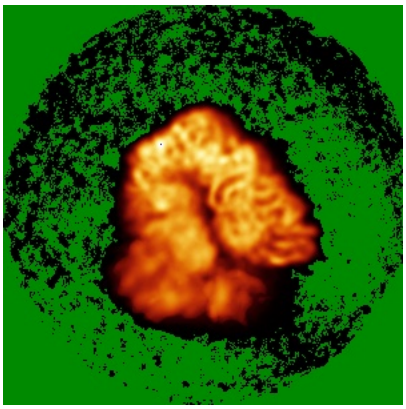


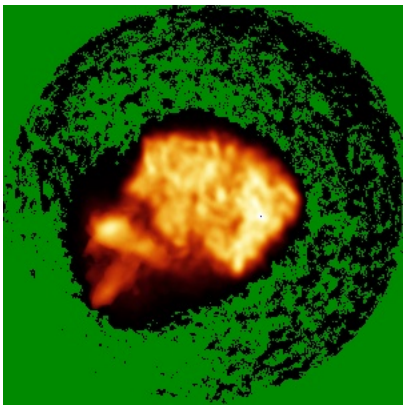
Z Index: 185

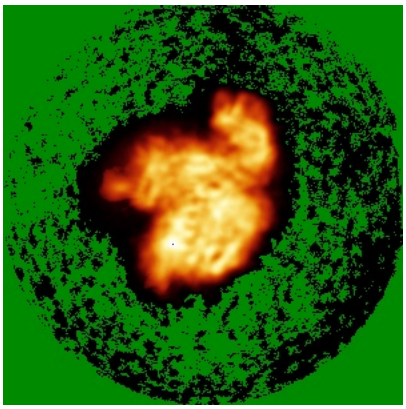
The images above show the largest variance slices of the map in three orthogonal directions.

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

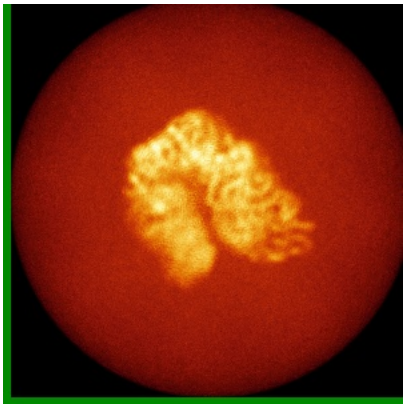
6.4.1 Primary map

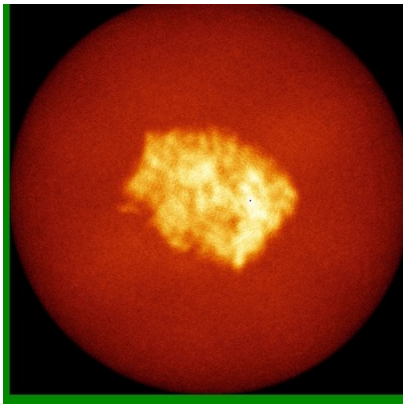

X

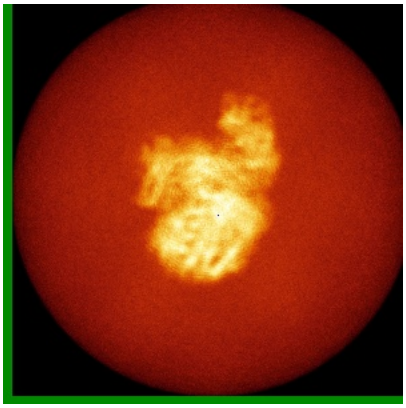

Y


Z

6.4.2 Raw 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.

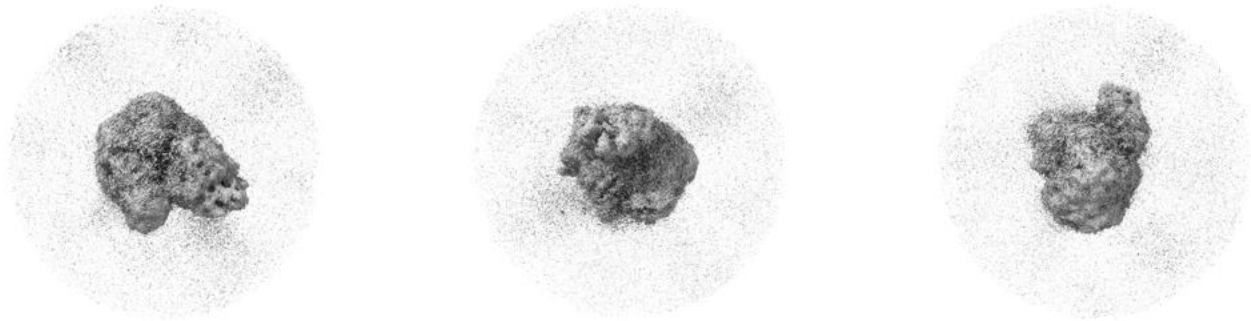
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.00167. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

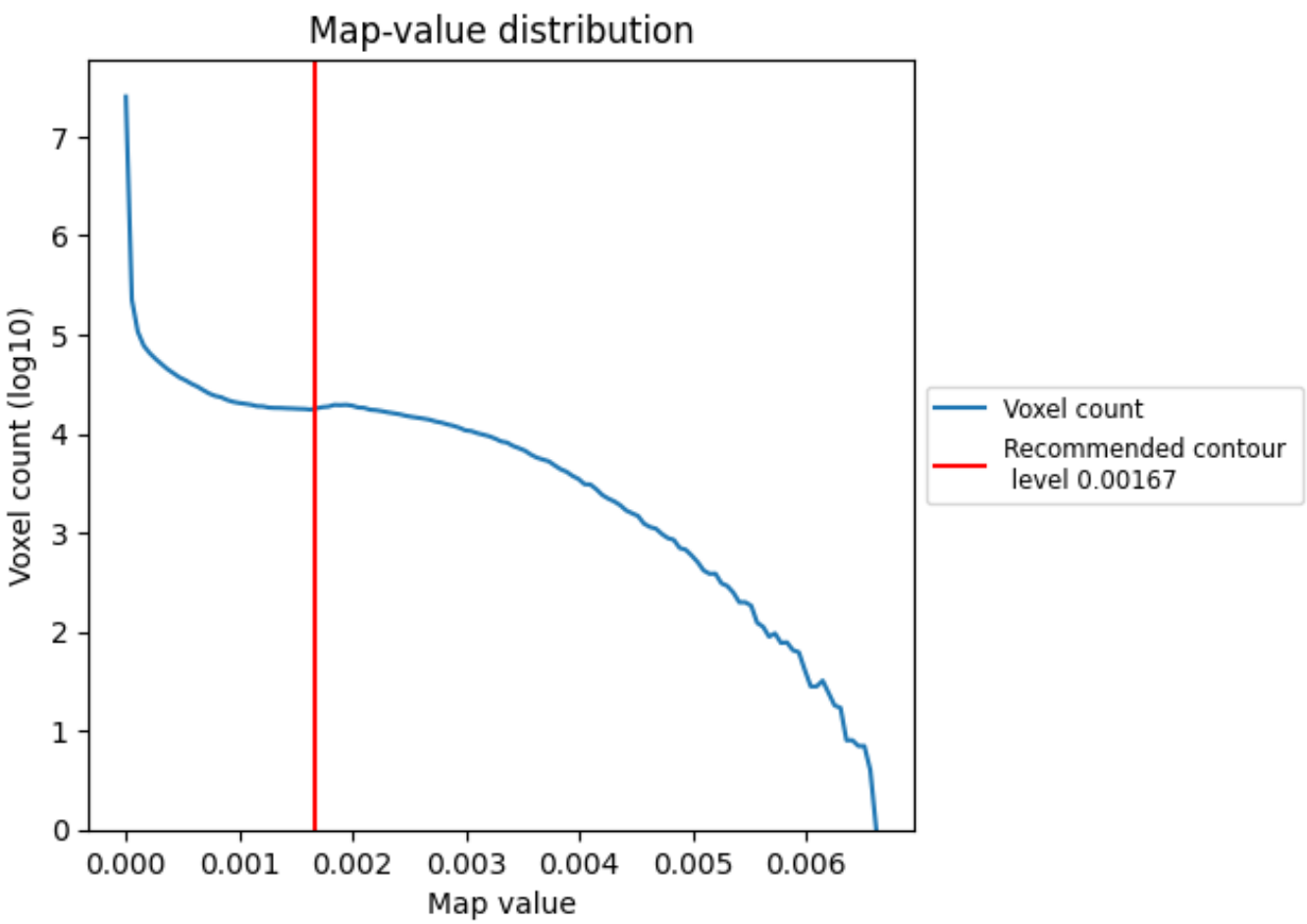
6.6 Mask visualisation (i)

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

7 Map analysis (i)

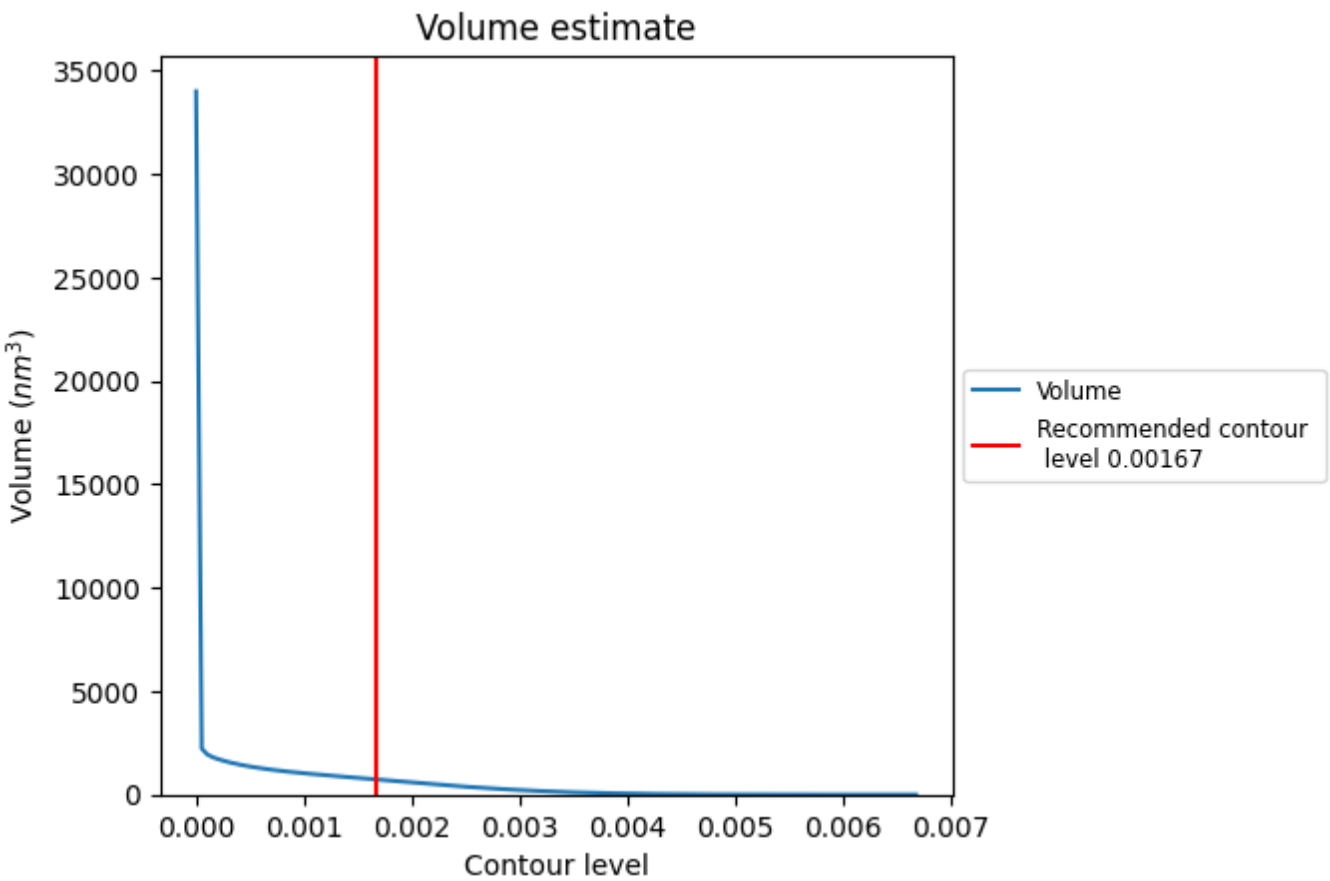
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

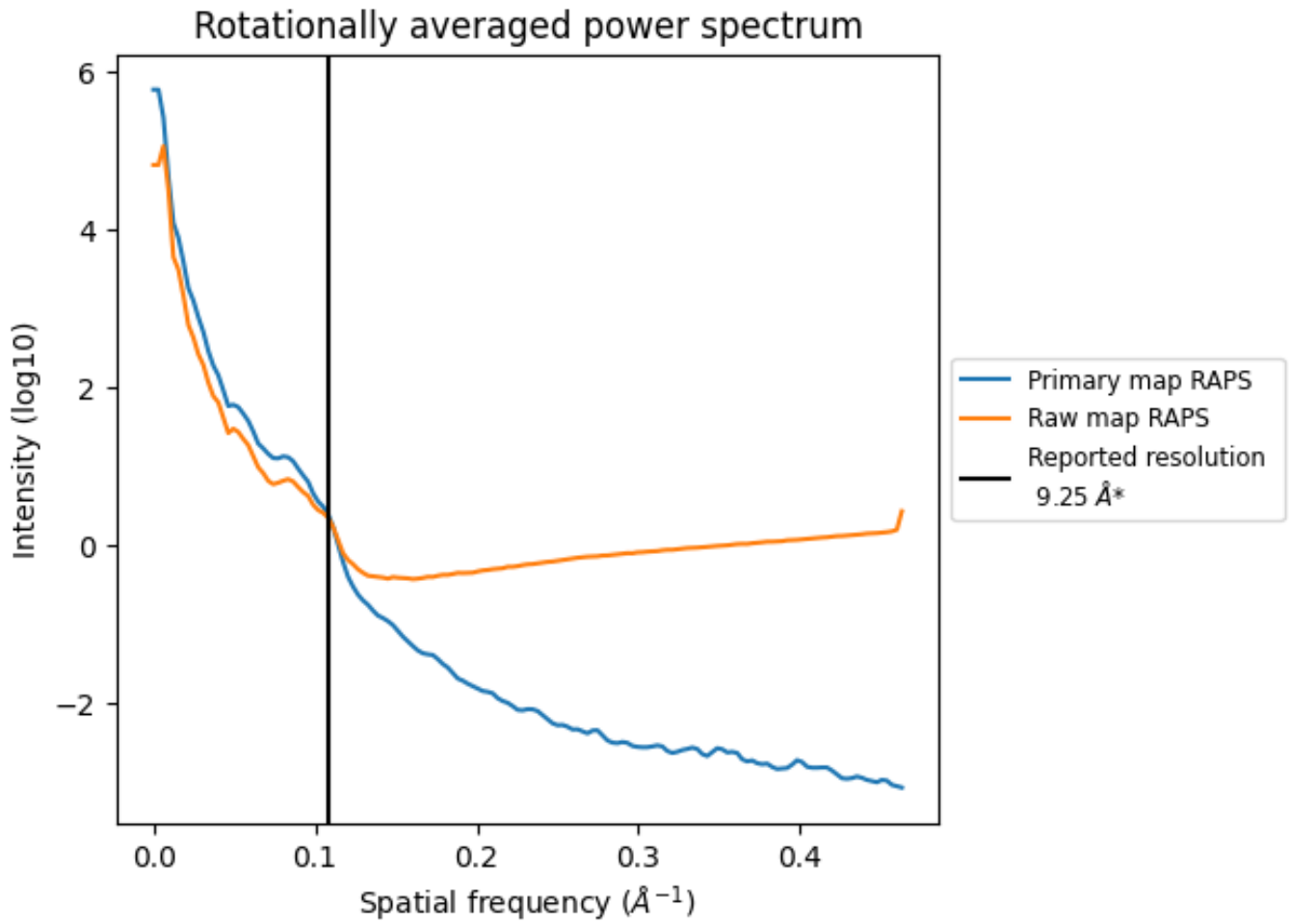
7.2 Volume estimate (i)



The volume at the recommended contour level is 733 nm^3; this corresponds to an approximate mass of 662 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)

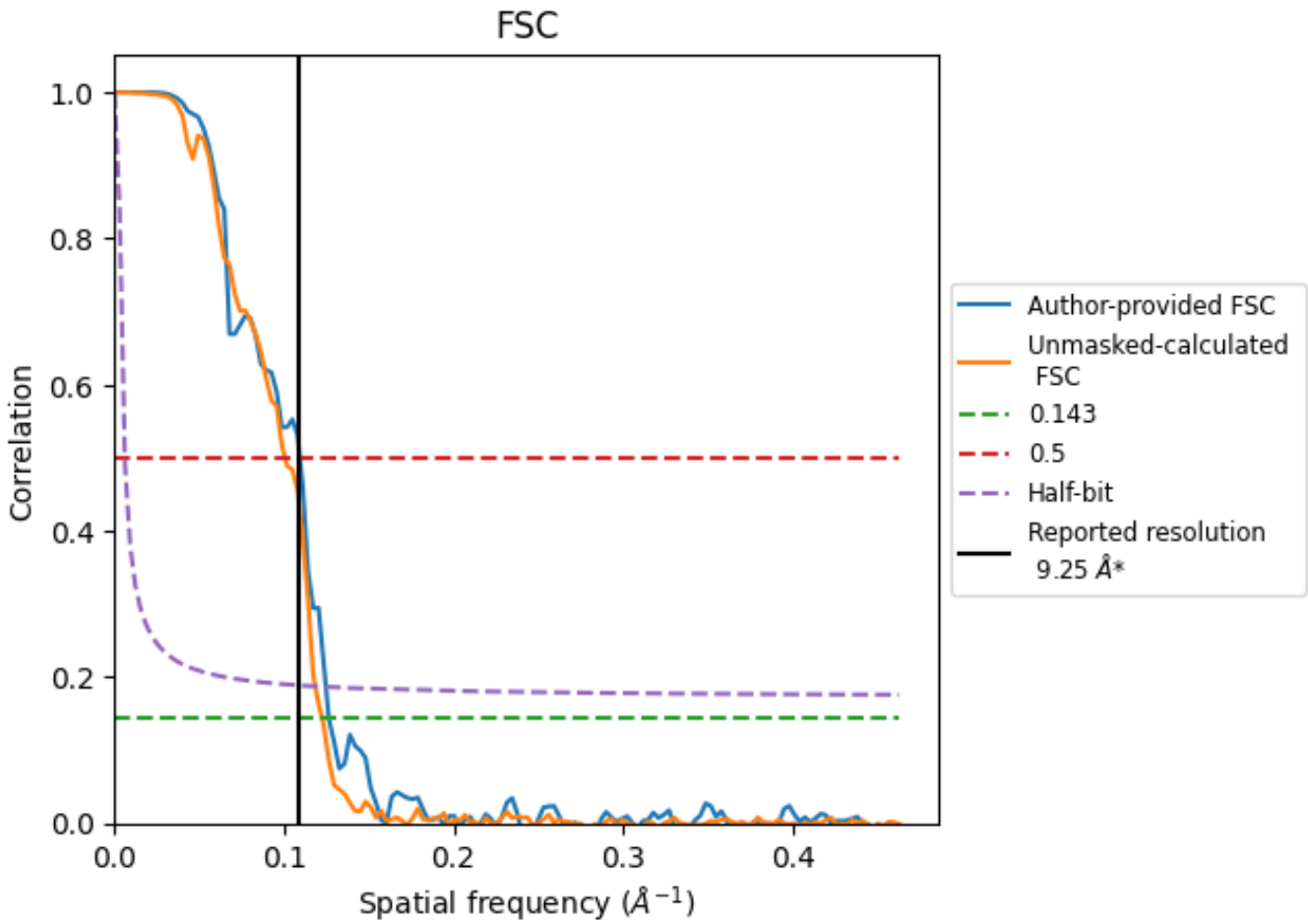


*Reported resolution corresponds to spatial frequency of 0.108 Å^{-1}

8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.108 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	9.25	-	-
Author-provided FSC curve	7.91	9.14	8.02
Unmasked-calculated*	8.17	9.94	8.45

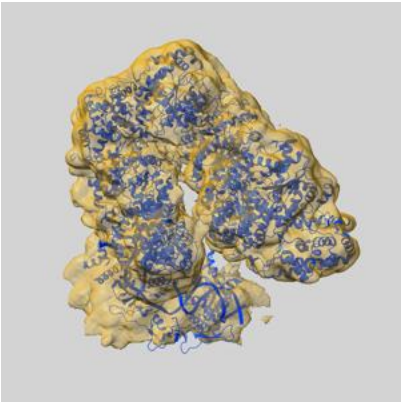
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 7.91 differs from the reported value 9.25 by more than 10 %

The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 8.17 differs from the reported value 9.25 by more than 10 %

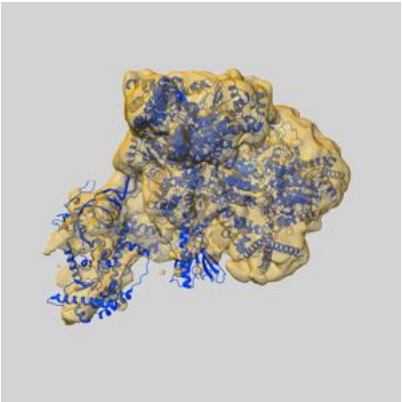
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22588 and PDB model 7K04. Per-residue inclusion information can be found in section 3 on page 7.

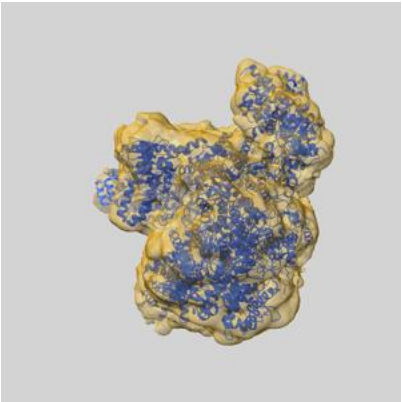
9.1 Map-model overlay (i)



X



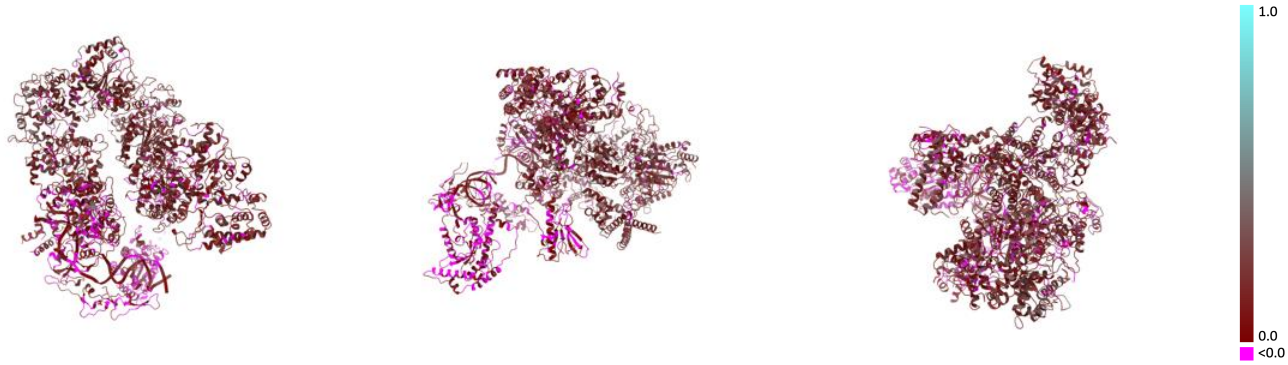
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.00167 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.

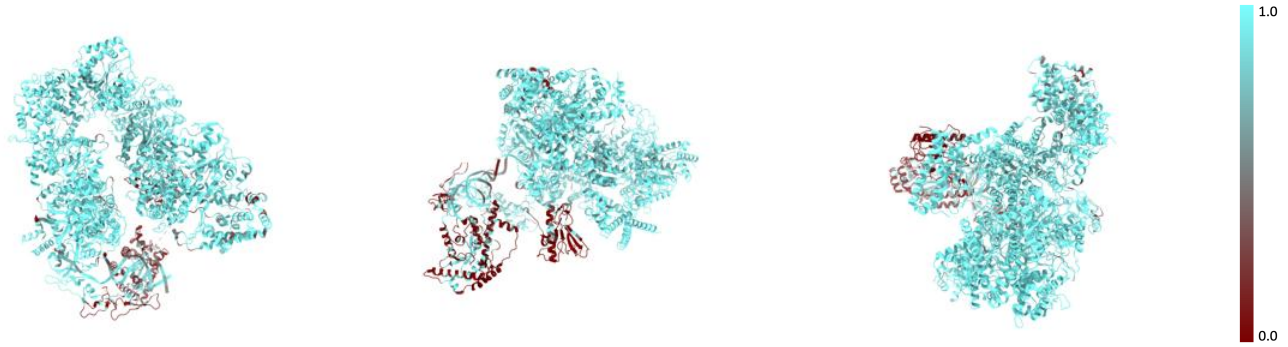
9.2 Q-score mapped to coordinate model (i)



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.

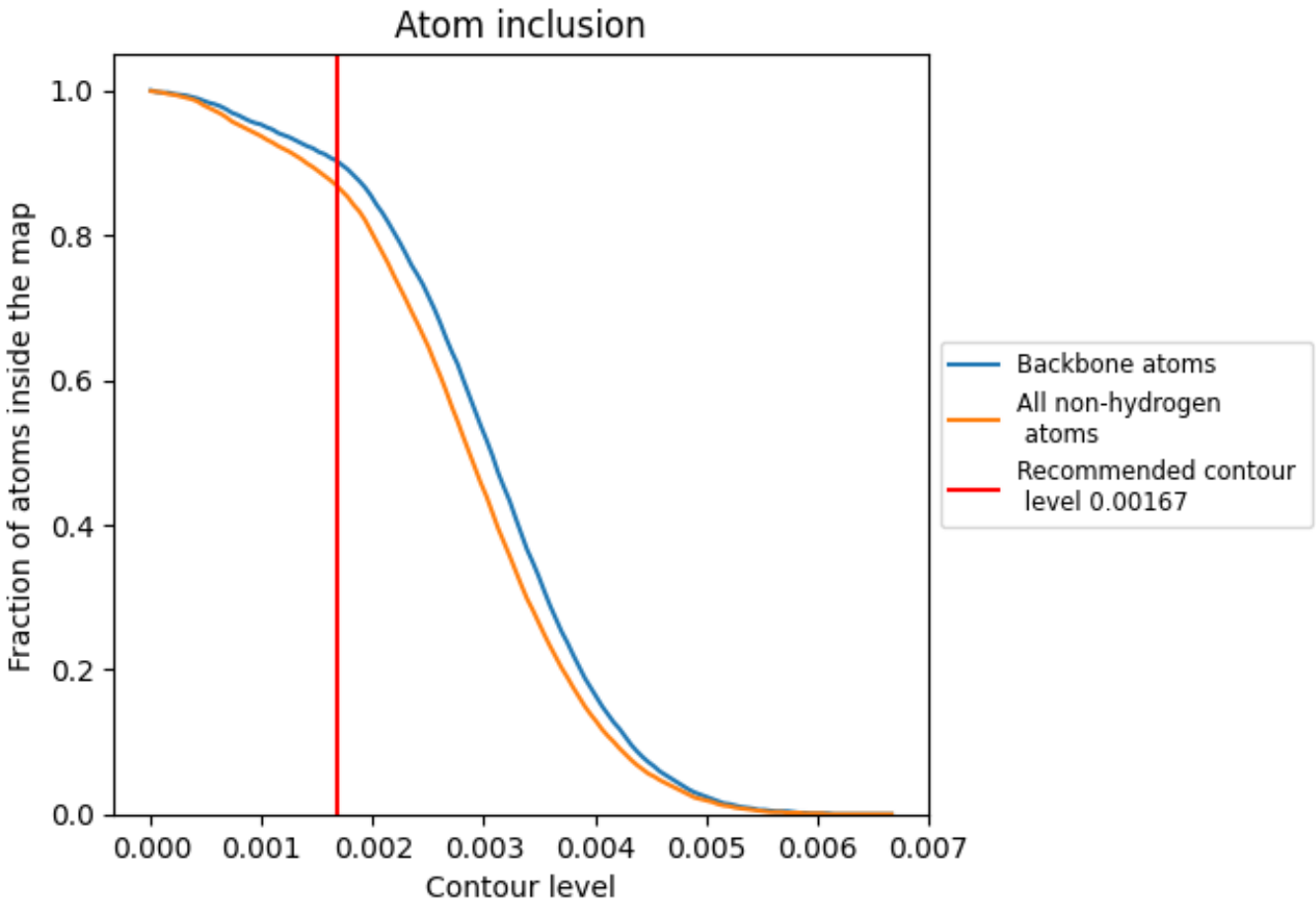
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.00167).

9.4 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.00167) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8690	0.1220
0	0.9280	0.1490
1	0.7370	0.1430
2	0.9660	0.1740
4	0.9600	0.1740
5	0.9920	0.1370
6	0.9270	0.1710
7	0.9660	0.1010
A	0.4730	0.0230
E	0.8670	0.0600
W	0.7990	0.0730
Y	0.6950	0.0460