wwPDB EM Validation Summary Report (i)

Aug 24, 2026 – 08:24 pm BST

PDB ID	:	9Q9M / pdb_00009q9m
EMDB ID	:	EMD-52964
Title	:	Cryo-EM structure of human Mre11-Rad50-Nbs1 (MRN) complex bound to DNA and telomeric factor TRF2
Authors	:	Cui, H.J.; Lammens, K.; Hopfner, K.P.; Fan, Y.L.; Kuybu, F.
Deposited on	:	2025-02-26
Resolution	:	2.81 Å(reported)
Based on initial model	:	.

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:

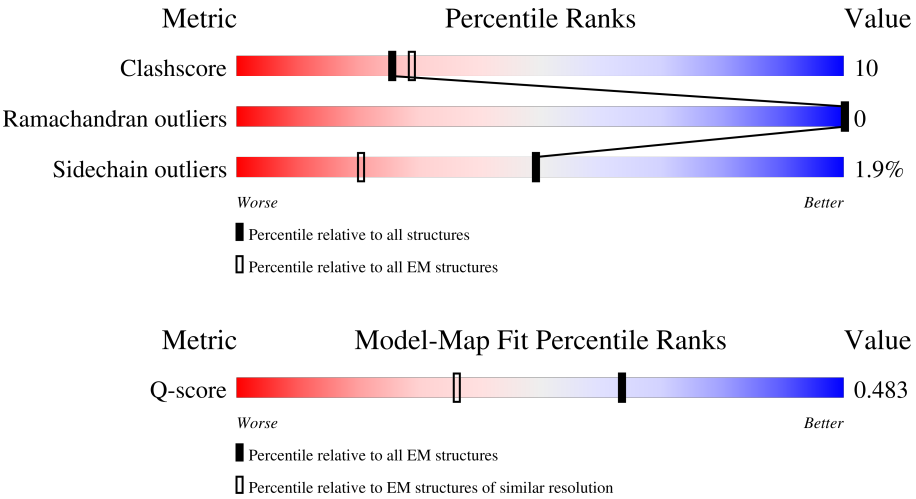
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.81 Å.

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



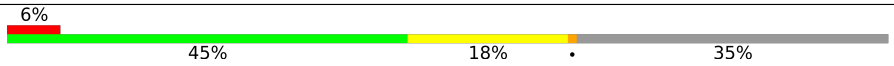
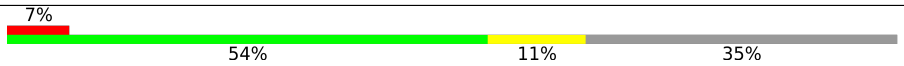
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11740 (2.31 - 3.31)

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	J	559	97%
2	P	64	6%, 31%, 9%, 59%
3	T	64	27%, 14%, 59%
4	F	754	5%, 8%, 89%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	A	1312	
5	B	1312	
6	D	738	
6	E	738	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17361 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 Telomeric repeat-binding factor 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	J	18	154	97	22	35	0	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	-4	GLY	-	expression tag	UNP Q15554
J	-3	PRO	-	expression tag	UNP Q15554
J	-2	ALA	-	expression tag	UNP Q15554
J	-1	SER	-	expression tag	UNP Q15554
J	0	GLY	-	expression tag	UNP Q15554
J	?	-	ALA	deletion	UNP Q15554
J	542	SER	-	expression tag	UNP Q15554
J	543	LEU	-	expression tag	UNP Q15554
J	544	GLU	-	expression tag	UNP Q15554
J	545	HIS	-	expression tag	UNP Q15554
J	546	HIS	-	expression tag	UNP Q15554
J	547	HIS	-	expression tag	UNP Q15554
J	548	HIS	-	expression tag	UNP Q15554
J	549	HIS	-	expression tag	UNP Q15554
J	550	HIS	-	expression tag	UNP Q15554
J	551	HIS	-	expression tag	UNP Q15554
J	552	HIS	-	expression tag	UNP Q15554
J	553	HIS	-	expression tag	UNP Q15554
J	554	HIS	-	expression tag	UNP Q15554

- Molecule 2 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	P	26	520	260	52	182	26	0	0

- Molecule 3 is a DNA chain called DNA (64-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	T	26	Total	C	N	O	P	0	0
			546	260	130	130	26		

- Molecule 4 is a protein called Nibrin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	82	Total	C	N	O	S	0	0
			681	440	120	120	1		

- Molecule 5 is a protein called DNA repair protein RAD50.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	A	465	Total	C	N	O	S	0	0
			3760	2360	658	718	24		
5	B	470	Total	C	N	O	S	1	0
			3811	2394	669	724	24		

- Molecule 6 is a protein called Double-strand break repair protein MRE11.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	478	Total	C	N	O	S	0	0
			3898	2477	679	726	16		
6	E	480	Total	C	N	O	S	0	0
			3917	2489	685	727	16		

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	709	SER	-	expression tag	UNP P49959
D	710	GLY	-	expression tag	UNP P49959
D	711	GLY	-	expression tag	UNP P49959
D	712	SER	-	expression tag	UNP P49959
D	713	LEU	-	expression tag	UNP P49959
D	714	GLU	-	expression tag	UNP P49959
D	715	VAL	-	expression tag	UNP P49959
D	716	LEU	-	expression tag	UNP P49959
D	717	PHE	-	expression tag	UNP P49959
D	718	GLN	-	expression tag	UNP P49959
D	719	GLY	-	expression tag	UNP P49959
D	720	PRO	-	expression tag	UNP P49959
D	721	ASP	-	expression tag	UNP P49959
D	722	TYR	-	expression tag	UNP P49959
D	723	LYS	-	expression tag	UNP P49959

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	724	ASP	-	expression tag	UNP P49959
D	725	ASP	-	expression tag	UNP P49959
D	726	ASP	-	expression tag	UNP P49959
D	727	ASP	-	expression tag	UNP P49959
D	728	LYS	-	expression tag	UNP P49959
D	729	GLY	-	expression tag	UNP P49959
D	730	THR	-	expression tag	UNP P49959
D	731	ASP	-	expression tag	UNP P49959
D	732	TYR	-	expression tag	UNP P49959
D	733	LYS	-	expression tag	UNP P49959
D	734	ASP	-	expression tag	UNP P49959
D	735	ASP	-	expression tag	UNP P49959
D	736	ASP	-	expression tag	UNP P49959
D	737	ASP	-	expression tag	UNP P49959
D	738	LYS	-	expression tag	UNP P49959
E	709	SER	-	expression tag	UNP P49959
E	710	GLY	-	expression tag	UNP P49959
E	711	GLY	-	expression tag	UNP P49959
E	712	SER	-	expression tag	UNP P49959
E	713	LEU	-	expression tag	UNP P49959
E	714	GLU	-	expression tag	UNP P49959
E	715	VAL	-	expression tag	UNP P49959
E	716	LEU	-	expression tag	UNP P49959
E	717	PHE	-	expression tag	UNP P49959
E	718	GLN	-	expression tag	UNP P49959
E	719	GLY	-	expression tag	UNP P49959
E	720	PRO	-	expression tag	UNP P49959
E	721	ASP	-	expression tag	UNP P49959
E	722	TYR	-	expression tag	UNP P49959
E	723	LYS	-	expression tag	UNP P49959
E	724	ASP	-	expression tag	UNP P49959
E	725	ASP	-	expression tag	UNP P49959
E	726	ASP	-	expression tag	UNP P49959
E	727	ASP	-	expression tag	UNP P49959
E	728	LYS	-	expression tag	UNP P49959
E	729	GLY	-	expression tag	UNP P49959
E	730	THR	-	expression tag	UNP P49959
E	731	ASP	-	expression tag	UNP P49959
E	732	TYR	-	expression tag	UNP P49959
E	733	LYS	-	expression tag	UNP P49959
E	734	ASP	-	expression tag	UNP P49959
E	735	ASP	-	expression tag	UNP P49959

Continued on next page...

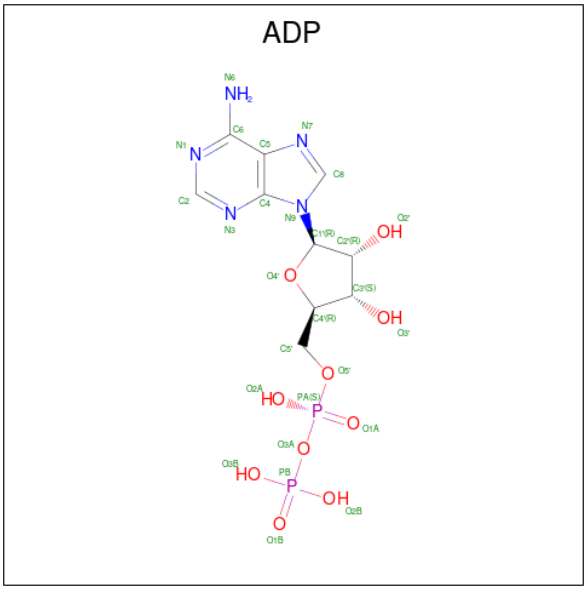
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	736	ASP	-	expression tag	UNP P49959
E	737	ASP	-	expression tag	UNP P49959
E	738	LYS	-	expression tag	UNP P49959

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

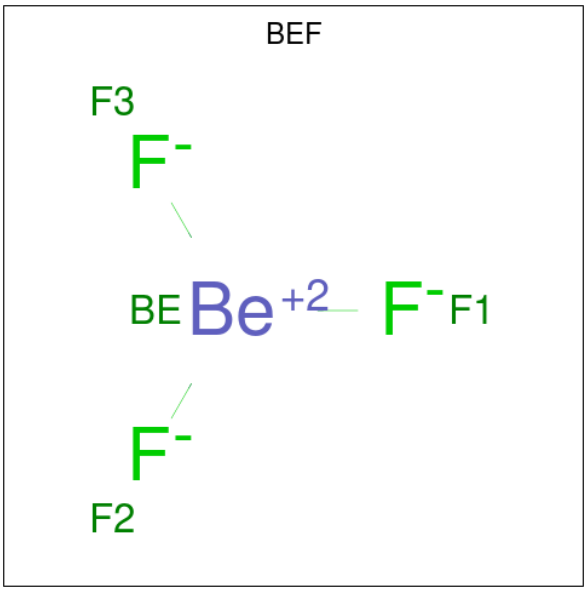
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 9 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
9	A	1	Total Be F 4 1 3	0
9	A	1	Total Be F 4 1 3	0

- Molecule 10 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	D	2	Total Mn 2 2	0
10	E	2	Total Mn 2 2	0

- Molecule 11 is water.

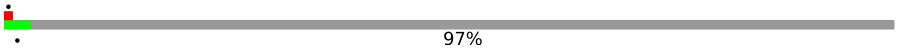
Mol	Chain	Residues	Atoms	AltConf
11	A	2	Total O 2 2	0
11	B	2	Total O 2 2	0
11	D	1	Total O 1 1	0
11	E	1	Total O 1 1	0

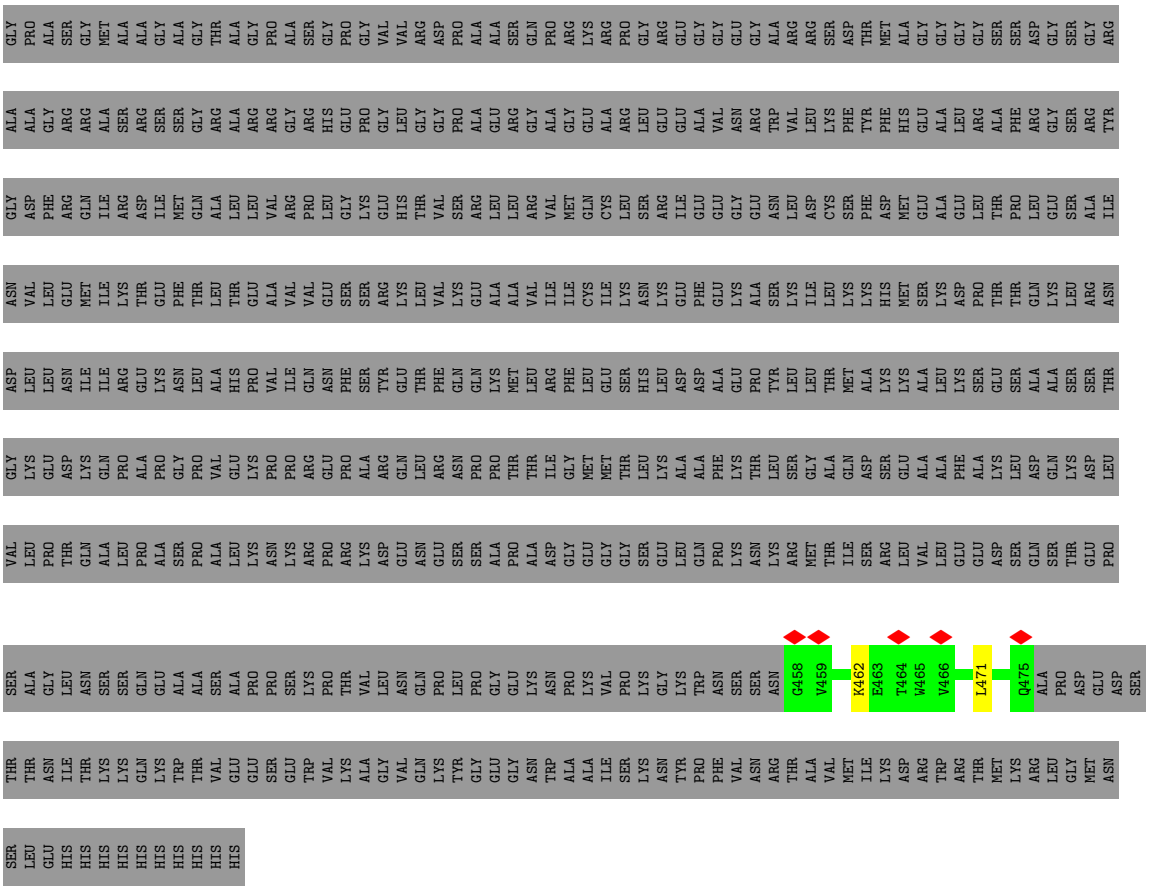
3 Residue-property plots (i)

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: Telomeric repeat-binding factor 2

Chain J:

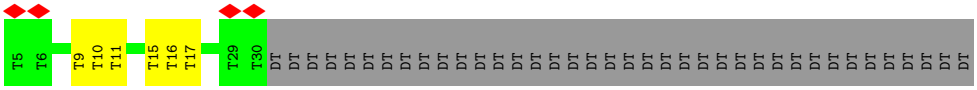




• Molecule 2: DNA (64-MER)

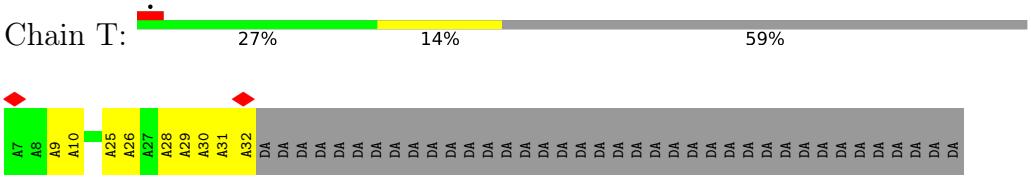
Chain P:

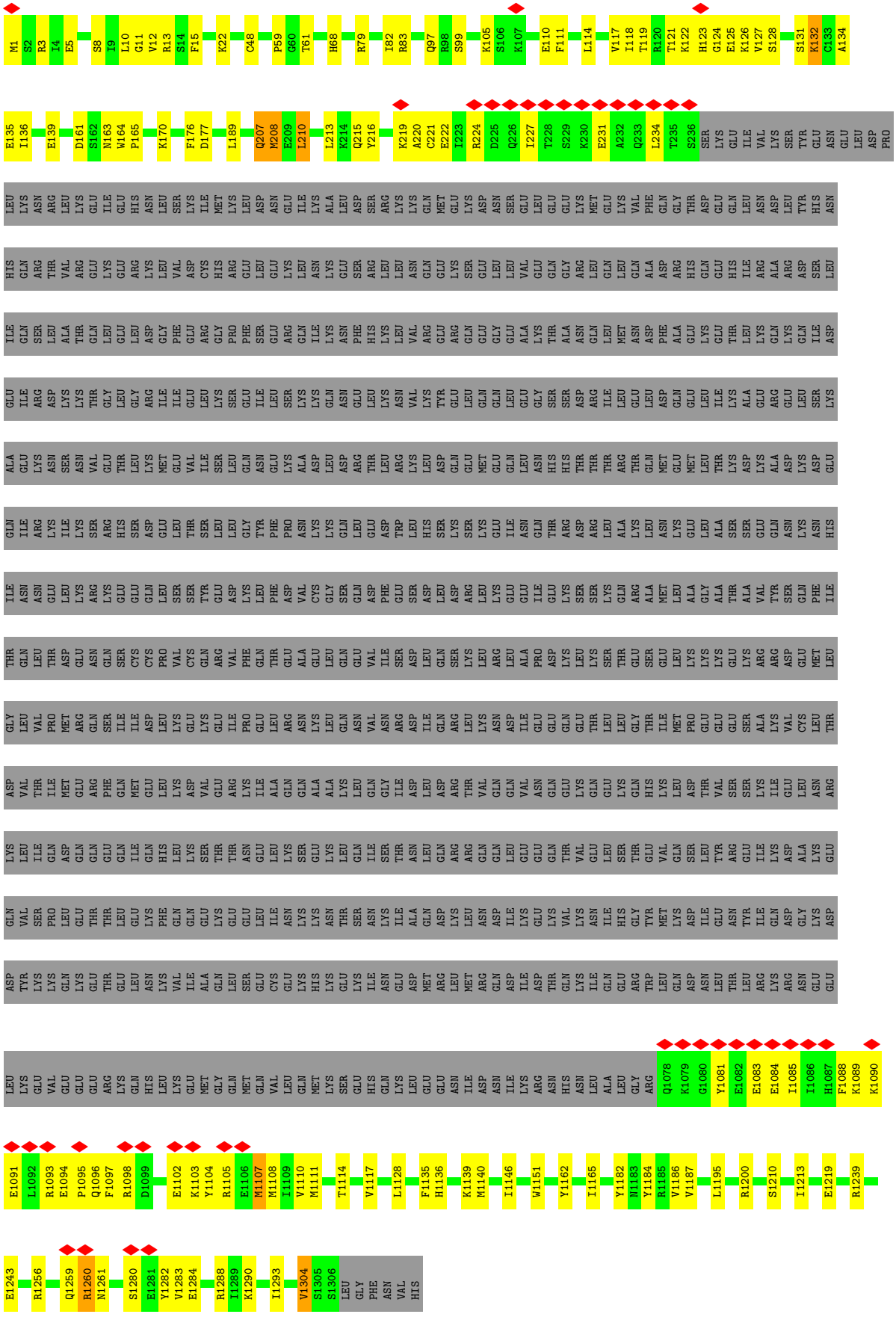




• Molecule 3: DNA (64-MER)

Chain T:

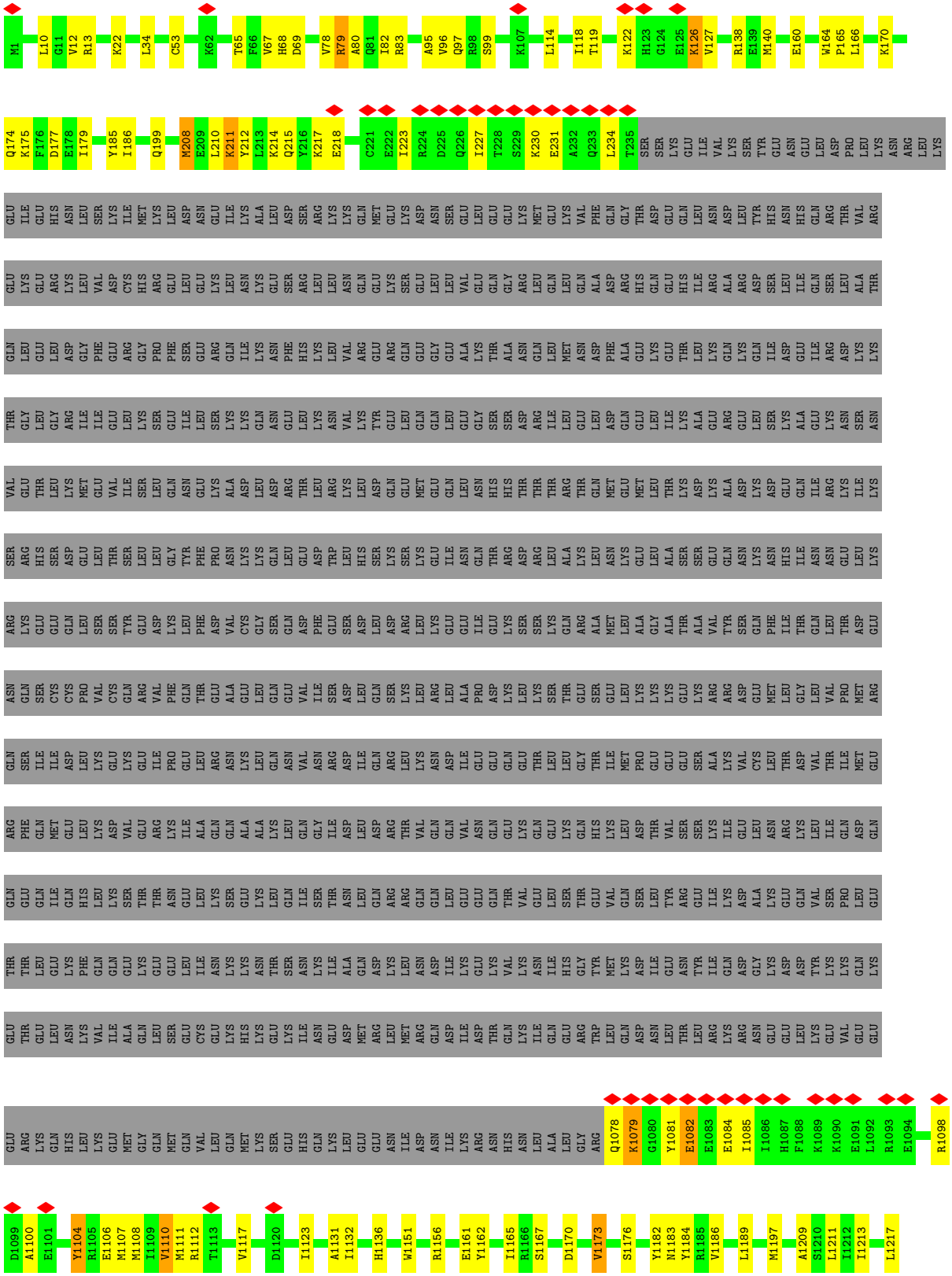

27%
14%
59%
A7 A8 A9 A10 A25 A26 A27 A28 A29 A30 A31 A32 DA DA DA

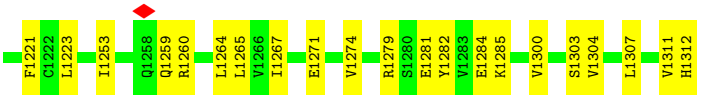


• Molecule 5: DNA repair protein RAD50

Chain B:

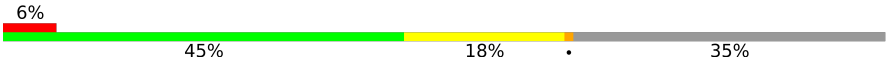


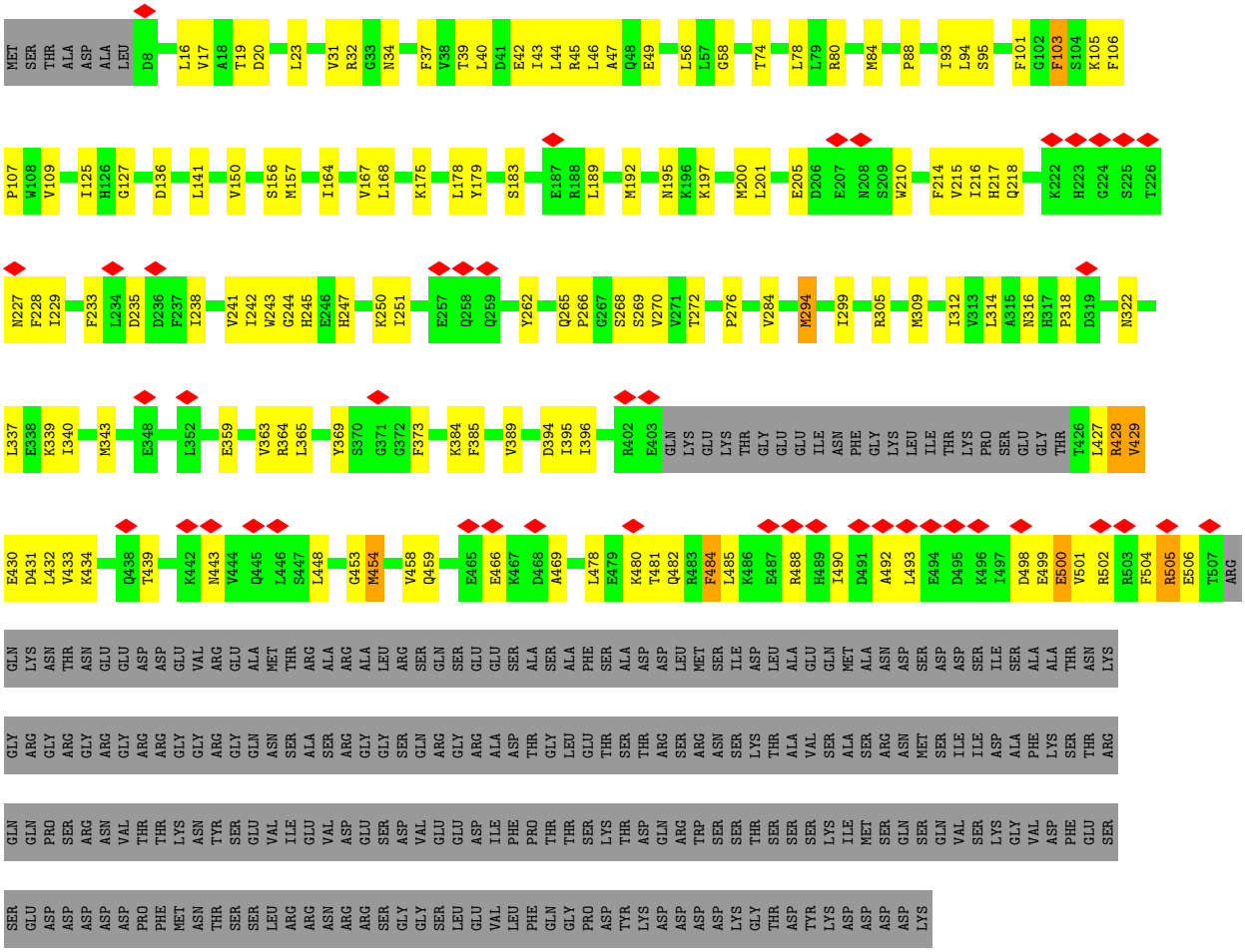




• Molecule 6: Double-strand break repair protein MRE11

Chain D:

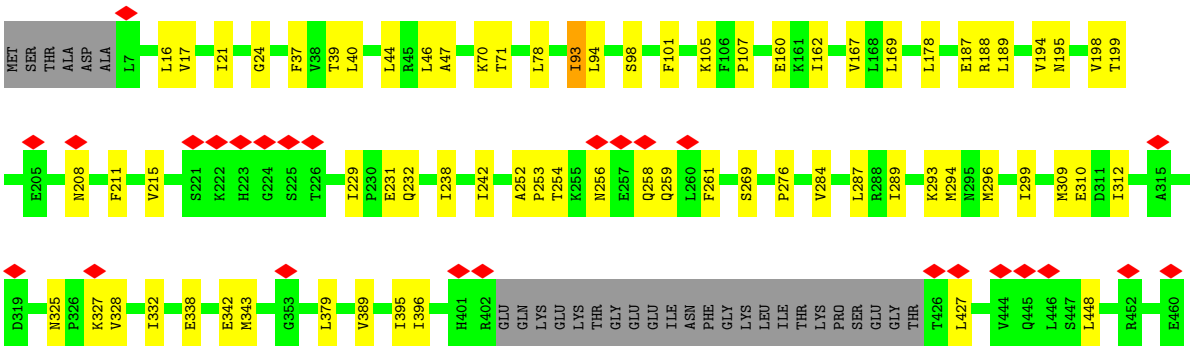


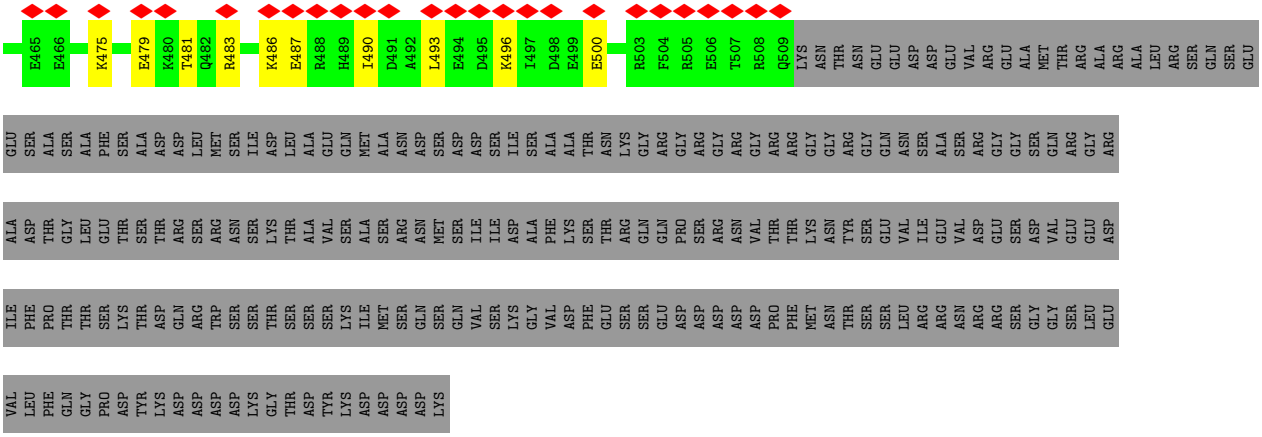


• Molecule 6: Double-strand break repair protein MRE11

Chain E:






E465 E466 K475 E479 K480 T481 Q482 R483 K486 E487 R488 H489 I490 D491 A492 L493 E494 D495 K496 I497 D498 E499 E500 R503 F504 R505 E506 T507 R508 Q509
LYS ASN THR ASN GLU GLU ASP ASP GLU VAL ARG GLU ALA MET THR ARG ALA ARG ALA LEU ARG SER GLN SER GLU
GLU SER ALA SER ALA PHE SER ALA ASP ASP LEU MET SER ILE ASP LEU ALA GLU GLN MET ALA ASN ASP SER ASP ASP SER ILE SER ALA ALA THR ASN LYS GLY ARG GLY ARG GLY ARG GLY ARG ARG GLY GLY ARG GLY GLN ASN SER ALA SER ARG GLY GLY SER GLN ARG GLY ARG
ALA ASP THR GLY LEU GLU THR SER THR ARG SER ARG ASN SER LYS THR ALA VAL SER ALA SER ARG ASN MET SER ILE ILE ASP ALA PHE LYS SER THR ARG GLN GLN PRO SER ARG ASN VAL THR THR LYS ASN TYR SER GLU VAL ILE GLU VAL ASP GLU SER ASP VAL GLU GLU ASP
ILE PHE PRO THR THR SER LYS THR ASP GLN ARG TRP SER SER THR SER SER SER LYS ILE MET SER GLN SER GLN VAL SER LYS GLY VAL ASP PHE GLU SER SER GLU ASP ASP ASP ASP ASP PRO PHE MET ASN THR SER SER LEU ARG ARG ASN ARG ARG ARG SER GLY GLY SER LEU GLU
VAL LEU PHE GLN GLY PRO ASP TYR LYS ASP ASP ASP ASP LYS GLY THR ASP TYR LYS ASP ASP ASP ASP LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	208916	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	3.206	Depositor
Minimum map value	-1.595	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	261.72, 261.72, 261.72	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.727, 0.727, 0.727	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, MN, ADP, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	J	0.12	0/156	0.36	0/210
2	P	0.42	0/571	0.84	0/880
3	T	0.46	0/623	0.72	0/958
4	F	0.40	0/695	0.67	1/931 (0.1%)
5	A	0.46	1/3809 (0.0%)	0.71	3/5106 (0.1%)
5	B	0.43	1/3865 (0.0%)	0.65	7/5180 (0.1%)
6	D	0.42	5/3981 (0.1%)	0.62	8/5367 (0.1%)
6	E	0.25	1/4000 (0.0%)	0.40	0/5392
All	All	0.40	8/17700 (0.0%)	0.62	19/24024 (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
4	F	0	1
5	A	0	4
5	B	0	4
6	D	0	3
All	All	0	12

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	453	GLY	C-N	-6.88	1.24	1.34
5	A	208	MET	C-O	6.72	1.31	1.24
6	D	384	LYS	C-N	6.72	1.43	1.33
6	E	312	ILE	C-N	6.27	1.41	1.33
6	D	228	PHE	C-N	-6.00	1.28	1.33

The worst 5 of 19 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	429	VAL	N-CA-C	-6.83	104.12	113.00
5	A	207	GLN	O-C-N	-6.60	114.50	122.22
6	D	105	LYS	N-CA-C	-6.38	105.46	113.18
4	F	748	PRO	N-CA-C	-6.36	100.90	111.26
5	A	1090	LYS	N-CA-C	-5.88	106.64	113.88

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1256	ARG	Sidechain
5	A	1260	ARG	Sidechain
5	A	13	ARG	Sidechain
5	A	79	ARG	Sidechain
4	F	745	ARG	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	J	154	0	135	3	0
2	P	520	0	313	6	0
3	T	546	0	287	6	0
4	F	681	0	695	27	0
5	A	3760	0	3833	100	0
5	B	3811	0	3886	80	0
6	D	3898	0	3853	103	0
6	E	3917	0	3879	63	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	27	0	12	0	0
8	B	27	0	12	1	0
9	A	8	0	0	0	0
10	D	2	0	0	0	0
10	E	2	0	0	0	0
11	A	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	B	2	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
All	All	17361	0	16905	351	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 10.

The worst 5 of 351 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:234:LEU:HD23	5:B:1085:ILE:HD11	1.34	1.04
5:A:125:GLU:HG2	5:A:126:LYS:H	1.25	1.01
6:D:448:LEU:HD11	6:D:481:THR:HG21	1.41	0.99
6:D:484:PHE:HE1	6:D:488:ARG:HH11	0.98	0.97
5:B:234:LEU:HD23	5:B:1085:ILE:CD1	1.94	0.96

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	J	16/559 (3%)	16 (100%)	0	0	100	100
4	F	78/754 (10%)	76 (97%)	2 (3%)	0	100	100
5	A	461/1312 (35%)	438 (95%)	23 (5%)	0	100	100
5	B	467/1312 (36%)	455 (97%)	12 (3%)	0	100	100
6	D	474/738 (64%)	457 (96%)	17 (4%)	0	100	100
6	E	476/738 (64%)	464 (98%)	12 (2%)	0	100	100
All	All	1972/5413 (36%)	1906 (97%)	66 (3%)	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	J	17/460 (4%)	17 (100%)	0	100	100
4	F	73/682 (11%)	73 (100%)	0	100	100
5	A	421/1222 (34%)	414 (98%)	7 (2%)	53	81
5	B	426/1222 (35%)	416 (98%)	10 (2%)	44	76
6	D	435/659 (66%)	426 (98%)	9 (2%)	47	78
6	E	437/659 (66%)	429 (98%)	8 (2%)	51	80
All	All	1809/4904 (37%)	1775 (98%)	34 (2%)	49	79

5 of 34 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	E	199	THR
6	E	208	ASN
6	E	342	GLU
5	B	1123	ILE
5	B	1110	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 23 such sidechains are listed below:

Mol	Chain	Res	Type
6	D	459	GLN
6	E	219	ASN
6	E	65	ASN
6	E	256	ASN
5	A	215	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 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	$\#\|Z\| > 2$
8	ADP	A	1402	7,9	27,29,29	1.35	4 (14%)	42,45,45	1.94	11 (26%)
9	BEF	A	1404	8	0,3,3	-	-	-		
9	BEF	A	1403	8	0,3,3	-	-	-		
8	ADP	B	1402	7,9	27,29,29	1.34	4 (14%)	42,45,45	1.92	11 (26%)

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
8	ADP	A	1402	7,9	-	4/16/32/32	0/3/3/3
8	ADP	B	1402	7,9	-	3/16/32/32	0/3/3/3

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1402	ADP	C5-C4	4.37	1.47	1.39
8	B	1402	ADP	C5-C4	4.32	1.47	1.39
8	A	1402	ADP	C5-C6	2.59	1.48	1.41
8	B	1402	ADP	C5-C6	2.54	1.48	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	1402	ADP	C5-N7	-2.34	1.34	1.39

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	B	1402	ADP	C5-C4-N3	-6.08	118.82	126.75
8	A	1402	ADP	C5-C4-N3	-6.07	118.83	126.75
8	A	1402	ADP	N3-C4-N9	4.99	135.30	127.08
8	B	1402	ADP	N3-C4-N9	4.95	135.25	127.08
8	A	1402	ADP	C2-N3-C4	3.81	120.75	111.75

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1402	ADP	C5'-O5'-PA-O3A
8	B	1402	ADP	C5'-O5'-PA-O3A
8	A	1402	ADP	O4'-C4'-C5'-O5'
8	A	1402	ADP	C3'-C4'-C5'-O5'
8	A	1402	ADP	C5'-O5'-PA-O1A

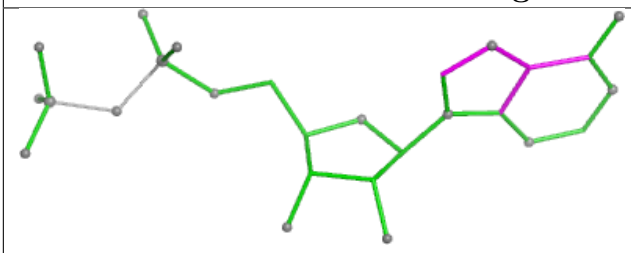
There are no ring outliers.

1 monomer is involved in 1 short contact:

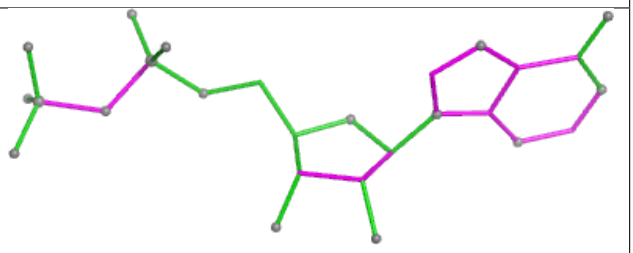
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1402	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

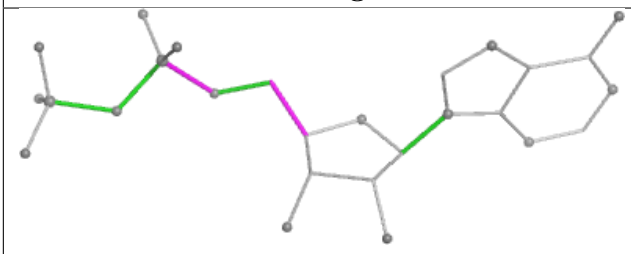
Ligand ADP A 1402



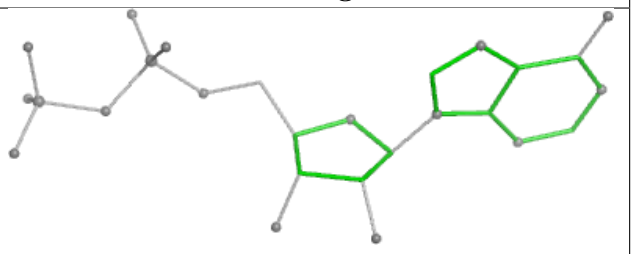
Bond lengths



Bond angles

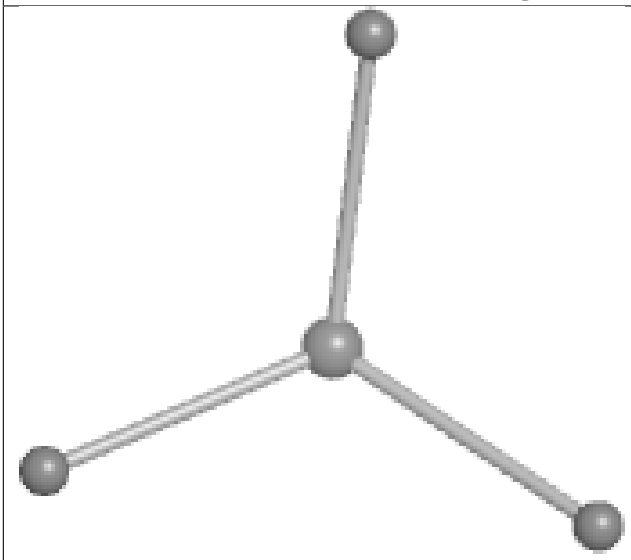


Torsions

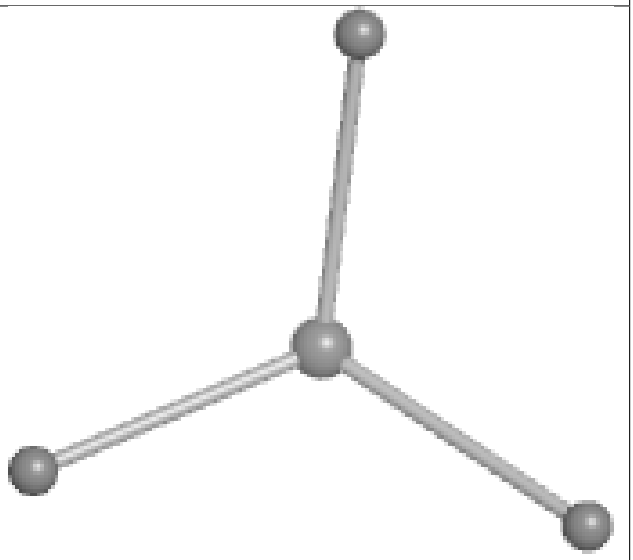


Rings

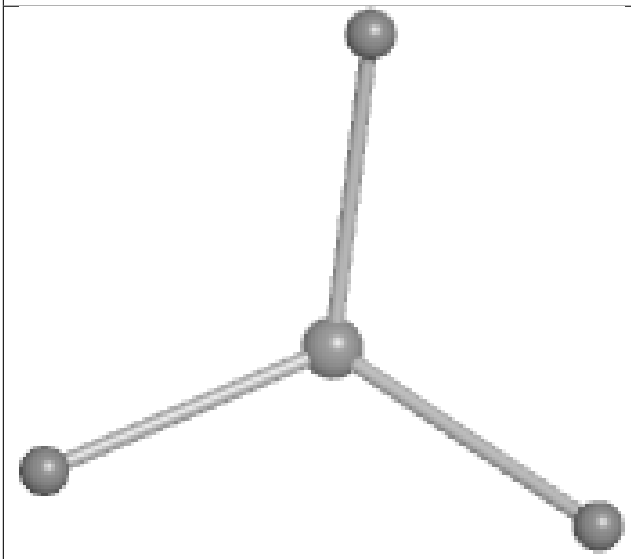
Ligand BEF A 1404



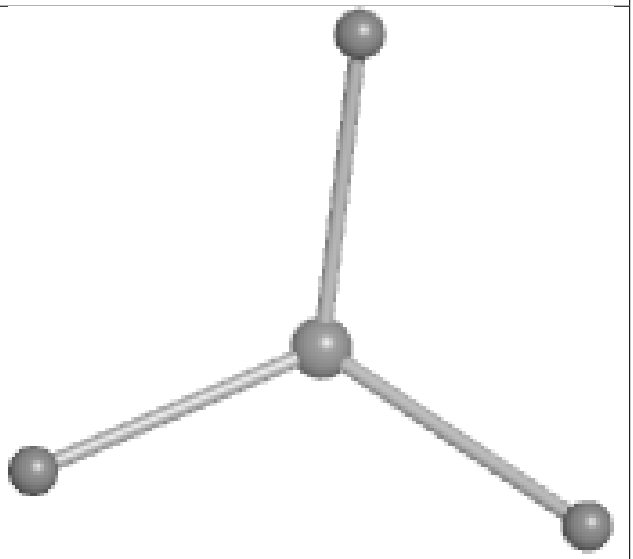
Bond lengths



Bond angles

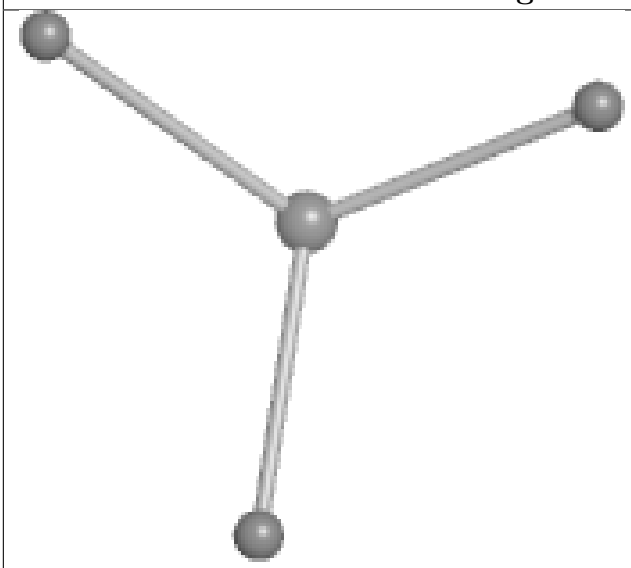


Torsions

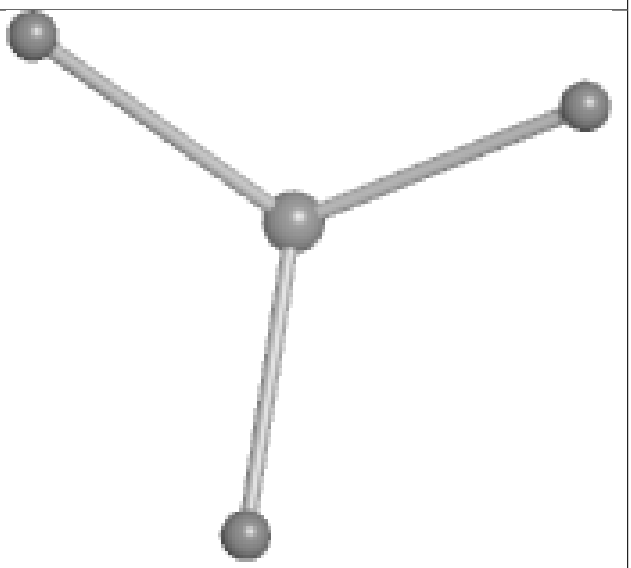


Rings

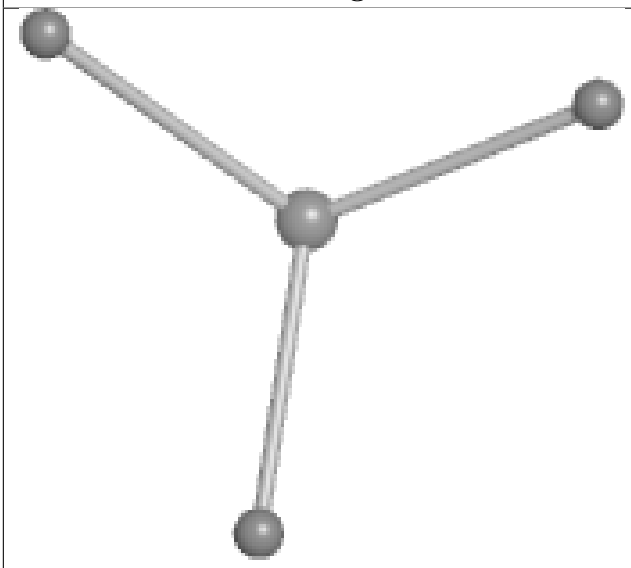
Ligand BEF A 1403



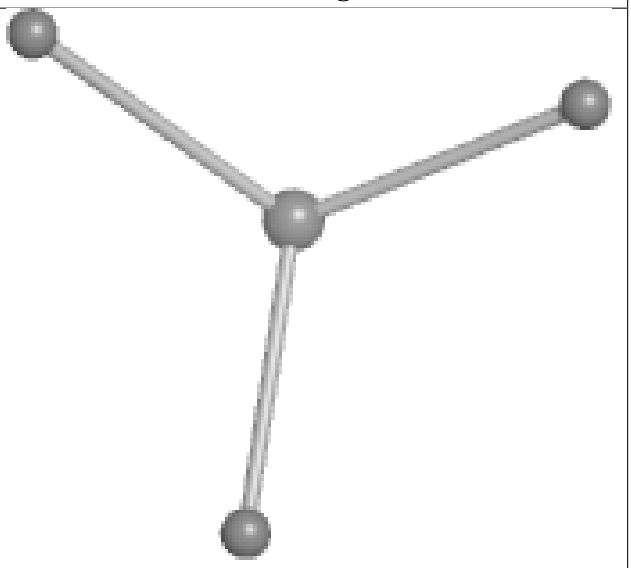
Bond lengths



Bond angles

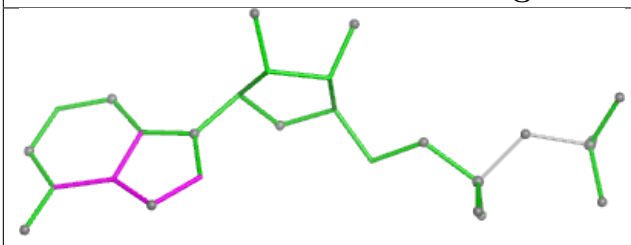


Torsions

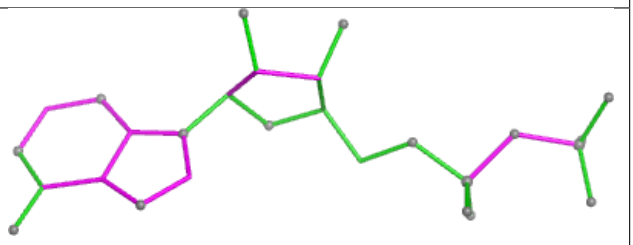


Rings

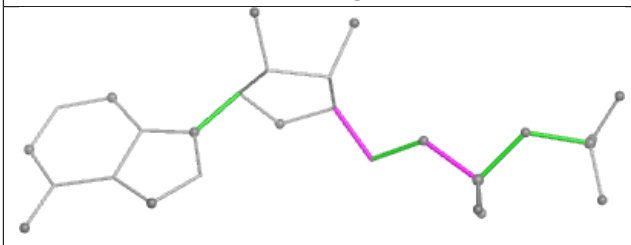
Ligand ADP B 1402



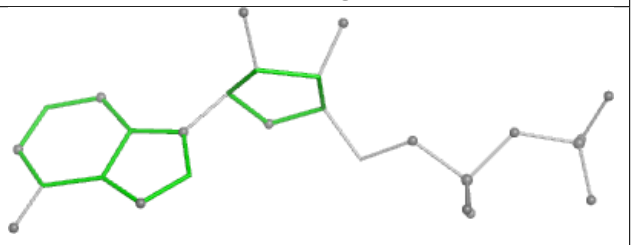
Bond lengths



Bond angles



Torsions



Rings

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.

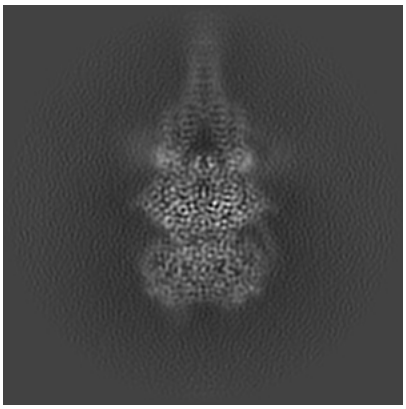
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52964. These allow visual inspection of the internal detail of the map and identification of artifacts.

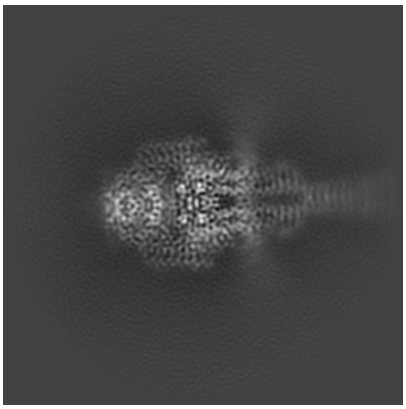
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

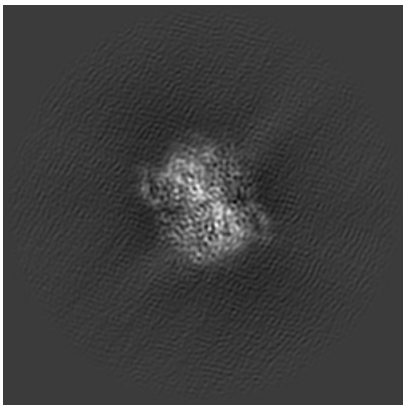
6.1.1 Primary map



X

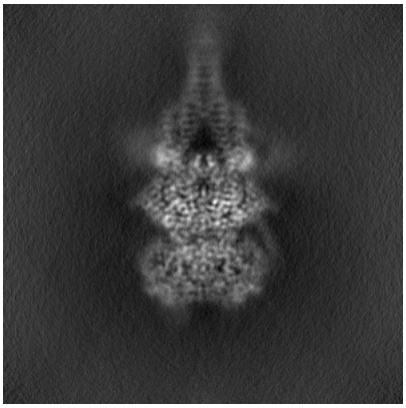


Y

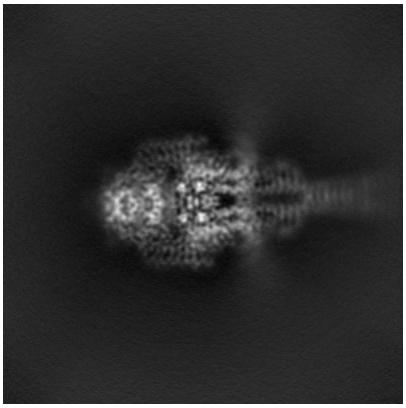


Z

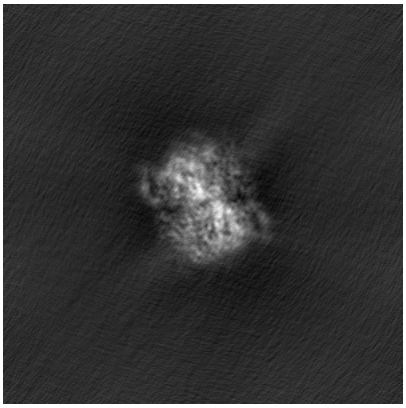
6.1.2 Raw map



X



Y



Z

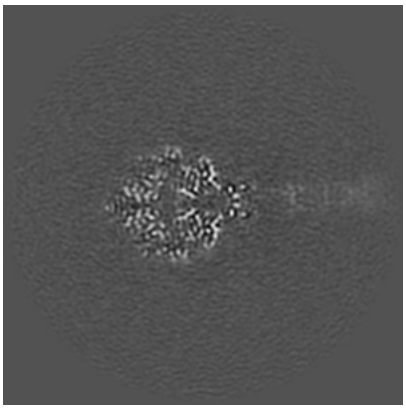
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

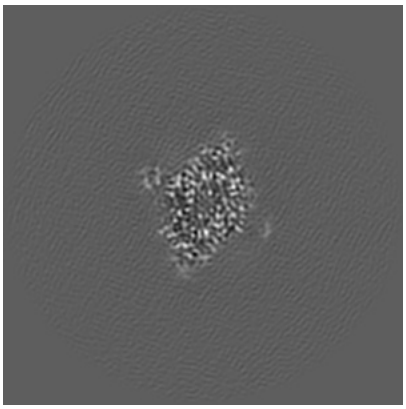
6.2.1 Primary map



X Index: 180

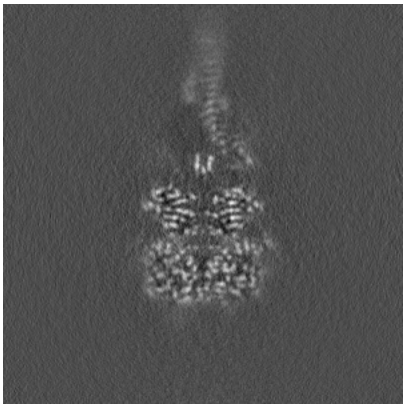


Y Index: 180

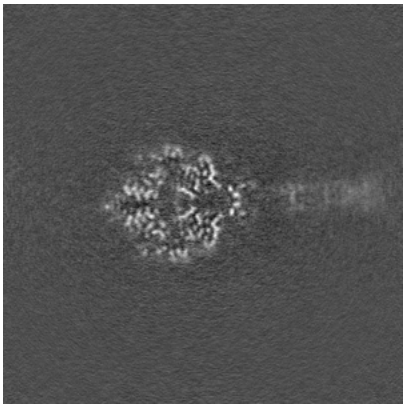


Z Index: 180

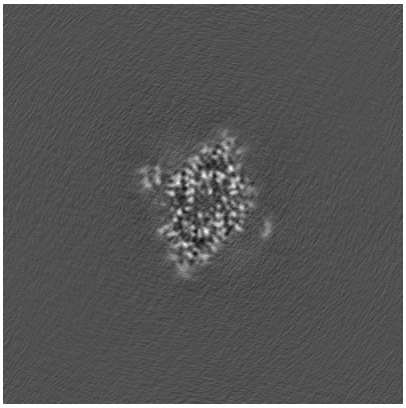
6.2.2 Raw map



X Index: 180



Y Index: 180

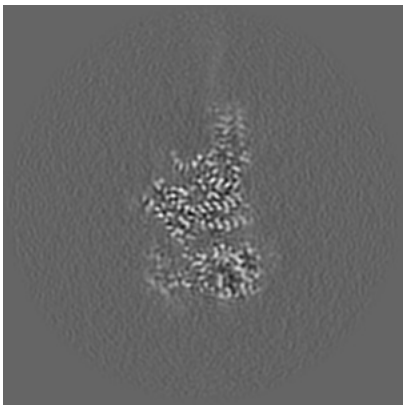


Z Index: 180

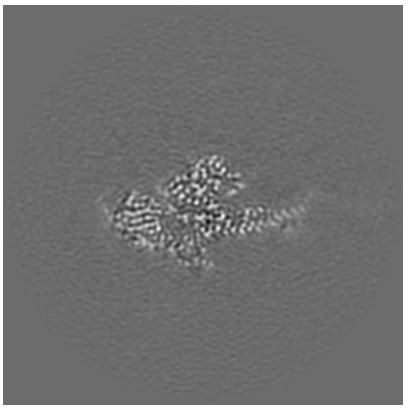
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

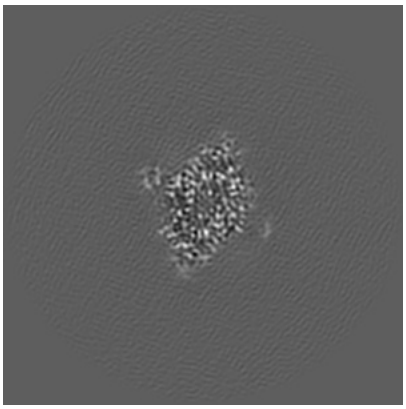
6.3.1 Primary map



X Index: 169

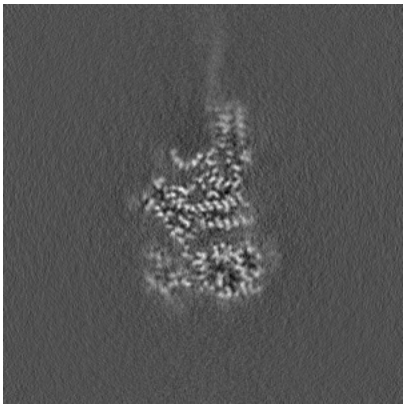


Y Index: 201

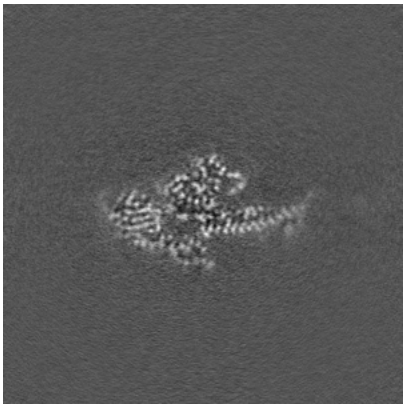


Z Index: 180

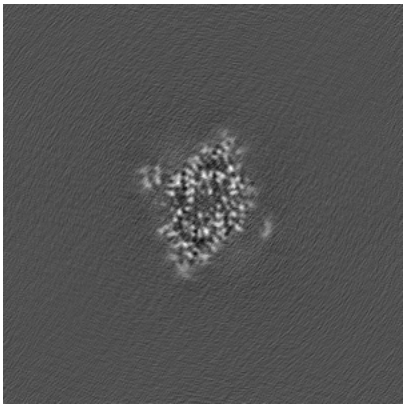
6.3.2 Raw map



X Index: 169



Y Index: 202

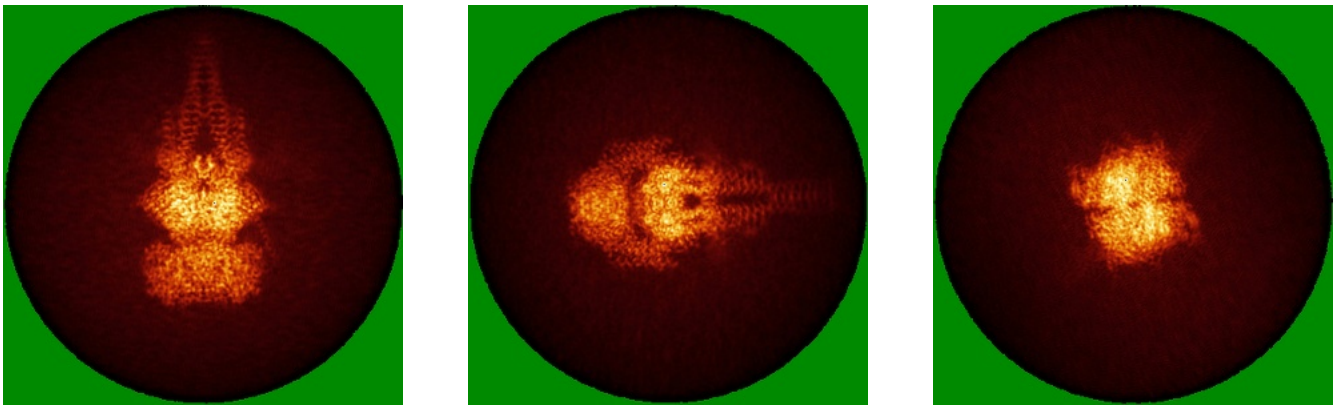


Z Index: 180

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

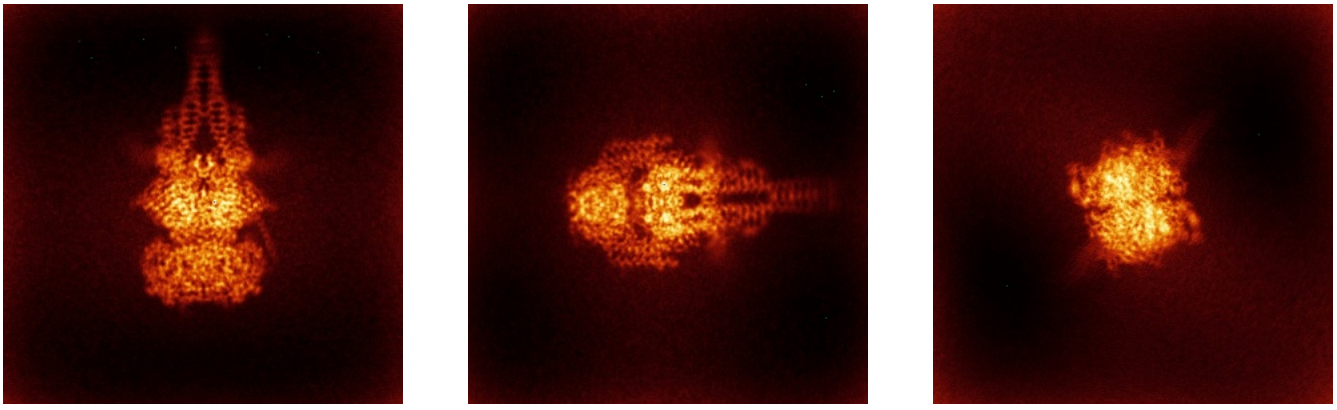
6.4 Orthogonal standard-deviation projections (False-color) (i)

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 0.3. 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.

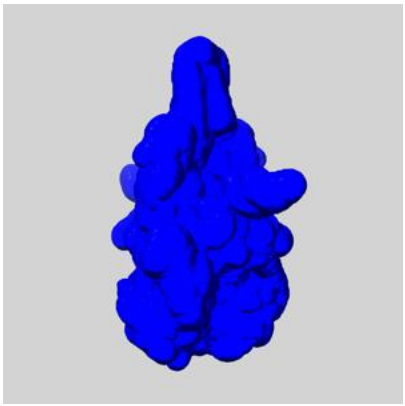
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

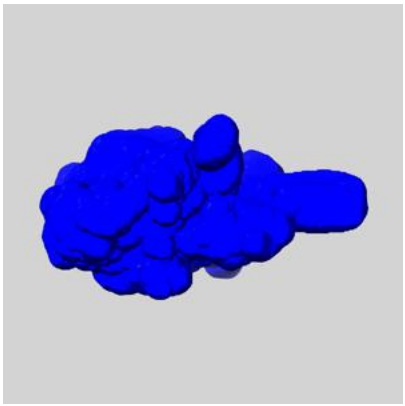
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

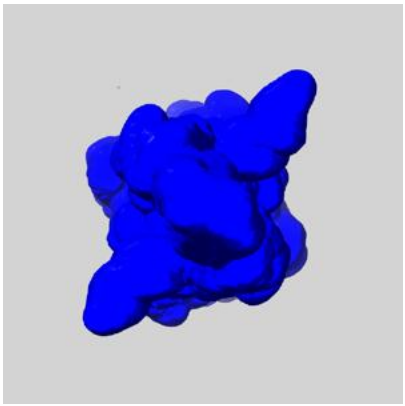
6.6.1 emd_52964_msk_1.map (i)



X



Y

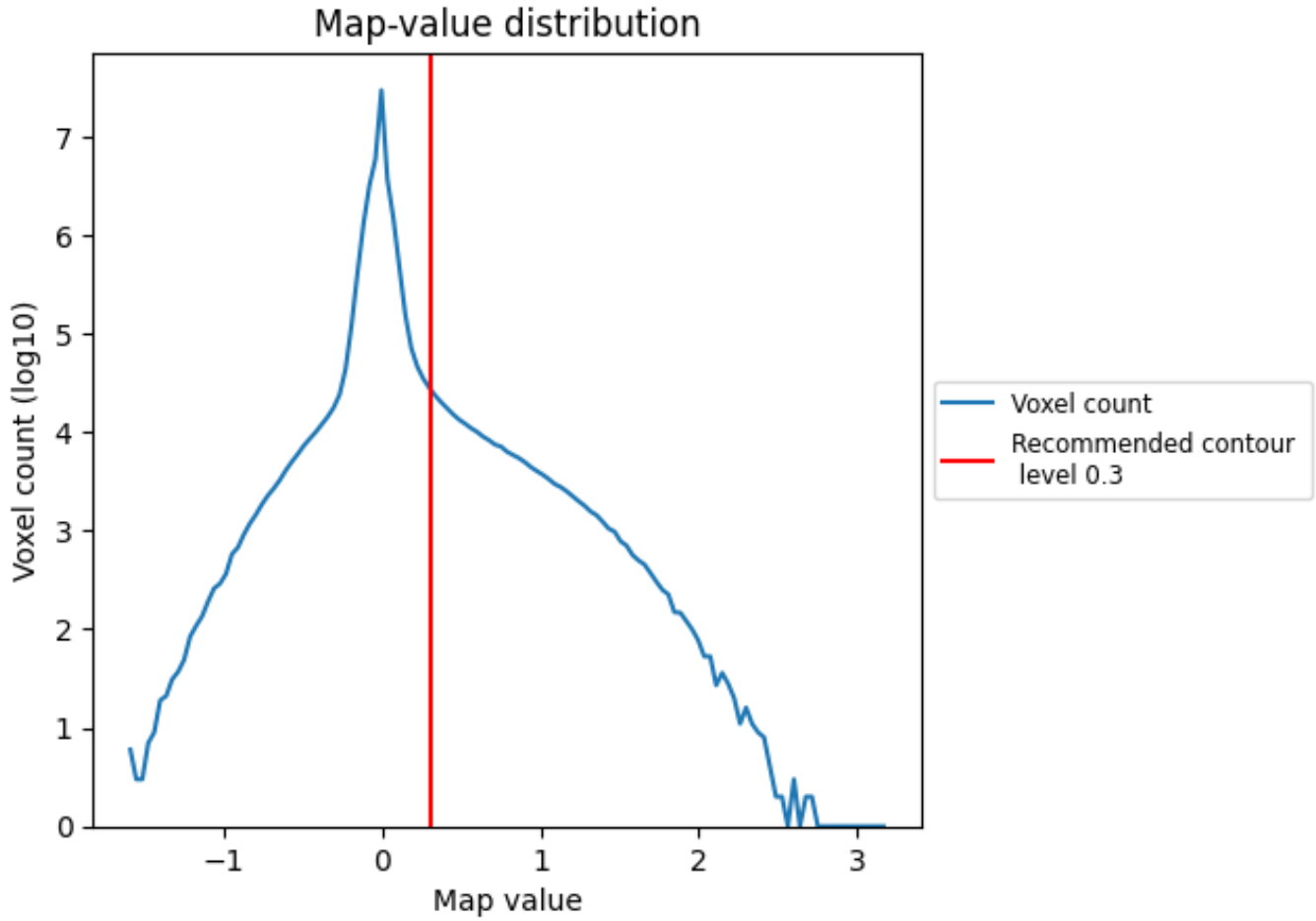


Z

7 Map analysis

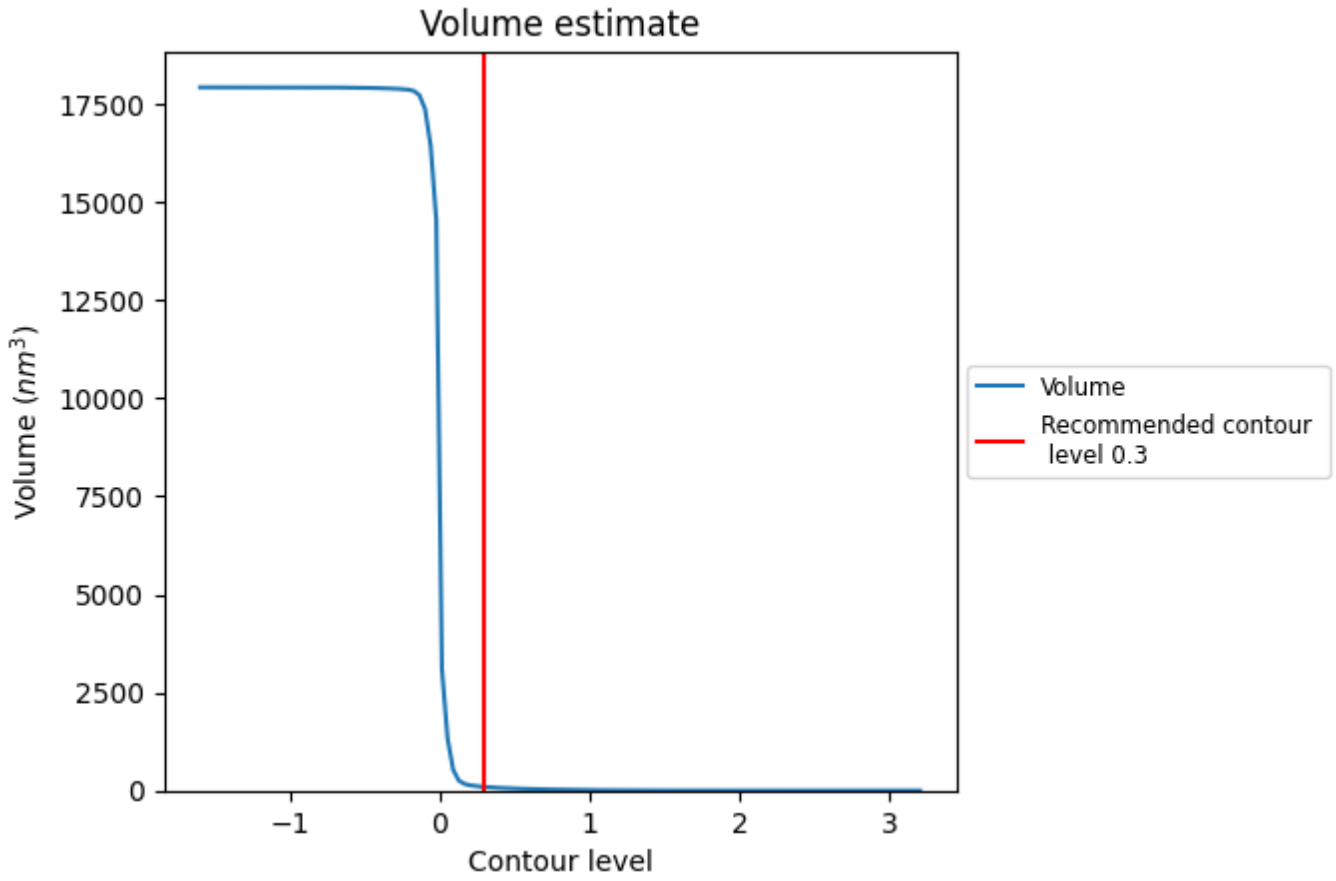
This section contains the results of statistical analysis of the map.

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.

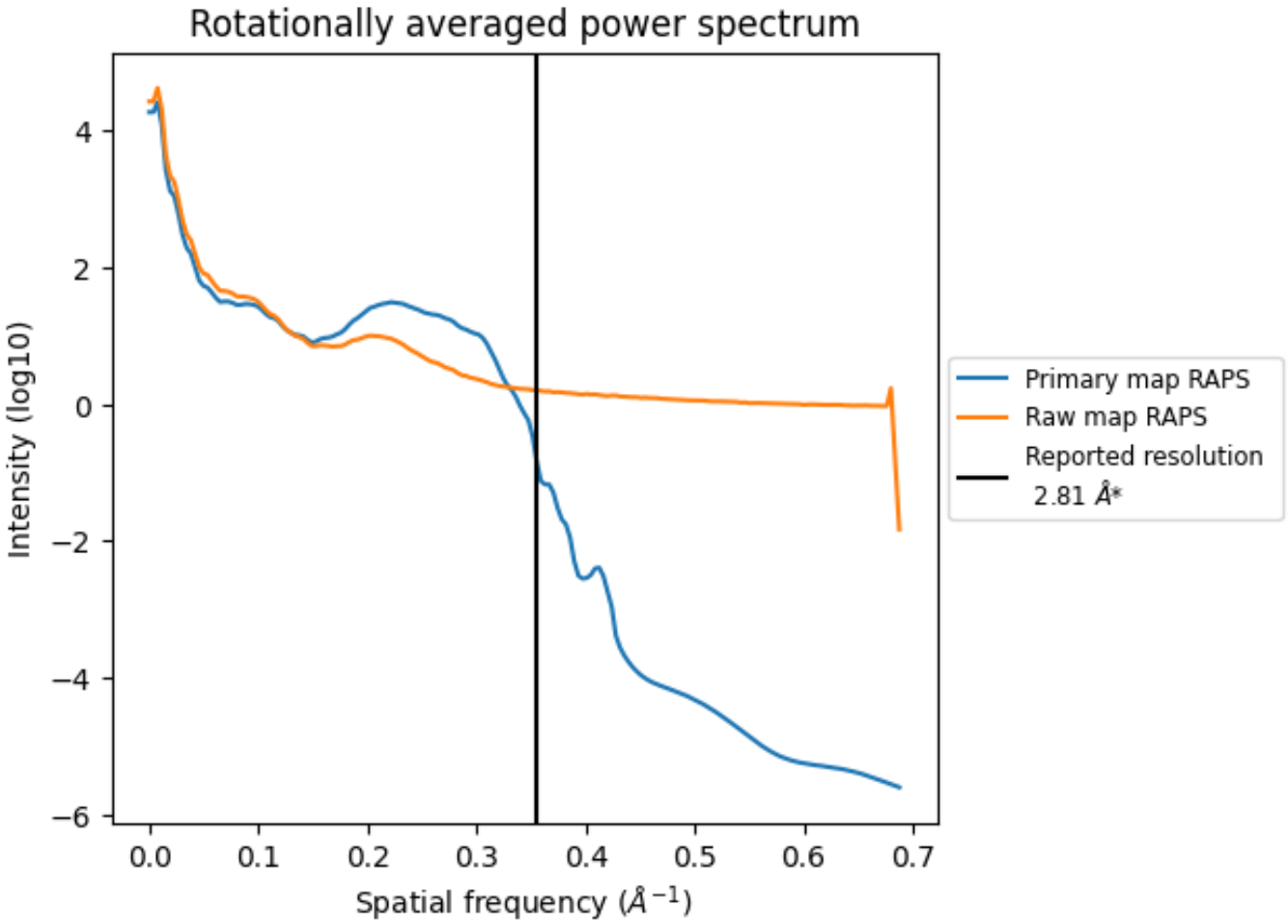
7.2 Volume estimate (i)



The volume at the recommended contour level is 93 nm^3; this corresponds to an approximate mass of 84 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)

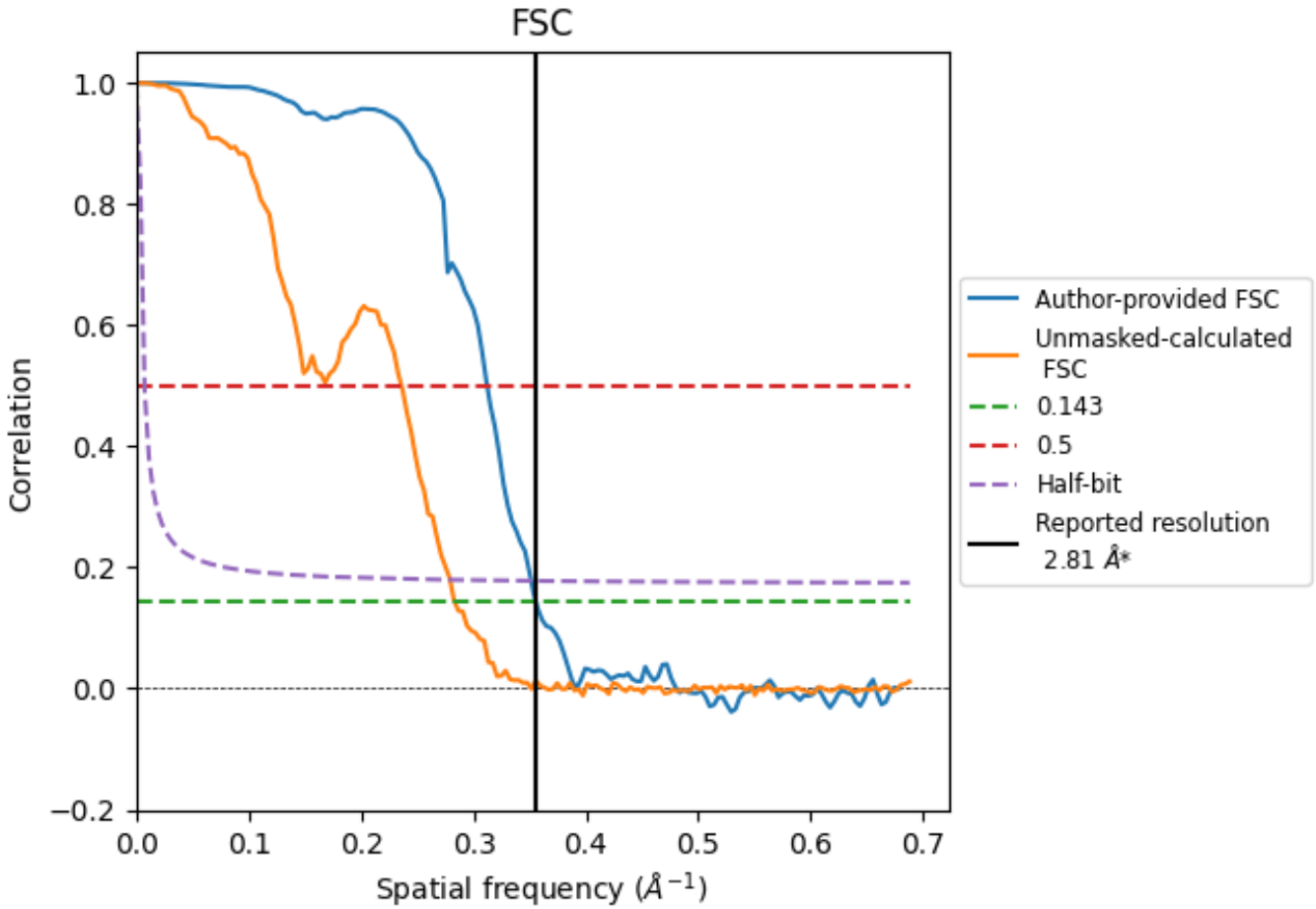


*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.356 Å^{-1}

8.2 Resolution estimates (i)

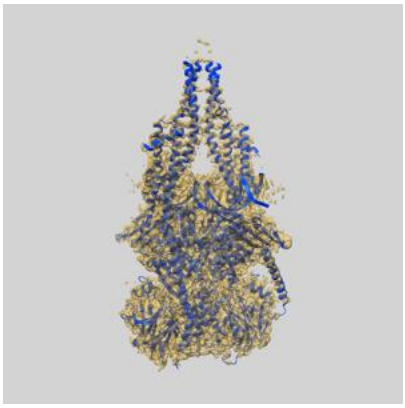
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.81	-	-
Author-provided FSC curve	2.81	3.20	2.85
Unmasked-calculated*	3.53	4.24	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.53 differs from the reported value 2.81 by more than 10 %

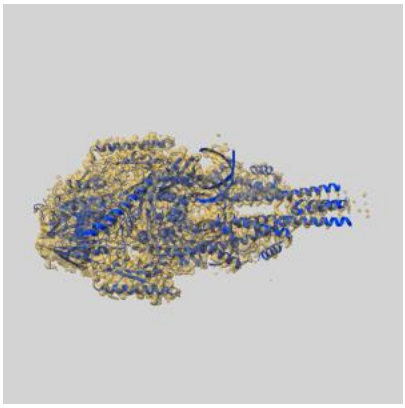
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52964 and PDB model 9Q9M. Per-residue inclusion information can be found in section 3 on page 9.

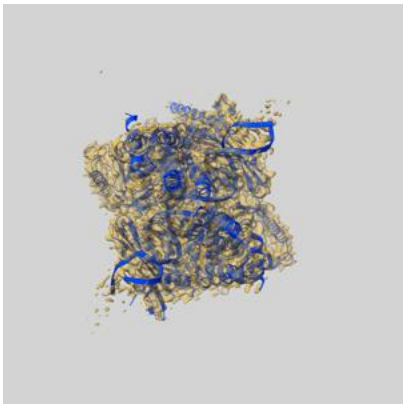
9.1 Map-model overlay



X



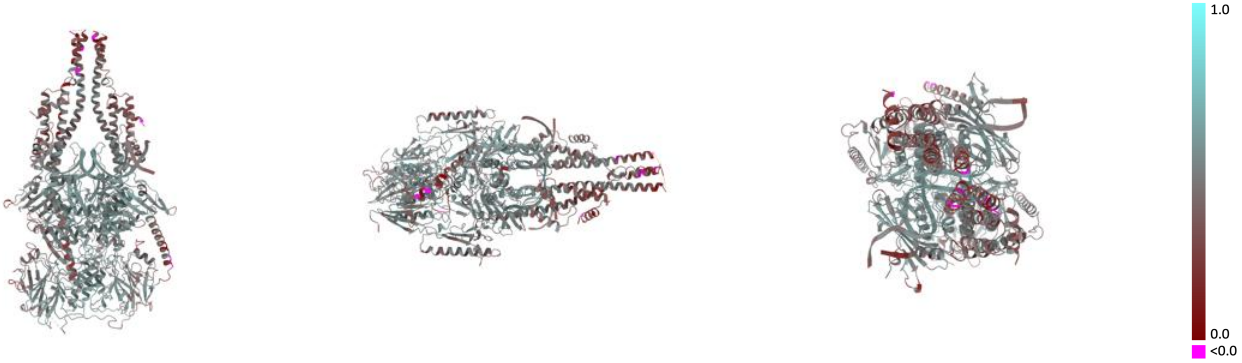
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.3 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.

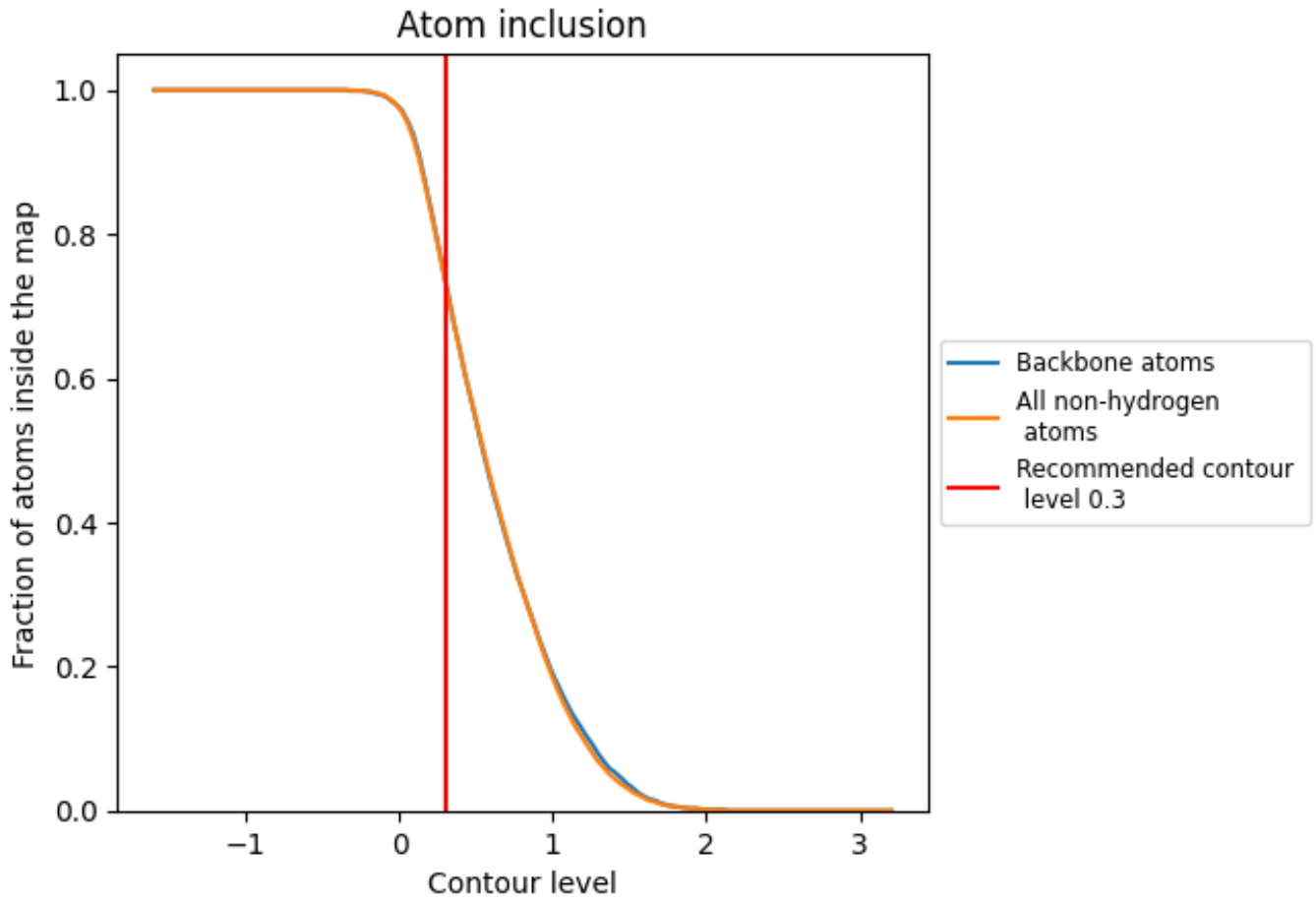
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.3).

9.4 Atom inclusion (i)



At the recommended contour level, 74% of all backbone atoms, 73% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7340	0.4830
A	0.7610	0.5010
B	0.7690	0.5020
D	0.7310	0.4790
E	0.7380	0.4620
F	0.4600	0.3900
J	0.5230	0.4130
P	0.7500	0.4860
T	0.8080	0.5250

