



## wwPDB EM Validation Summary Report ⓘ

Sep 2, 2024 – 12:20 PM JST

PDB ID : 8Y3Y  
EMDB ID : EMD-38907  
Title : The Cryo-EM structure of anti-phage defense associated DSR2 tetramer bound with two DSAD1 inhibitors (opposite side)  
Authors : Wang, R.W.; Xu, Q.; Wu, Z.X.; Li, J.L.; Shi, Z.B.; Li, F.X.  
Deposited on : 2024-01-29  
Resolution : 3.33 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](mailto: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.dev112  
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) : 2.38.2

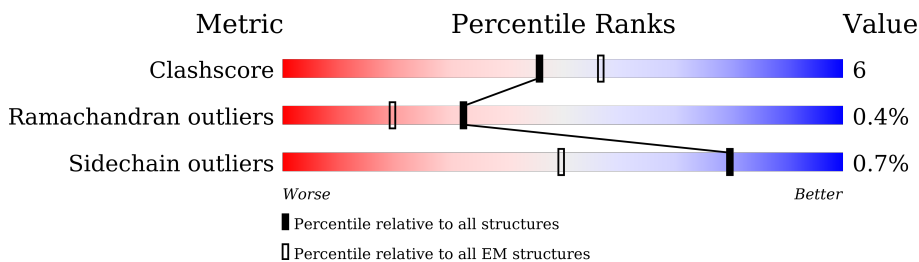
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.33 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  $\geq 3$ , 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	1005	
1	B	1005	
1	D	1005	
1	E	1005	
2	C	120	
2	F	120	

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 33586 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 SIR2-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	957	Total 7968	C 5155	N 1282	O 1499	S 32	0	0
1	B	958	Total 7996	C 5178	N 1290	O 1497	S 31	0	0
1	D	957	Total 7968	C 5155	N 1282	O 1499	S 32	0	0
1	E	958	Total 7996	C 5178	N 1290	O 1497	S 31	0	0

- Molecule 2 is a protein called DSR anti-defence 1.

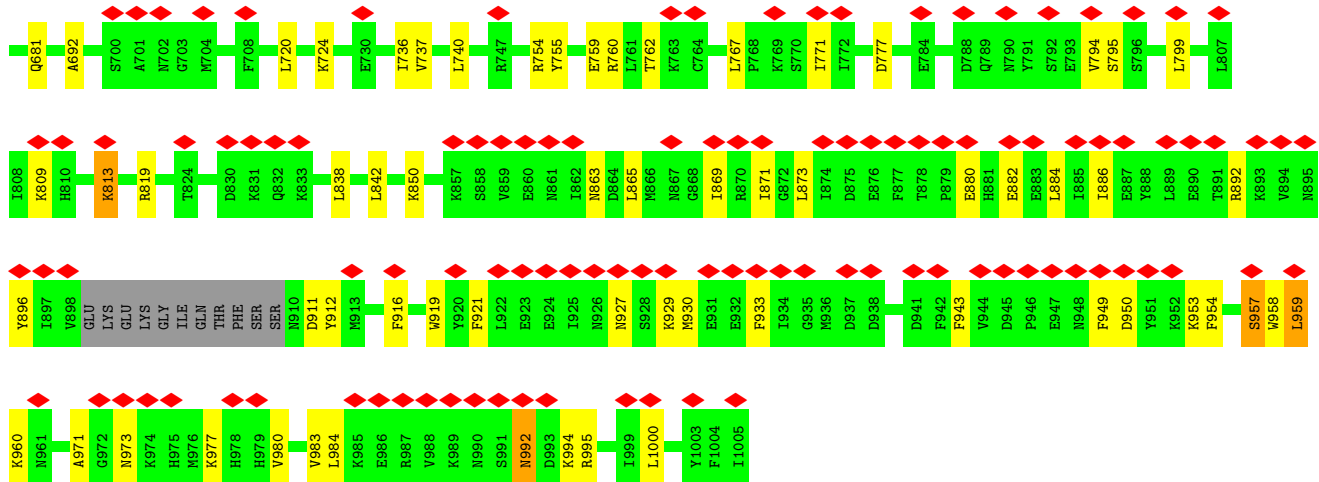
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	102	Total 829	C 544	N 133	O 150	S 2	0	0
2	F	102	Total 829	C 544	N 133	O 150	S 2	0	0

### 3 Residue-property plots

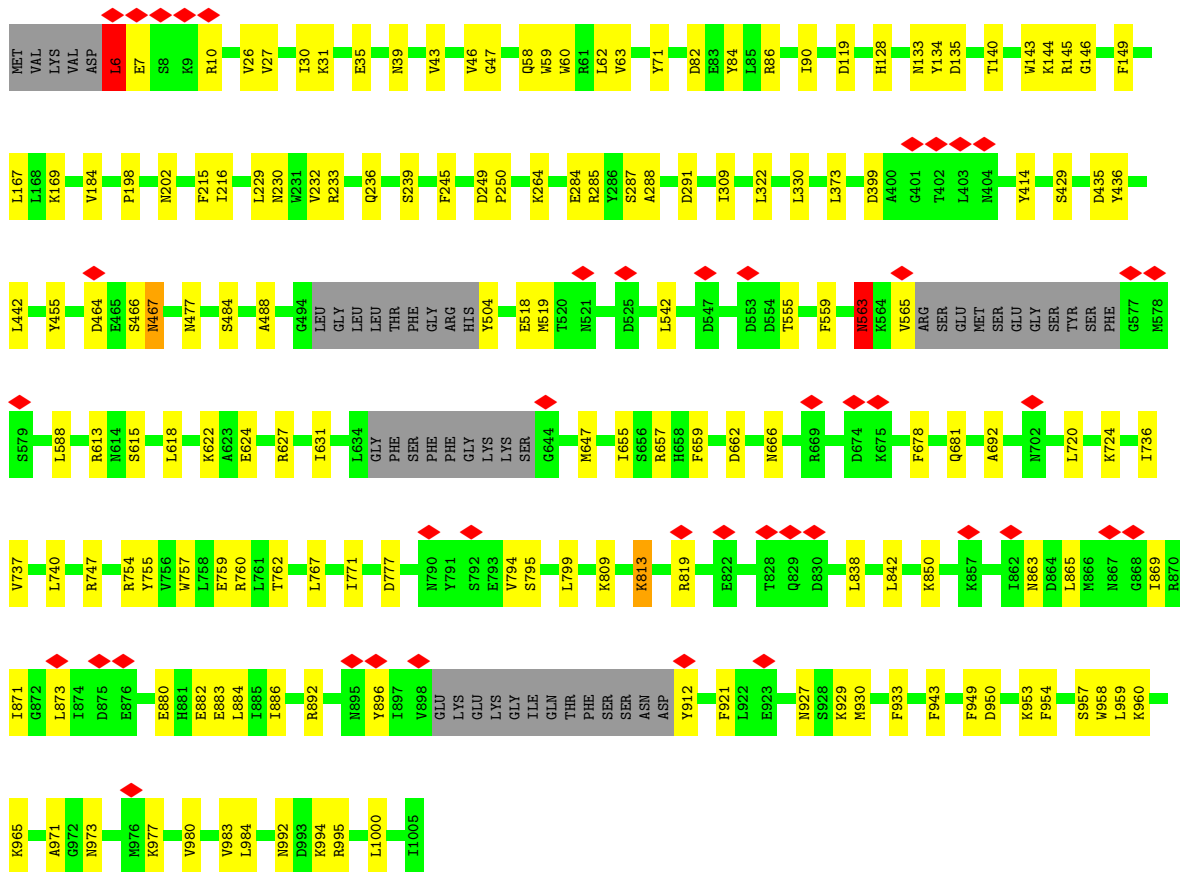
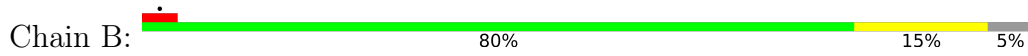
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: SIR2-like domain-containing protein

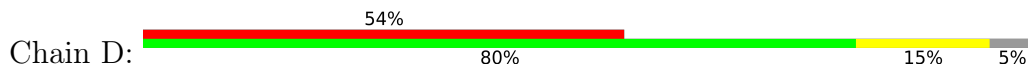




• Molecule 1: SIR2-like domain-containing protein

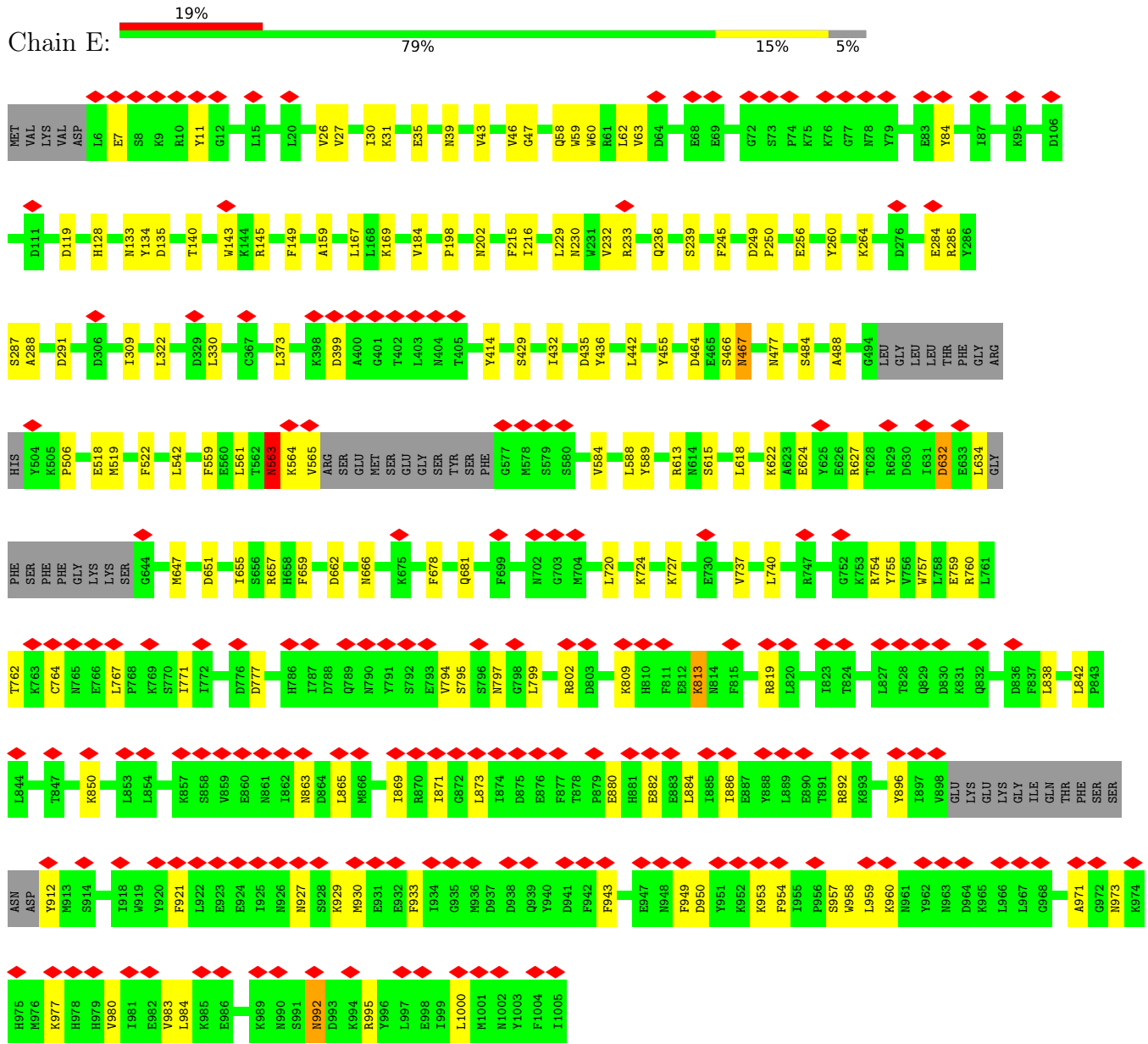


• Molecule 1: SIR2-like domain-containing protein

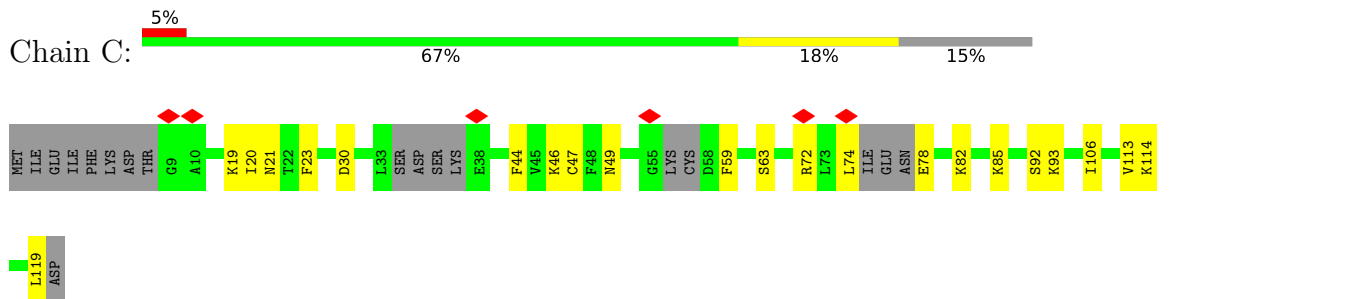


MET	VAL	LYS	VAL	ASP	LEU	GLU	SER	LYS	ARG	TRR	G12	E13	K14	L15	K16	E17	V18	F19	L20	M21	L22	D23	N24	N25	V26	V27	E28	C29	I30	K31	E32	E35	R38	N39	G40	K41	L42	L43	F44	F45	V46	G47	V50	S54	D55	Q58	W59	W60	R61	L62	V63	D64	K65	Y66								
H67	E68	E69	L70	Y71	G72	S73	P74	K75	K76	G77	N78	Y79	S80	S81	D82	E83	Y84	L85	R86	F91	Y92	N93	V94	K95	A99	G102	I103	D106	F107	F108	Q109	V110	D111	K112	P113	T114	N115	P116	H117	H118	D119	K120	G121	I121	M124	N125	P126	L127	H128	N133	Y134	D135	T140									
A141	C142	W143	K144	R145	G146	K147	Y148	F149	S150	V151	E156	D157	V158	A159	S163	S164	R165	Y166	L167	K169	G172	D173	F174	R175	K176	G177	F178	K186	E187	Y190	N196	Y197	L198	L199	I200	S201	N202	L203	M204	K205	T206	D270	A271	I207	I208	A209	T210	H211	T212	I213	V214	F215	I216									
G217	Y218	G219	L220	G221	D222	Y223	N224	I225	L229	N230	W231	V232	R233	Q236	K237	D238	S239	F240	H241	K242	P243	F245	I246	R247	T248	D249	P250	S251	P252	I253	E254	N255	E256	T257	L258	I259	K264	G265	L266	R267	I268	I269	D270	A271	A272	S273	L274	I275	D276	S277	E279	Y280	D281	Y282								
L283	E284	R285	Y286	S287	A288	W289	M290	D291	L292	L293	I294	E295	S296	Q297	K300	F301	I302	T303	K304	D305	D306	E307	V308	I309	D310	I316	S317	P318	L319	F320	I321	L322	Q323	Y324	I325	R326	K327	I328	D329	L330	K331	H332	V333	F334	E335	Y336	D337	L338	M343	G415	V347	R348	F354	G355	R359							
E362	L363	K364	E365	S366	C367	D368	E369	R370	S371	K372	S374	K375	Q377	Y378	E379	R380	F381	N382	F385	N386	F387	F388	E389	K390	I394	C395	M396	A397	K398	D399	A400	G401	T402	L403	N404	T405	S406	I407	E408	I409	N410	S411	L412	A413	Y414	H415	G416	K417	Y418	D419	V420	K423	F424									
E427	Q428	S429	V430	S431	I432	E433	D434	D435	Y436	F441	L442	E450	L454	Y455	S456	N457	I458	I459	L460	N461	S462	I463	D464	E465	N467	G468	C469	A371	Y471	N477	S484	A488	V489	T490	PHE	ASN	GLY	LEU	GLY	LEU	LEU	THR	PHE	GLY	ARG	HIS	TYS	LYS	P506													
F507	T508	D509	E510	F511	L512	A513	R514	E515	E516	R517	E518	M519	T520	F521	F522	M523	I524	M531	P532	F533	E534	F535	Q536	K537	K538	Y539	K540	I541	L542	L545	S546	T555	R563	K564	V565	R566	E571	F576	G577	M578	S579	S580	M583	R587	L588	Y589	D590	F594	E597													
M598	C599	L600	M601	F602	E607	F608	V611	L612	R613	M614	S615	M616	S617	L618	L619	I620	E621	K622	A623	E624	I625	E626	R627	T628	R629	D630	I631	ASP	GLU	LEU	PHE	SER	PHE	PHE	GLY	LYS	SER	G644	F645	F646	M647	V653	M654	R657	H658	F659	R660	I661	D662	D663	I664	R665	M666	F744								
L667	E668	R669	S670	C671	R675	F678	Q681	E686	Y687	O690	I691	A692	E693	E694	K697	Q698	F699	S700	A701	M702	G703	M704	N705	Q711	F712	I713	S714	E715	A716	K717	A718	A719	A720	L720	Y721	F722	K724	L728	S729	E730	E731	G732	K735	I736	V737	K738	A739	L740	F744													
P745	E746	R747	D748	I751	R754	Y755	L758	E759	R760	L761	T762	K763	C764	M765	E766	L767	P768	K769	S770	I771	I772	S773	I774	D777	F778	L779	V780	L781	E784	K785	H786	I787	D788	Q789	M790	Y791	S792	E793	V794	S795	S796	L799	Y800	S801	L807	I808	K809	H810	F811	E812	K813	M814										
F815	I816	S817	K818	R819	L820	S821	E822	I823	T824	L825	C826	L827	T828	Q829	D830	Q831	Q832	K833	Q834	I835	D836	F837	L838	F839	K840	L841	L842	F843	L844	L845	S846	T847	N848	A849	K850	L853	L854	S855	F856	K857	S858	V859	E860	M861	I862	M863	D864	L865	M866	M867	G868	I869	R870	L871	G872	L873	I874	D875				
E876	F877	I878	P879	E880	H881	E882	E883	L884	L885	I886	E887	E890	T891	K892	K893	V894	N895	Y896	I897	W958	L959	K960	I961	Y962	N963	D964	K965	L966	I970	A971	G972	N973	K974	H975	N976	K977	N980	F921	L922	E923	E924	I925	N926	N927	S928	S929	K929	N930	I931	E932	D933	I934	G935	M936	D937	I939	E938	M1001	N1002	Y940	F1004	I1005
F942	F943	N944	D945	F946	E947	N948	F949	D950	Y951	K952	F954	N955	P956	S957	N958	L959	K960	I961	Y962	N963	D964	K965	L966	I970	A971	G972	N973	K974	H975	N976	K977	N980	F921	L922	E923	E924	I925	N926	N927	S928	S929	K929	N930	I931	E932	D933	I934	G935	M936	D937	I939	E938	M1001	N1002	Y940	F1004	I1005					

• Molecule 1: SIR2-like domain-containing protein

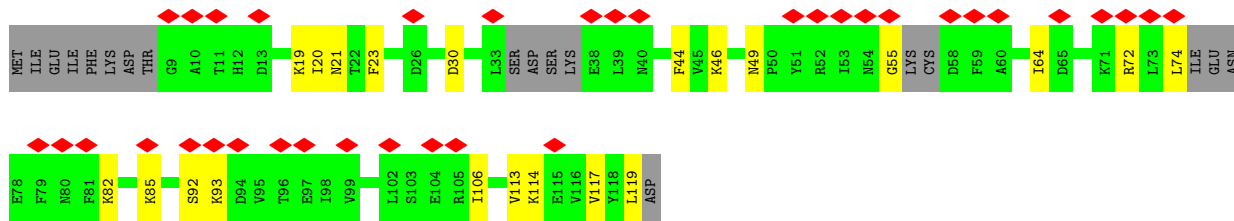


• Molecule 2: DSR anti-defence 1



• Molecule 2: DSR anti-defence 1







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	91205	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	13000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	3.660	Depositor
Minimum map value	-0.368	Depositor
Average map value	0.031	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.6	Depositor
Map size ( $\text{\AA}$ )	430.91998, 430.91998, 430.91998	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.0773, 1.0773, 1.0773	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.39	0/8150	0.55	2/10979 (0.0%)
1	B	0.38	0/8178	0.55	3/11014 (0.0%)
1	D	0.39	0/8150	0.55	3/10979 (0.0%)
1	E	0.39	0/8178	0.55	2/11014 (0.0%)
2	C	0.44	0/847	0.63	0/1144
2	F	0.44	0/847	0.63	0/1144
All	All	0.39	0/34350	0.55	10/46274 (0.0%)

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
1	A	0	6
1	B	0	3
1	D	0	4
1	E	0	4
2	C	0	1
2	F	0	1
All	All	0	19

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	442	LEU	CA-CB-CG	6.87	131.09	115.30
1	B	442	LEU	CA-CB-CG	6.85	131.05	115.30
1	A	442	LEU	CA-CB-CG	6.84	131.04	115.30
1	E	442	LEU	CA-CB-CG	6.83	131.01	115.30
1	E	959	LEU	CA-CB-CG	5.54	128.04	115.30

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	563	ASN	Peptide
1	A	565	VAL	Peptide
1	A	568	GLU	Peptide
1	A	794	VAL	Peptide
1	A	911	ASP	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	7968	0	7798	101	0
1	B	7996	0	7845	102	0
1	D	7968	0	7798	93	0
1	E	7996	0	7845	102	0
2	C	829	0	820	15	0
2	F	829	0	820	14	0
All	All	33586	0	32926	397	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 6.

The worst 5 of 397 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:B:912:TYR:HH	2:C:78:GLU:N	1.50	1.10
1:A:562:THR:O	1:A:566:ARG:HB2	1.61	0.99
1:D:892:ARG:O	1:D:896:TYR:HB2	1.73	0.88
1:B:892:ARG:O	1:B:896:TYR:HB2	1.73	0.88
1:A:892:ARG:O	1:A:896:TYR:HB2	1.73	0.88

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	949/1005 (94%)	872 (92%)	74 (8%)	3 (0%)	37 66
1	B	948/1005 (94%)	871 (92%)	74 (8%)	3 (0%)	37 66
1	D	949/1005 (94%)	870 (92%)	76 (8%)	3 (0%)	37 66
1	E	948/1005 (94%)	870 (92%)	74 (8%)	4 (0%)	30 61
2	C	94/120 (78%)	74 (79%)	19 (20%)	1 (1%)	12 41
2	F	94/120 (78%)	74 (79%)	19 (20%)	1 (1%)	12 41
All	All	3982/4260 (94%)	3631 (91%)	336 (8%)	15 (0%)	32 61

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	958	TRP
1	B	958	TRP
1	D	958	TRP
1	E	958	TRP
1	A	795	SER

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	879/923 (95%)	873 (99%)	6 (1%)	81 88
1	B	881/923 (95%)	874 (99%)	7 (1%)	79 87
1	D	879/923 (95%)	873 (99%)	6 (1%)	81 88

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	881/923 (95%)	875 (99%)	6 (1%)	81	88
2	C	94/113 (83%)	93 (99%)	1 (1%)	70	82
2	F	94/113 (83%)	93 (99%)	1 (1%)	70	82
All	All	3708/3918 (95%)	3681 (99%)	27 (1%)	80	88

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	330	LEU
1	D	838	LEU
1	E	973	ASN
1	D	813	LYS
1	D	973	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 27 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	93	ASN
1	D	765	ASN
2	F	17	HIS
1	D	477	ASN
1	D	863	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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.

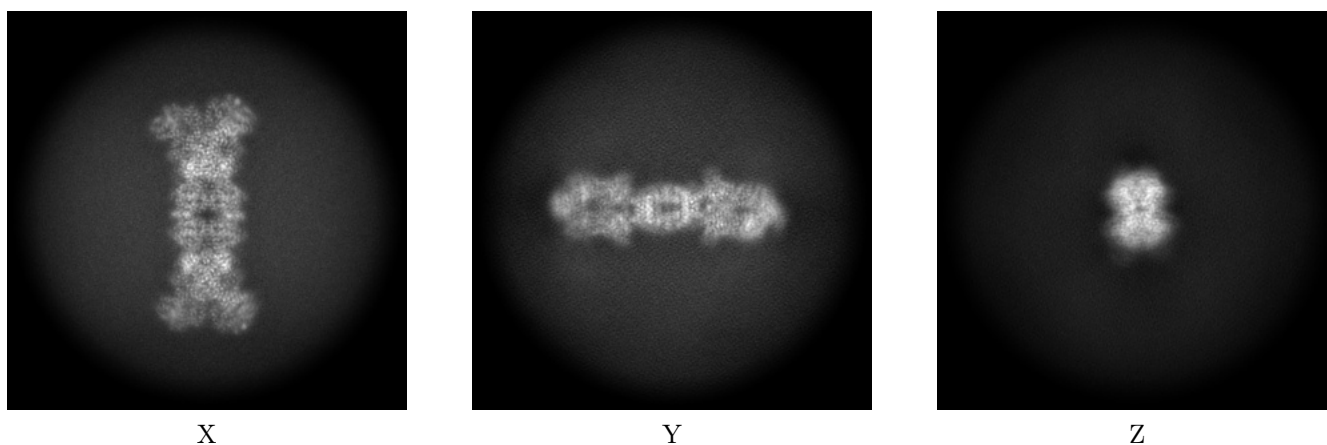
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38907. 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](#)

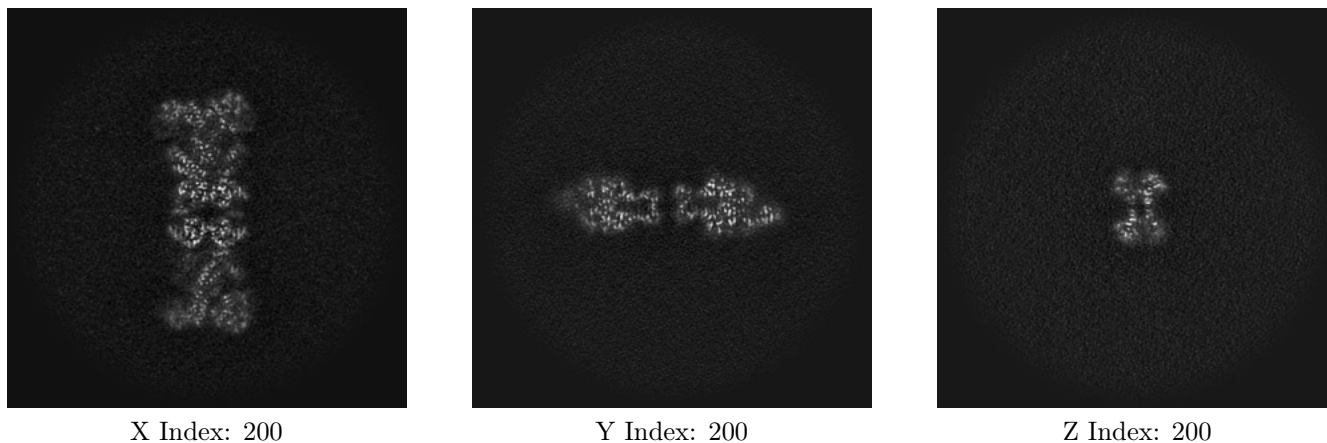
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

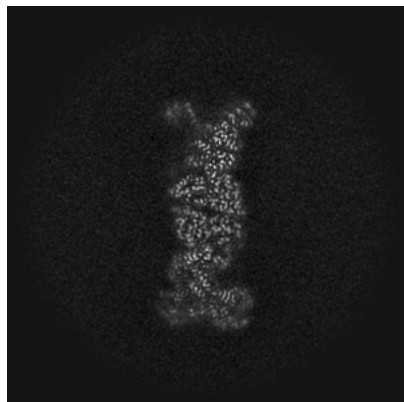
#### 6.2.1 Primary map



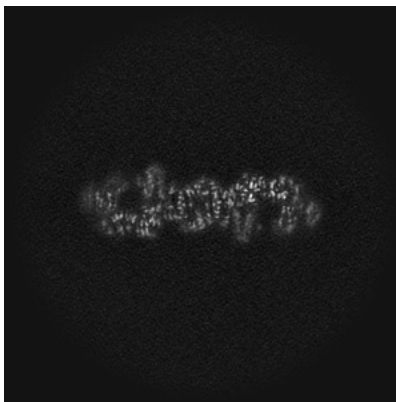
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [\(i\)](#)

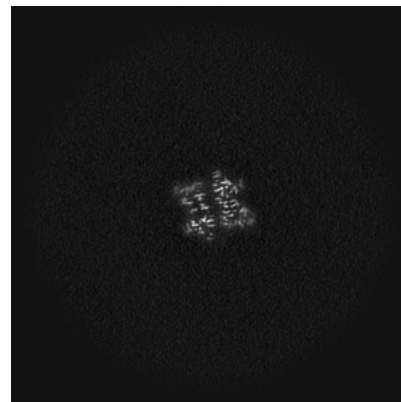
### 6.3.1 Primary map



X Index: 212



Y Index: 219

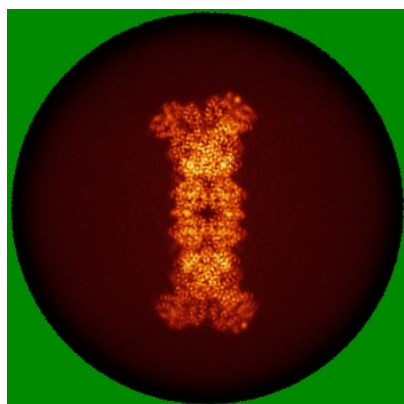


Z Index: 242

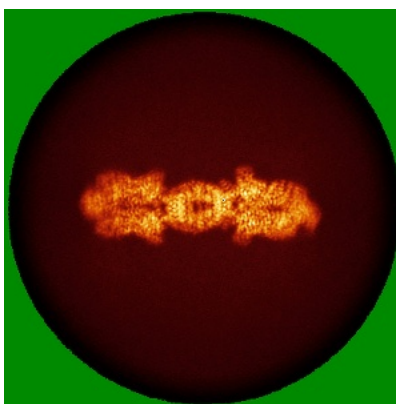
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [\(i\)](#)

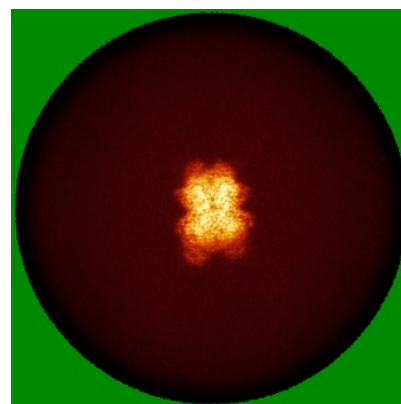
### 6.4.1 Primary map



X



Y



Z

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



## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

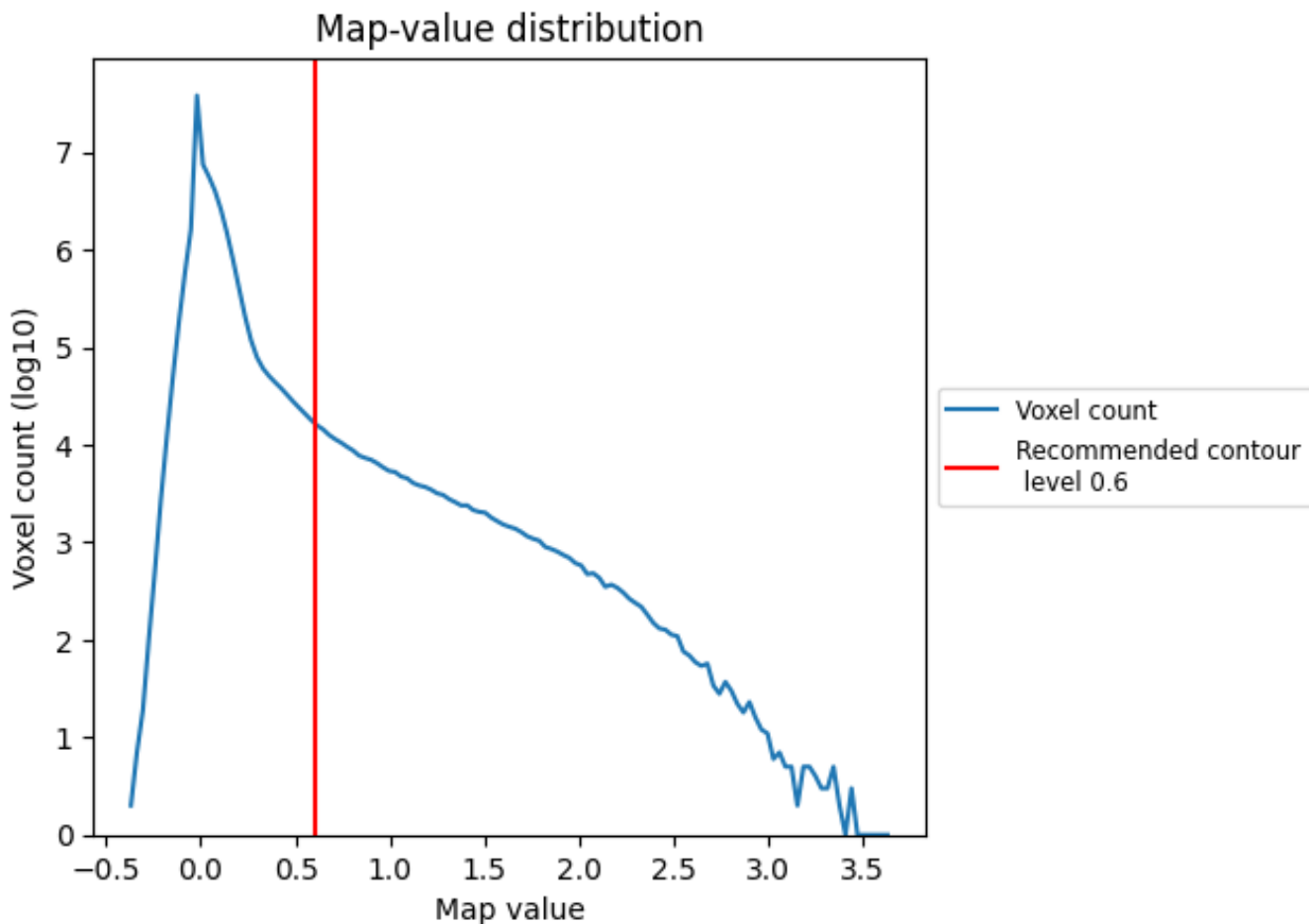
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

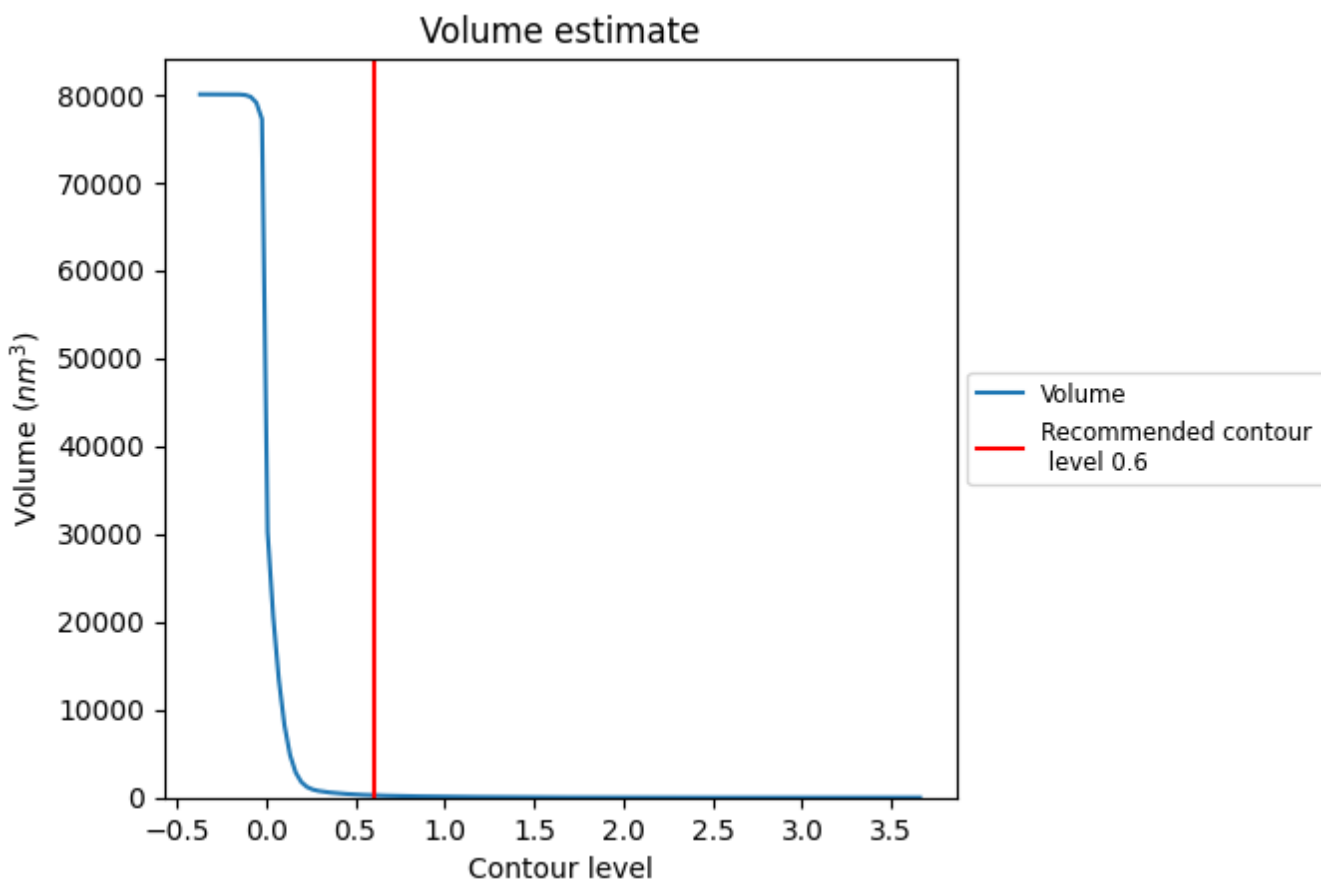
This section contains the results of statistical analysis of the map.

### 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.

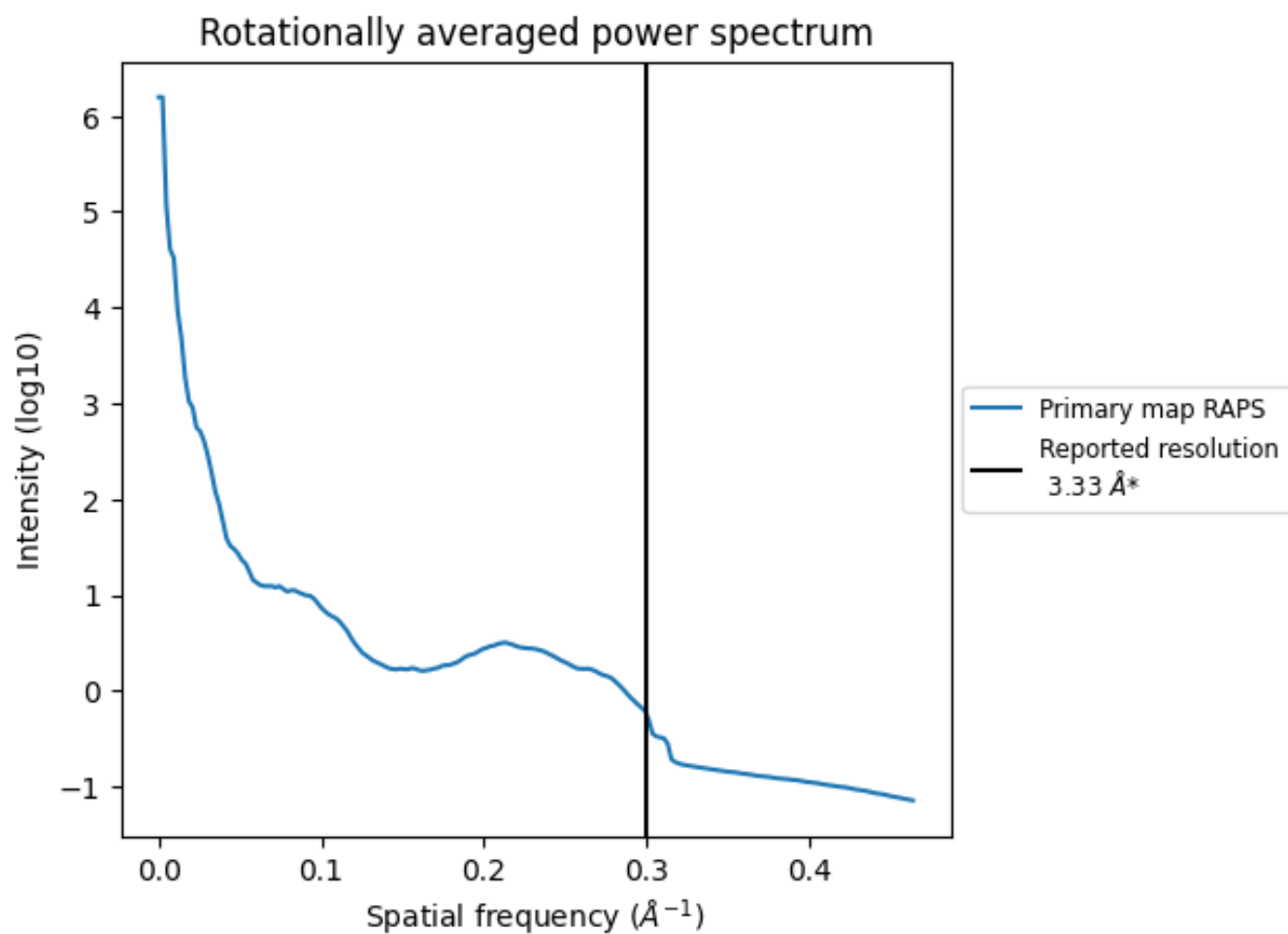
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 258 nm<sup>3</sup>; this corresponds to an approximate mass of 233 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 0.300 Å<sup>-1</sup>

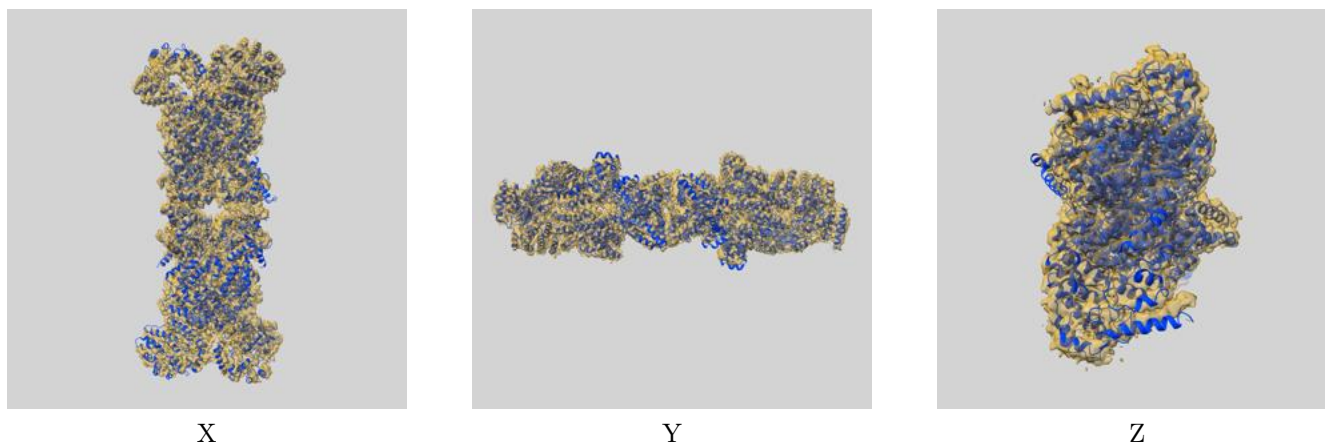
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

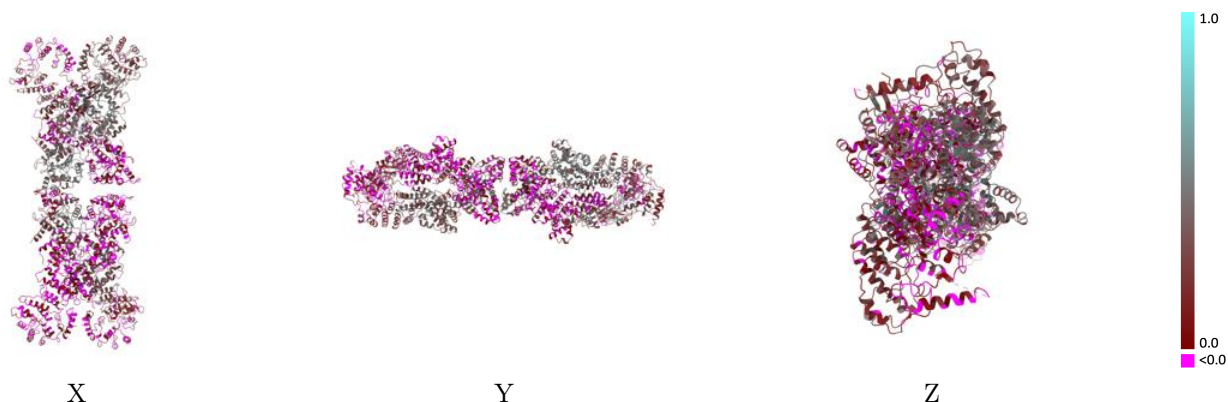
This section contains information regarding the fit between EMDB map EMD-38907 and PDB model 8Y3Y. Per-residue inclusion information can be found in section 3 on page 4.

### 9.1 Map-model overlay [i](#)



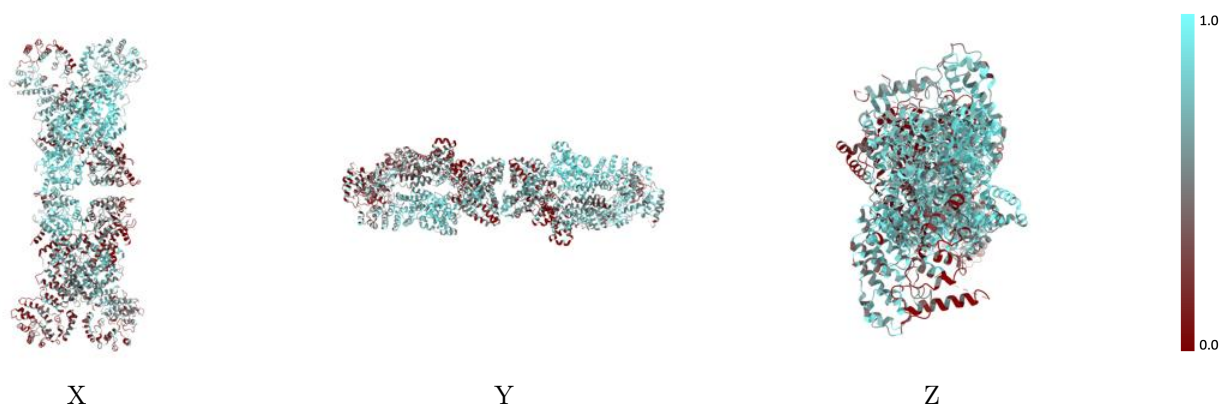
The images above show the 3D surface view of the map at the recommended contour level 0.6 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



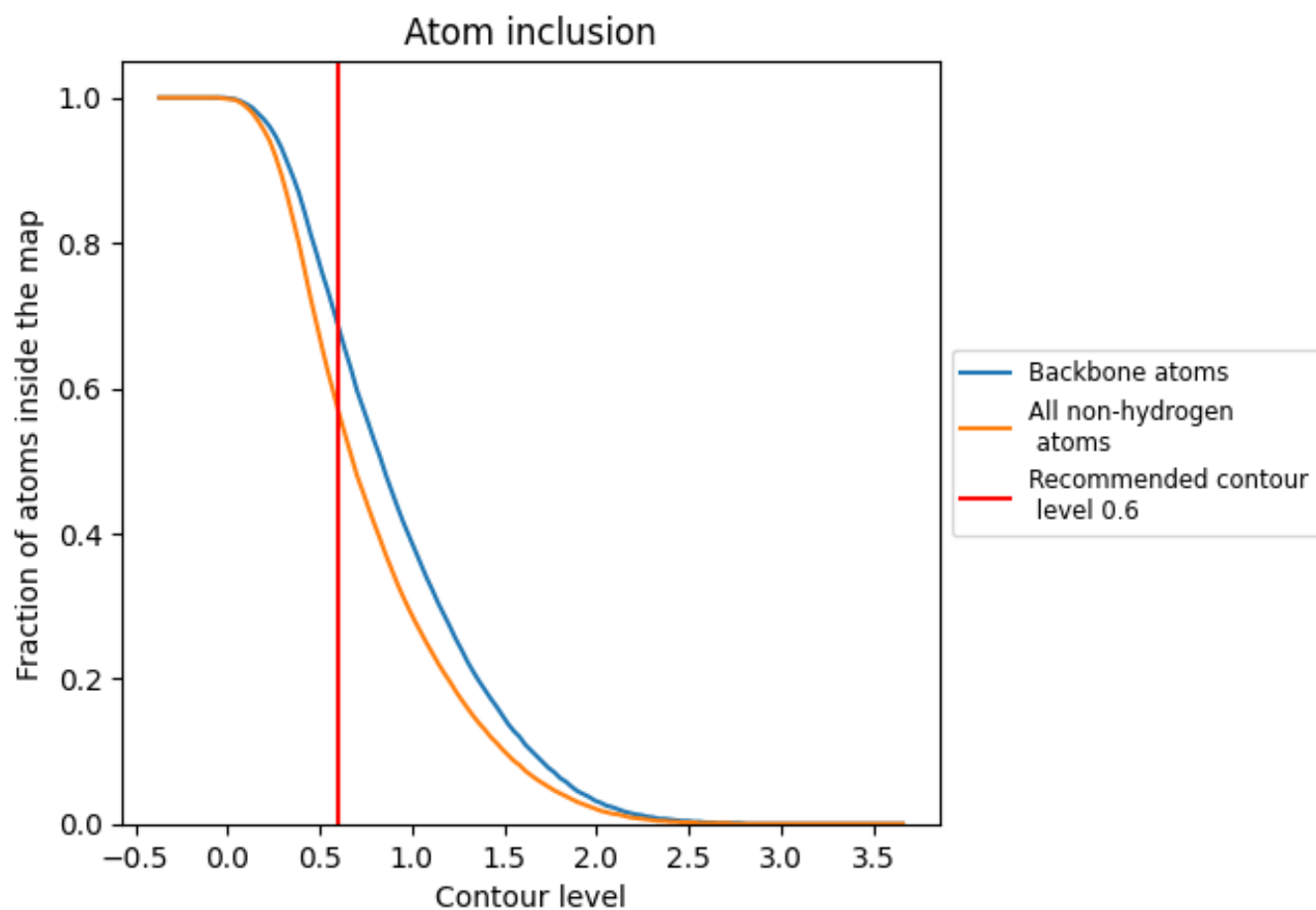
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.6).

## 9.4 Atom inclusion [i](#)

















At the recommended contour level, 68% of all backbone atoms, 57% 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 (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5700	 0.1840
A	 0.4570	 0.0680
B	 0.7900	 0.3750
C	 0.7200	 0.3560
D	 0.3710	 0.0170
E	 0.6490	 0.2540
F	 0.5240	 0.2310

