



wwPDB EM Validation Summary Report ⓘ

Sep 28, 2026 – 12:53 PM EDT

PDB ID : 11HT / pdb_000011ht
EMDB ID : EMD-75702
Title : Cryo-EM structure of the human ZNFX1 tetramer
Authors : Wang, F.; He, Q.; Li, H.
Deposited on : 2026-02-25
Resolution : 3.71 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

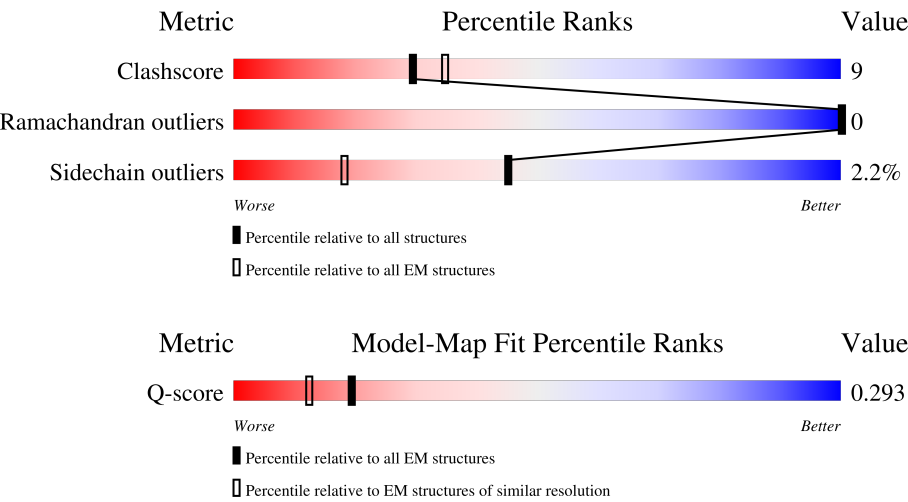
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.2
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.51

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 3.71 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	10534 (3.21 - 4.21)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1918	9% 53% 13% 33%
1	B	1918	19% 51% 16% 33%
1	C	1918	9% 52% 14% 33%
1	D	1918	19% 50% 16% 33%

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Mol	Chain	Length	Quality of chain
1	E	1918	7% 6% 91%
1	F	1918	7% 7% 91%

2 Entry composition [i](#)

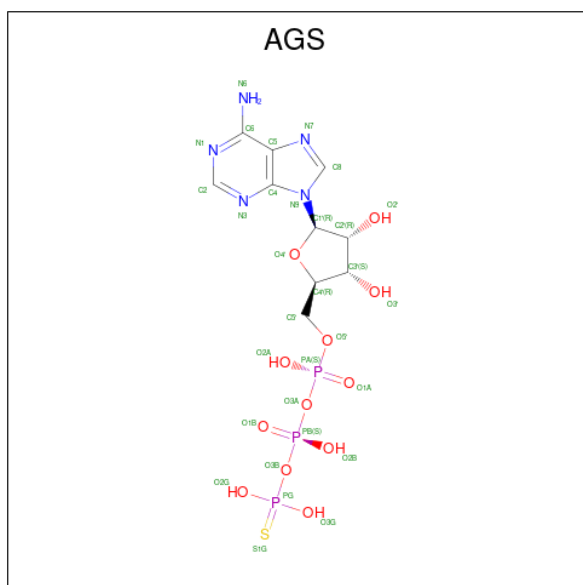
There are 2 unique types of molecules in this entry. The entry contains 44040 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NFX1-type zinc finger-containing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	B	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	C	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	D	1282	Total	C	N	O	S	0	0
			10307	6503	1814	1909	81		
1	E	172	Total	C	N	O	S	0	0
			1344	855	226	256	7		
1	F	172	Total	C	N	O	S	0	0
			1344	855	226	256	7		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$) (labeled as "Ligand of Interest" by depositor).

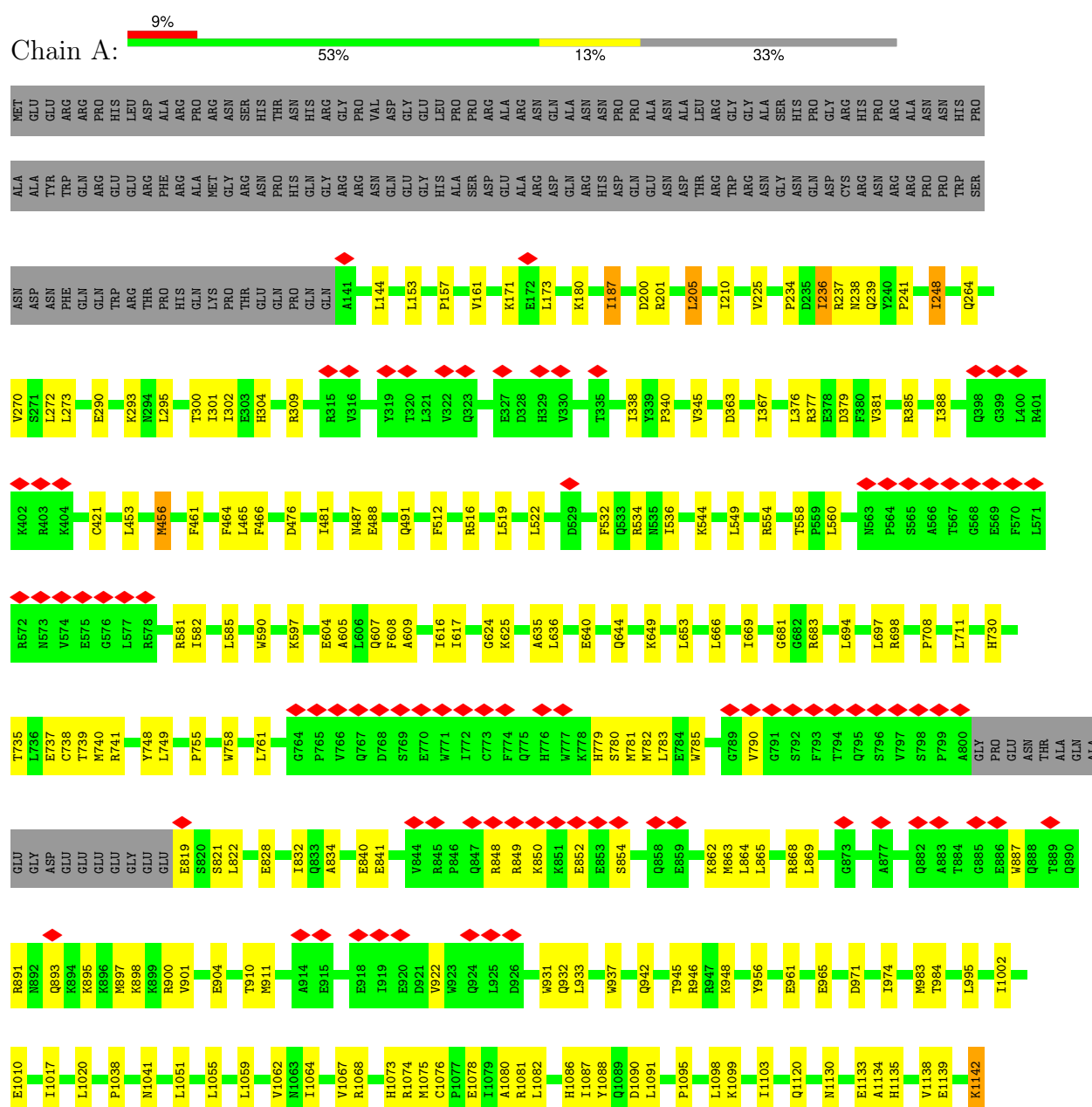


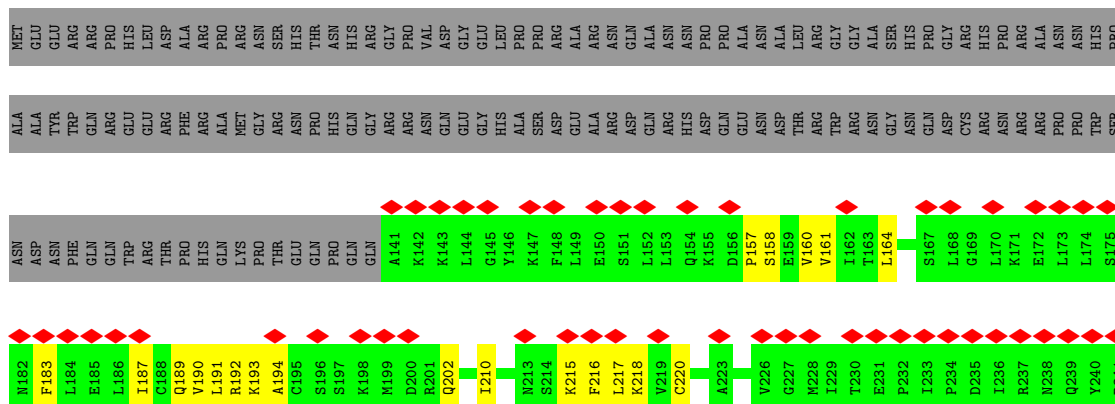
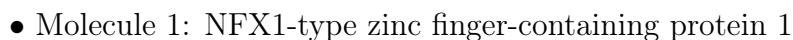
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	B	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	C	1	Total 31	C 10	N 5	O 12	P 3	S 1	0
2	D	1	Total 31	C 10	N 5	O 12	P 3	S 1	0

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: NFX1-type zinc finger-containing protein 1





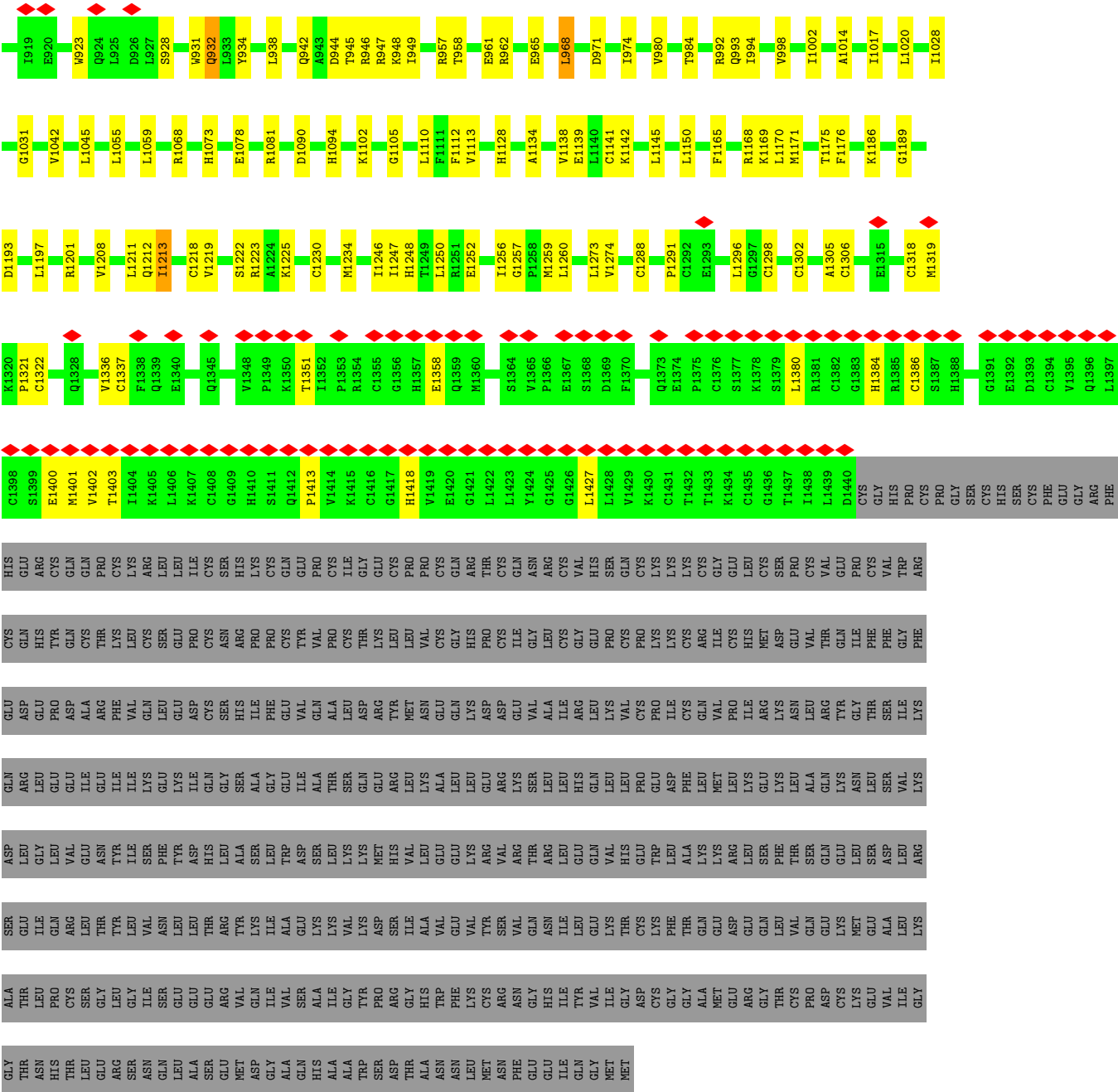
[illegible]

THR	LEU	PHE	LYS	LYS	LYS	ASP	SER
CYS	VAL	THR	LEU	LEU	ASN	GLU	PRO
PRO	GLN	THR	ALA	ALA	ASN	VAL	CYS
ASP	GLU	GLN	GLN	GLN	ARG	THR	GLU
CYS	LYS	GLU	ASN	LYS	TYR	ILE	VAL
LYS	MET	LEU	ASN	ASN	GLY	ILE	PRO
GLU	GLU	SER	LEU	LEU	THR	CYS	CYS
VAL	ALA	ASP	SER	ASP	GLN	PHE	VAL
ILE	LEU	LEU	VAL	VAL	ILE	GLY	THR
GLY	LEU	ARG	LYS	LYS	LYS	PHE	ARG
THR	ALA	SER	ASP	ASP	GLN	GLU	CYS
GLY	THR	GLU	LEU	LEU	ARG	ASP	GLN
ASN	LEU	ILE	GLY	GLY	LEU	GLU	HIS
HIS	PRO	ARG	LEU	LEU	LEU	PRO	TYR
THR	CYS	ARG	VAL	VAL	GLU	ASP	GLN
LEU	SER	THR	ARG	ARG	GLU	VAL	CYS
LEU	SER	LEU	GLN	GLN	GLY	ALA	CYS
GLU	GLY	THR	TYR	TYR	ILE	PHE	THR
ARG	LEU	TYR	ILE	ILE	ILE	ARG	LYS
SER	GLY	LEU	VAL	VAL	ILE	PHE	GLN
ASN	ILE	VAL	SER	SER	LYS	VAL	LEU
GLN	SER	ASN	PHE	PHE	GLU	GLN	CYS
LEU	GLU	LEU	TYR	TYR	LYS	ASP	PRO
ALA	GLU	LEU	ASP	ASP	ILE	ASP	CYS
ALA	GLU	THR	HIS	HIS	GLN	CYS	CYS
SER	GLU	THR	LEU	LEU	GLY	SER	ASN
GLU	ARG	ARG	LEU	LEU	GLY	ASN	ARG
MET	VAL	TYR	ALA	ALA	ILE	HIS	ARG
ASP	GLN	LYS	SER	SER	LYS	PRO	PRO
GLY	ILE	VAL	LEU	LEU	GLY	LEU	VAL
ALA	VAL	GLU	TRP	TRP	ALA	ALA	PRO
ALA	VAL	ALA	TRP	TRP	TRP	GLU	TYR
GLN	SER	GLU	ASP	ASP	ILE	VAL	VAL
HIS	ALA	LYS	SER	SER	ILE	GLN	ALA
ALA	ILE	LYS	LEU	LEU	THR	ALA	PRO
ALA	GLY	VAL	LEU	LEU	GLN	LEU	CYS
ALA	TRP	VAL	GLU	GLU	ASN	ASP	THR
ASN	PHE	GLU	GLU	GLU	GLN	LYS	LYS
LEU	LYS	VAL	LYS	LYS	LEU	HIS	GLY
MET	CYS	TYR	ARG	ARG	GLU	ASP	PRO
ASN	ARG	SER	VAL	VAL	ARG	ASP	CYS
PHE	ASN	SER	ARG	ARG	LYS	ASP	CYS
GLU	GLY	GLN	THR	THR	LEU	GLU	ILE
GLU	HIS	ASN	LEU	LEU	LEU	ALA	LEU
ILE	TYR	ILE	LEU	LEU	LEU	CYS	CYS
GLN	VAL	LEU	GLU	GLU	HIS	ARG	GLY
GLY	THR	GLU	GLN	GLN	GLY	LEU	GLY
MET	ILE	THR	VAL	VAL	ILE	ILE	ILE
MET	GLY	THR	ALA	ALA	PHE	CYS	LYS
MET	GLY	THR	LYS	LYS	THR	ILE	LYS
MET	ALA	GLN	LYS	LYS	CYS	GLN	ARG
MET	MET	GLU	GLU	GLU	VAL	VAL	CYS
MET	GLU	ASP	ASP	ASP	THR	THR	PRO
MET	ARG	GLU	LEU	LEU	ILE	ILE	CYS
MET	GLY	GLN	SER	SER	GLU	ASP	GLY
MET	GLY	THR	LEU	LEU	ASP	ILE	THR
MET	GLY	THR	ALA	ALA	PHE	CYS	ARG
MET	ALA	GLN	LYS	LYS	LEU	GLN	CYS
MET	MET	GLU	GLU	GLU	VAL	VAL	GLY
MET	GLU	ASP	ARG	ARG	THR	THR	THR
MET	ARG	GLU	LEU	LEU	LEU	LEU	THR
MET	GLY	GLN	GLY	GLY	GLY	GLY	GLY

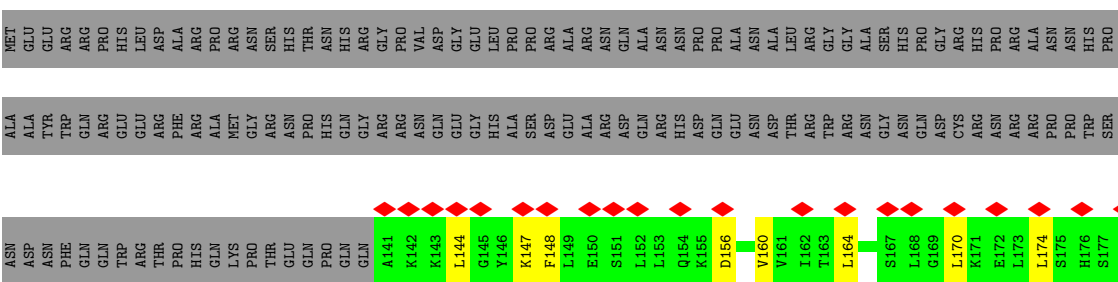
- Molecule 1: NFX1-type zinc finger-containing protein 1

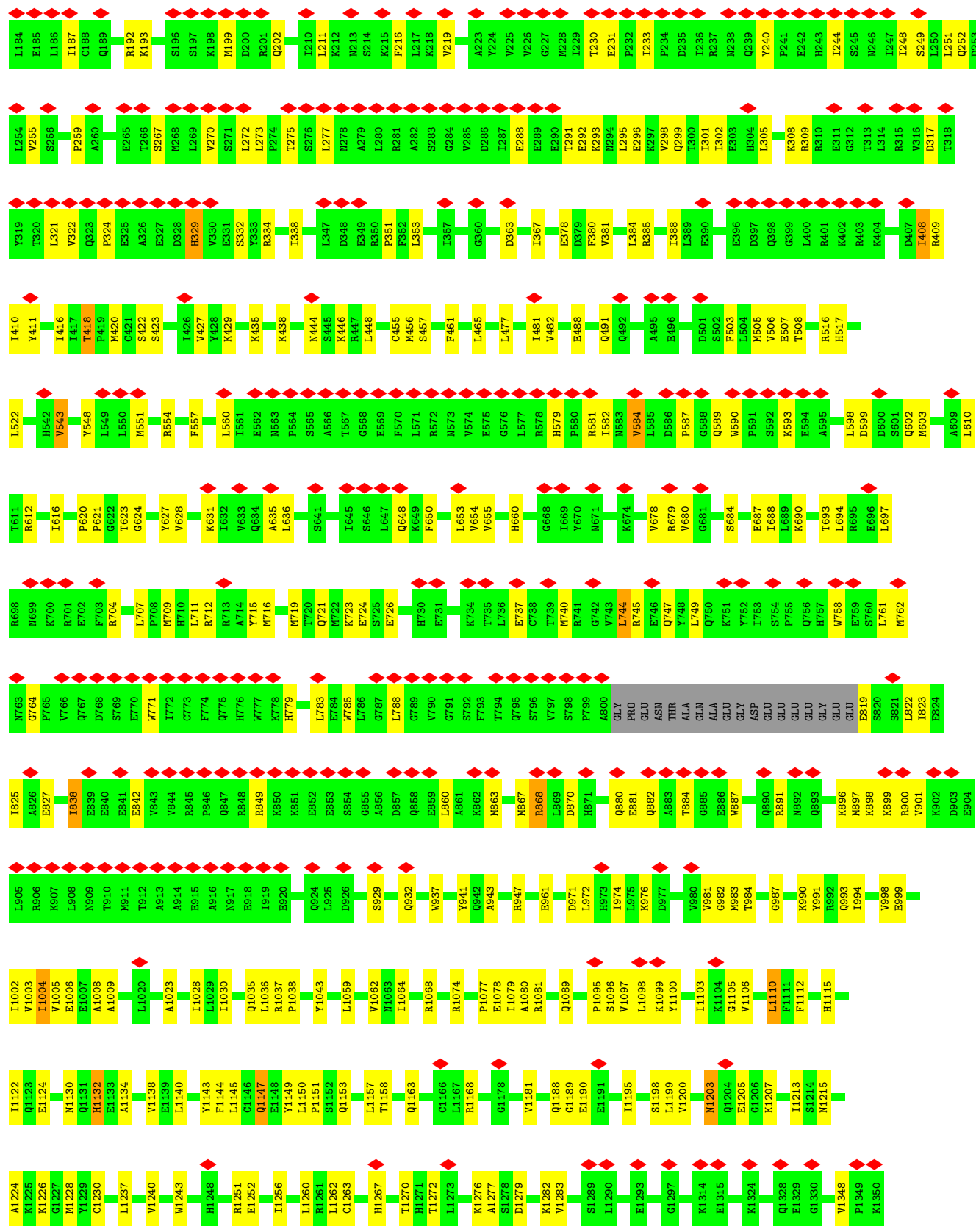


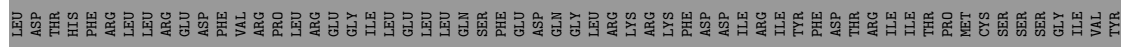
MET	GLU	ALA	ASP	ASN	P234	P351	L494	F608	R741	L831	V844	G764	F608	L494	P351	P234	GLU	ALA
	TYR	TYR	ASN	ASN	D235	F352	L336	L610	R745	A834	R845	F765	A609	L610	P351	D235	GLU	TYR
	TRP	TRP	PHE	GLN	R237	L353	M504	T611	E746		P846	F766	L612	M505	L353	R237	TRP	TYR
	ARG	GLN	GLN	GLN	R238	M506	E613	E613	Q747		R838	F767	E616	E613	M506	Q239	ARG	GLN
	PRO	ARG	TRP	TRP	Y240	S364	V506	L614	L761		E839	F768	L616	E616	Y511	Y240	PRO	ARG
	HIS	GLU	TRP	TRP				L616			E840	F769	E617	E616	F512		GLU	GLU
	LEU	GLU	ARG	ARG				E617				F770	E617	E617	F512		LEU	GLU
	ASP	ARG	PHE	PRO				K625				R849	F771	E617	F512		ASP	ARG
	ALA	ARG	GLN	HIS								R849	F772	E617	R516		ALA	ARG
	PRO	ARG	ALA	GLN				L519				R849	F773	E617	R516		PRO	ARG
ASN	ARG	MET	LYS				V525				R849	F774	E617	R516		ASN	ARG	
ARG	GLY	GLY	PRO				Q526				R849	F775	E617	R516		ARG	GLY	
ASN	THR	THR	THR				E527				R849	F776	E617	R516		ASN	THR	
THR	GLN	ASN	GLU				E528				R849	F777	E617	R516		THR	GLN	
HIS	PRO	HIS	GLN				D529				R849	F778	E617	R516		HIS	PRO	
ASN	PRO	GLN	PRO				R534				R849	F779	E617	R516		ASN	PRO	
GLY	HIS	GLY	GLN				F395				R849	F780	E617	R516		GLY	HIS	
GLY	GLY	ARG	GLY				E396				R849	F781	E617	R516		GLY	GLY	
PRO	ARG	ASN	ASN				D397				R849	F782	E617	R516		PRO	ARG	
VAL	ASN	ASN	ASN				Q398				R849	F783	E617	R516		VAL	ASN	
ASP	GLN	ASN	ASN				C399				R849	F784	E617	R516		ASP	GLN	
GLY	GLU	GLY	GLY				L400				R849	F785	E617	R516		GLY	GLU	
LEU	HIS	HIS	L152				E541				R849	F786	E617	R516		LEU	HIS	
ALA	ALA	ALA	L296				F543				R849	F787	E617	R516		ALA	ALA	
PRO	SER	SER	S158				K544				R849	F788	E617	R516		PRO	SER	
ARG	ASP	ASP	E296				F545				R849	F789	E617	R516		ARG	ASP	
ALA	GLU	GLU	V161				P546				R849	F790	E617	R516		ALA	GLU	
ALA	ALA	ALA	Q298				R547				R849	F791	E617	R516		ALA	ALA	
ASN	ASP	ASP	Q299				R554				R849	F792	E617	R516		ASN	ASP	
ASN	ASN	ASN	L170				Y555				R849	F793	E617	R516		ASN	ASN	
GLN	GLN	GLN	L173				N563				R849	F794	E617	R516		GLN	GLN	
ALA	GLN	GLN	E303				P564				R849	F795	E617	R516		ALA	GLN	
ASN	HIS	HIS	H304				S565				R849	F796	E617	R516		ASN	HIS	
ASN	ASP	ASP	L305				A566				R849	F797	E617	R516		ASN	ASP	
PRO	GLN	GLN	L314				T567				R849	F798	E617	R516		PRO	GLN	
ALA	GLU	GLU					M709				R849	F799	E617	R516		ALA	GLU	
ASN	ASN	ASN	I187				H710				R849	F800	E617	R516		ASN	ASN	
ALA	ASP	ASP	V190				G568				R849	F801	E617	R516		ALA	ASP	
LEU	THR	THR					L711				R849	F802	E617	R516		LEU	THR	
GLY	ARG	ARG	L321				E569				R849	F803	E617	R516		GLY	ARG	
GLY	TRP	TRP	C195				F570				R849	F804	E617	R516		GLY	TRP	
GLY	ARG	ARG	Q323				L571				R849	F805	E617	R516		GLY	ARG	
ALA	ASN	ASN	M199				R572				R849	F806	E617	R516		ALA	ASN	
SER	GLY	GLY	S203				M716				R849	F807	E617	R516		SER	GLY	
HIS	ASN	ASN	W204				K723				R849	F808	E617	R516		HIS	ASN	
GLY	ASN	ASN	L205				V574				R849	F809	E617	R516		GLY	ASN	
PRO	GLN	GLN					E575				R849	F810	E617	R516		PRO	GLN	
GLY	ASP	ASP	L208				Q727				R849	F811	E617	R516		GLY	ASP	
ARG	CYS	CYS					H730				R849	F812	E617	R516		ARG	CYS	
HIS	ARG	ARG	L217				E731				R849	F813	E617	R516		HIS	ARG	
PRO	ASN	ASN					L577				R849	F814	E617	R516		PRO	ASN	
ARG	ARG	ARG	L217				R578				R849	F815	E617	R516		ARG	ARG	
ALA	ARG	ALA	L221				Q747				R849	F816	E617	R516		ALA	ARG	
ASN	PRO	PRO	L221				E475				R849	F817	E617	R516		ASN	PRO	
ASN	PRO	PRO	M336				D476				R849	F818	E617	R516		ASN	PRO	
HIS	THR	THR	V225								R849	F819	E617	R516		HIS	THR	
THR	SEP	SEP	L338				T481				R849	F820	E617	R516		THR	SEP	



● Molecule 1: NFX1-type zinc finger-containing protein 1











4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	258760	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)	1200	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.095	Depositor
Minimum map value	-0.448	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.07	Depositor
Map size ($\text{\AA}$)	331.2, 331.2, 331.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.828, 0.828, 0.828	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: AGS

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	0.18	0/10508	0.45	0/14189
1	B	0.24	0/10508	0.53	0/14189
1	C	0.18	0/10508	0.47	0/14189
1	D	0.22	0/10508	0.51	0/14189
1	E	0.19	0/1361	0.53	0/1836
1	F	0.19	0/1361	0.55	0/1836
All	All	0.21	0/44754	0.50	0/60428

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	10307	0	10368	158	0
1	B	10307	0	10368	198	0
1	C	10307	0	10368	174	0
1	D	10307	0	10368	224	0
1	E	1344	0	1417	36	0
1	F	1344	0	1417	27	0
2	A	31	0	12	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	12	1	0
2	C	31	0	12	2	0
2	D	31	0	12	8	0
All	All	44040	0	44354	809	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 9.

The worst 5 of 809 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:734:LYS:HE3	1:B:857:ASP:HA	1.39	0.99
1:D:621:PRO:HG3	1:D:1035:GLN:HE21	1.28	0.94
1:B:1200:VAL:HG13	1:B:1237:LEU:CD2	2.05	0.85
1:D:621:PRO:HG3	1:D:1035:GLN:NE2	1.93	0.84
1:C:1068:ARG:HH22	1:C:1090:ASP:H	1.27	0.82

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	1278/1918 (67%)	1224 (96%)	54 (4%)	0	100	100
1	B	1278/1918 (67%)	1215 (95%)	63 (5%)	0	100	100
1	C	1278/1918 (67%)	1221 (96%)	57 (4%)	0	100	100
1	D	1278/1918 (67%)	1233 (96%)	45 (4%)	0	100	100
1	E	170/1918 (9%)	163 (96%)	7 (4%)	0	100	100
1	F	170/1918 (9%)	168 (99%)	2 (1%)	0	100	100
All	All	5452/11508 (47%)	5224 (96%)	228 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1162/1726 (67%)	1136 (98%)	26 (2%)	45	63
1	B	1162/1726 (67%)	1136 (98%)	26 (2%)	45	63
1	C	1162/1726 (67%)	1139 (98%)	23 (2%)	48	64
1	D	1162/1726 (67%)	1134 (98%)	28 (2%)	43	62
1	E	159/1726 (9%)	157 (99%)	2 (1%)	61	71
1	F	159/1726 (9%)	157 (99%)	2 (1%)	61	71
All	All	4966/10356 (48%)	4859 (98%)	107 (2%)	45	63

5 of 107 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	322	VAL
1	C	1213	ILE
1	D	1230	CYS
1	C	494	LEU
1	C	730	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	474	GLN
1	D	1147	GLN
1	C	685	ASN
1	D	1035	GLN
1	F	243	HIS

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](#)

4 ligands are 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$
2	AGS	A	2000	-	32,33,33	0.71	0	45,52,52	0.78	0
2	AGS	B	2000	-	32,33,33	0.46	1 (3%)	45,52,52	0.67	1 (2%)
2	AGS	C	2000	-	32,33,33	0.64	0	45,52,52	0.76	1 (2%)
2	AGS	D	2000	-	32,33,33	0.68	1 (3%)	45,52,52	0.56	0

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
2	AGS	A	2000	-	-	5/21/38/38	0/3/3/3
2	AGS	B	2000	-	-	5/21/38/38	0/3/3/3
2	AGS	C	2000	-	-	5/21/38/38	0/3/3/3
2	AGS	D	2000	-	-	2/21/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2000	AGS	PG-S1G	2.14	1.95	1.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2000	AGS	PG-S1G	2.01	1.95	1.90

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2000	AGS	PB-O3B-PG	-3.39	120.76	133.17
2	C	2000	AGS	PB-O3B-PG	-2.75	123.12	133.17

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

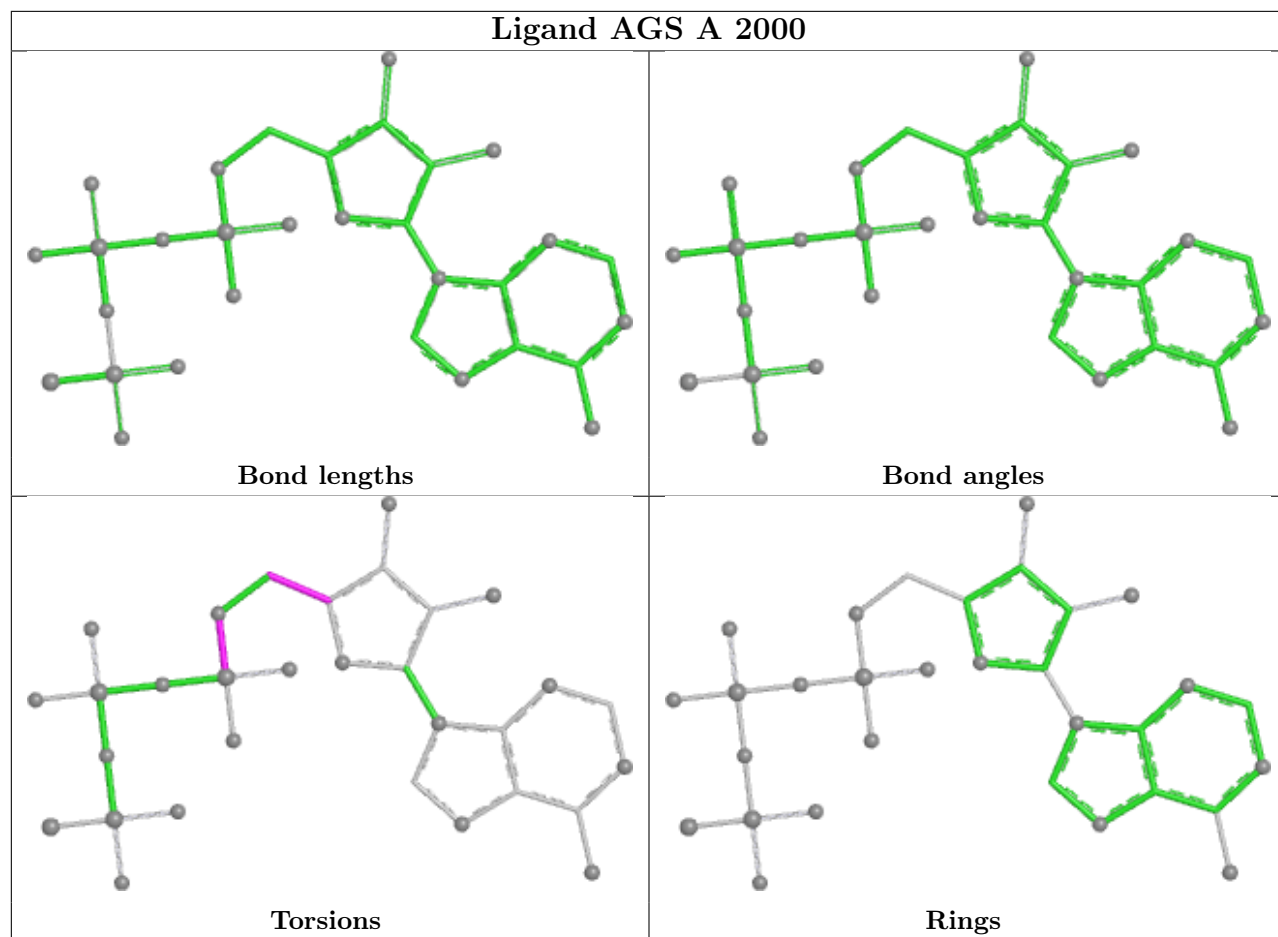
Mol	Chain	Res	Type	Atoms
2	A	2000	AGS	C5'-O5'-PA-O1A
2	A	2000	AGS	C5'-O5'-PA-O2A
2	A	2000	AGS	C5'-O5'-PA-O3A
2	B	2000	AGS	C5'-O5'-PA-O1A
2	B	2000	AGS	C5'-O5'-PA-O3A

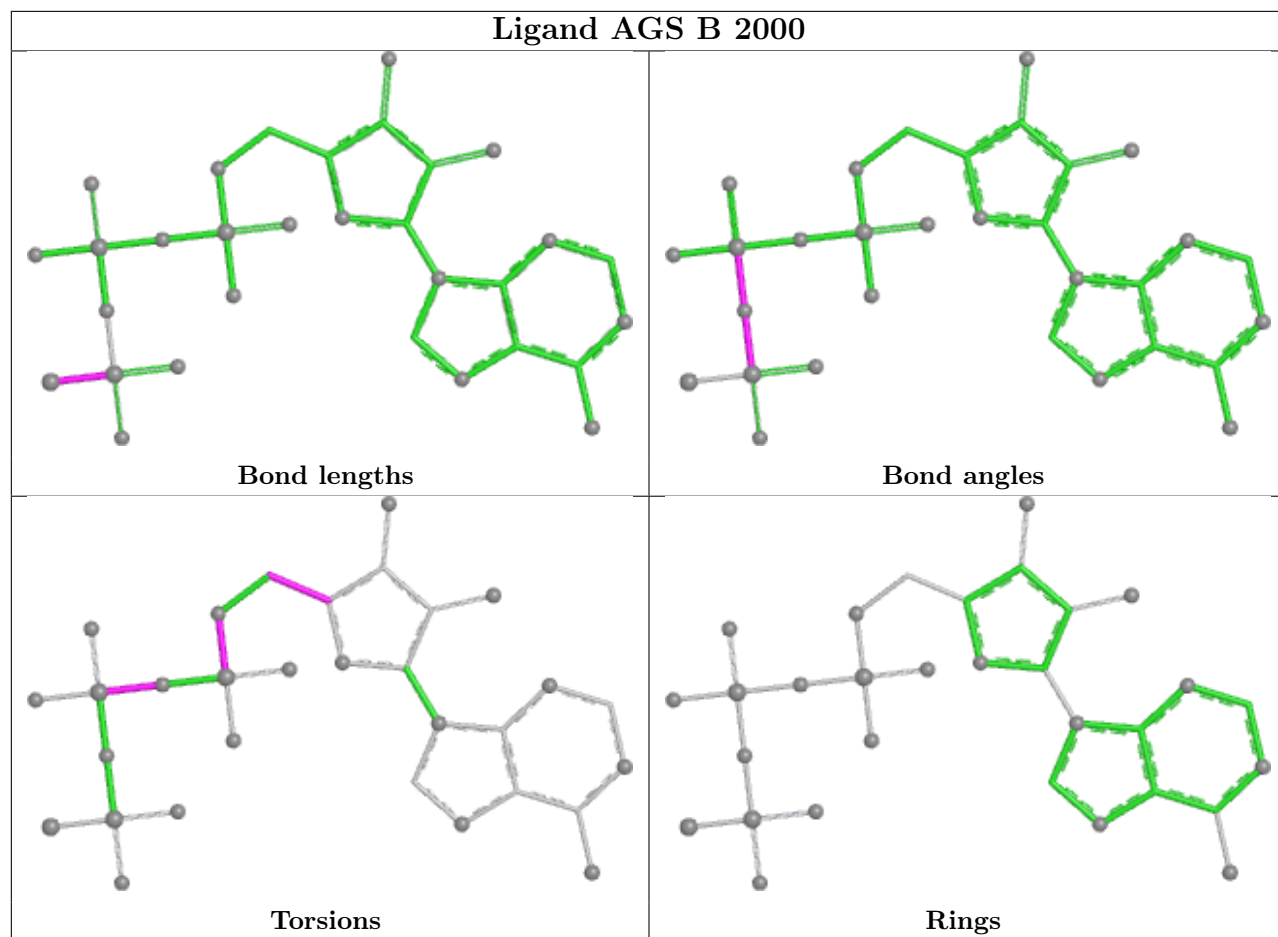
There are no ring outliers.

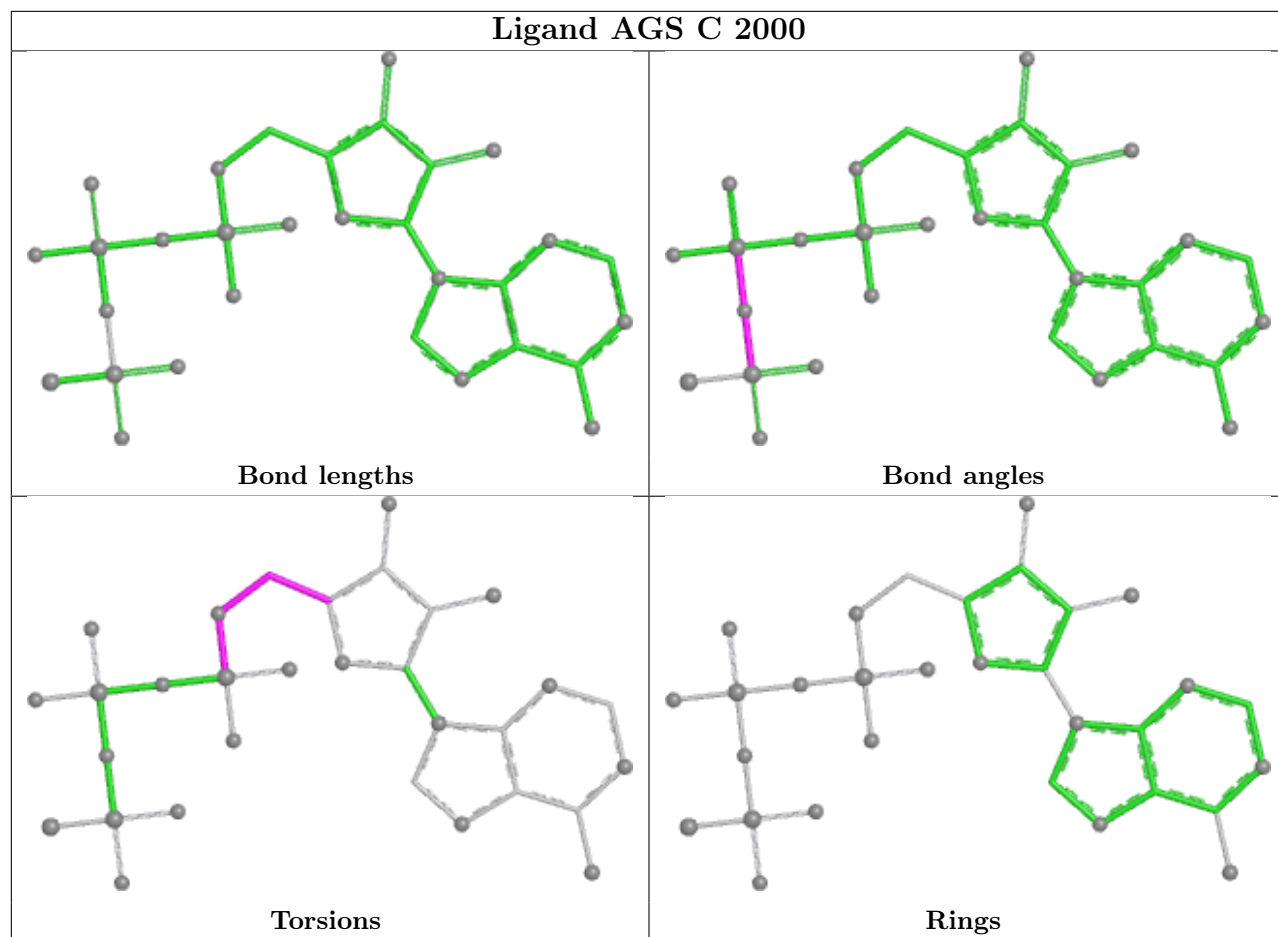
4 monomers are involved in 16 short contacts:

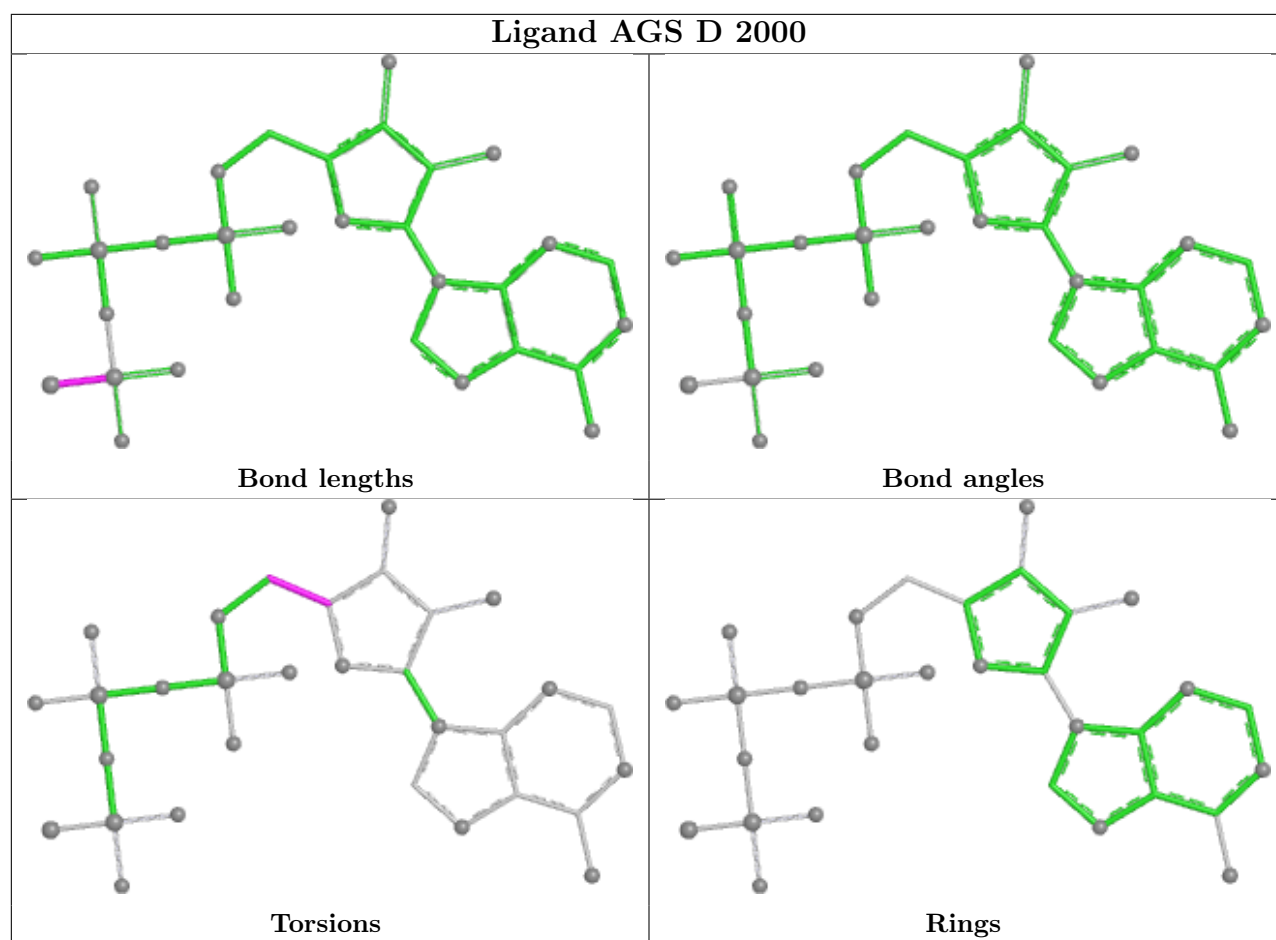
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2000	AGS	5	0
2	B	2000	AGS	1	0
2	C	2000	AGS	2	0
2	D	2000	AGS	8	0

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 than 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.









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.

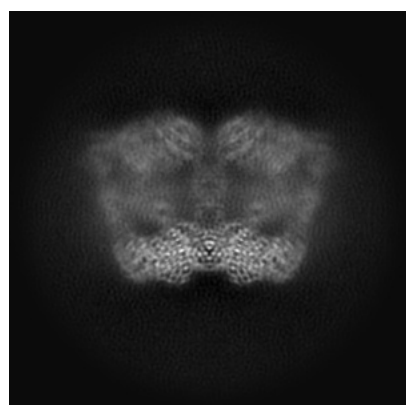
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-75702. These allow visual inspection of the internal detail of the map and identification of artifacts.

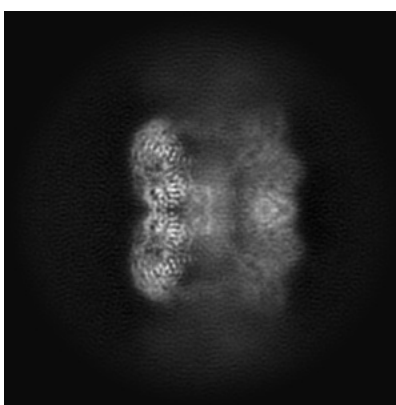
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

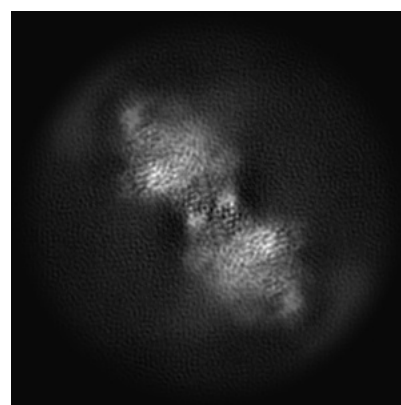
6.1.1 Primary map



X



Y

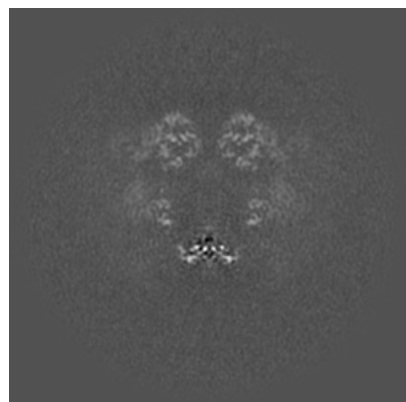


Z

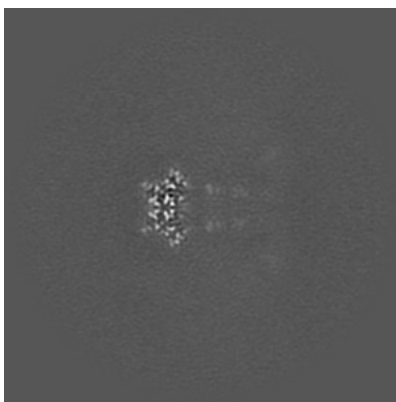
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

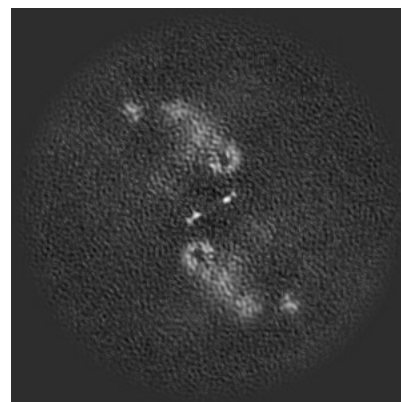
6.2.1 Primary map



X Index: 200



Y Index: 200

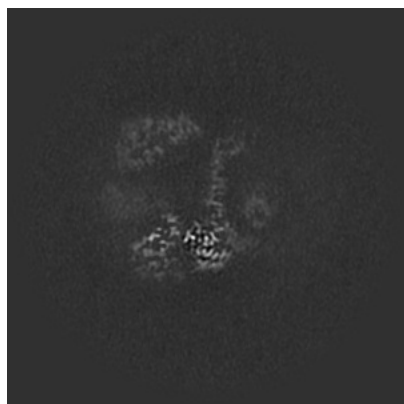


Z Index: 200

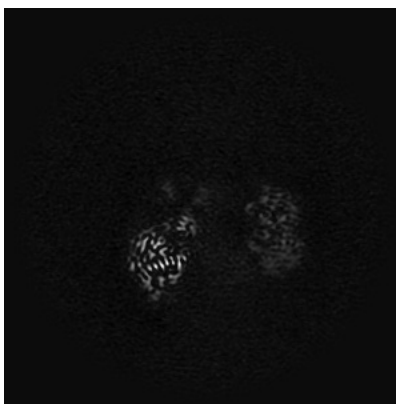
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

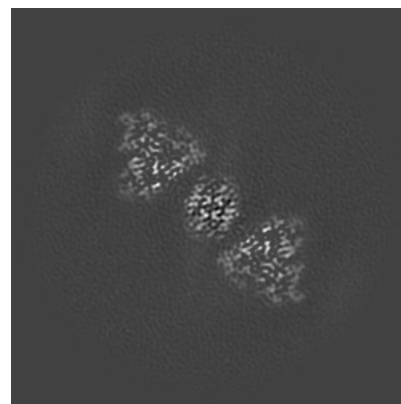
6.3.1 Primary map



X Index: 220



Y Index: 235

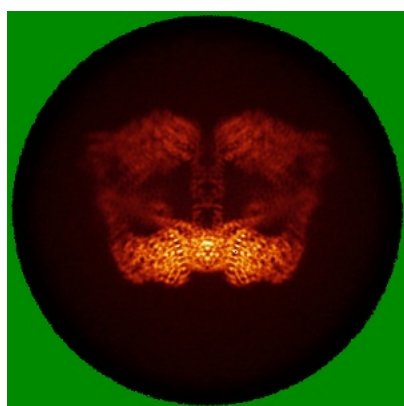


Z Index: 156

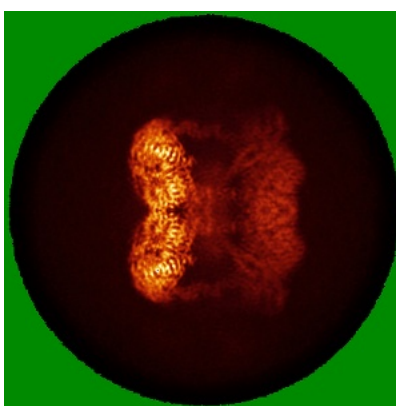
The images above show the largest variance slices of the map in three orthogonal directions.

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

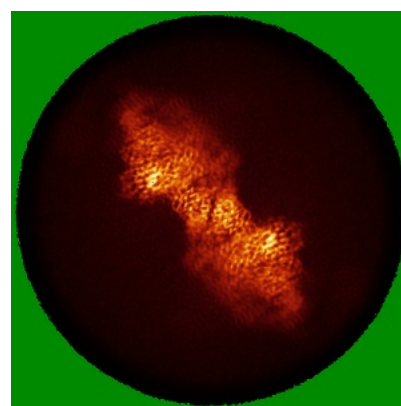
6.4.1 Primary map



X



Y

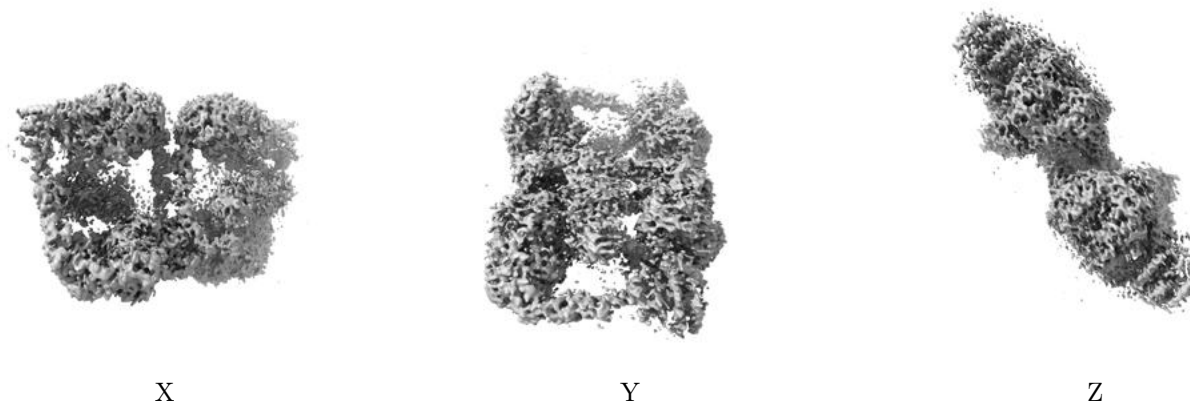


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

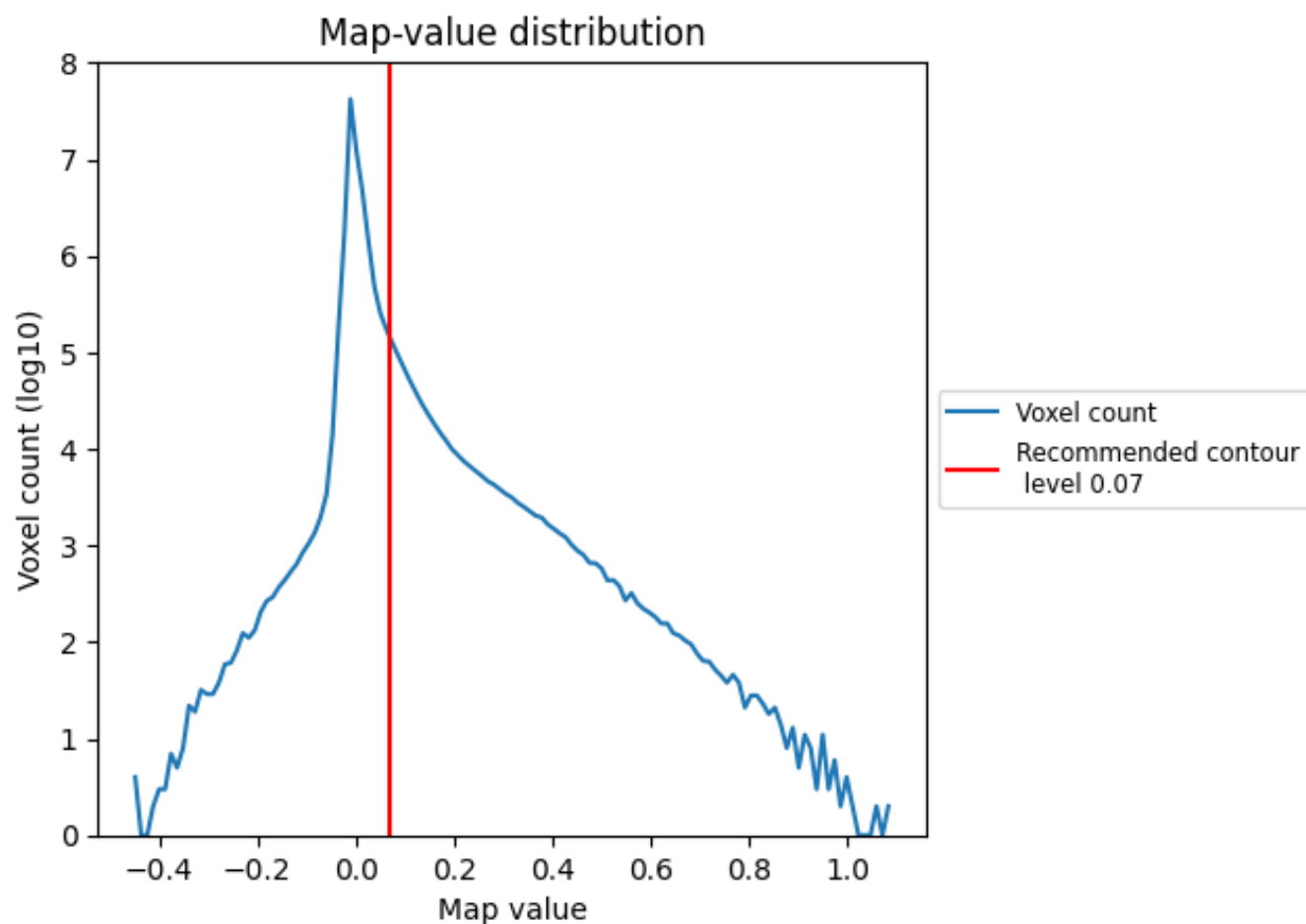
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

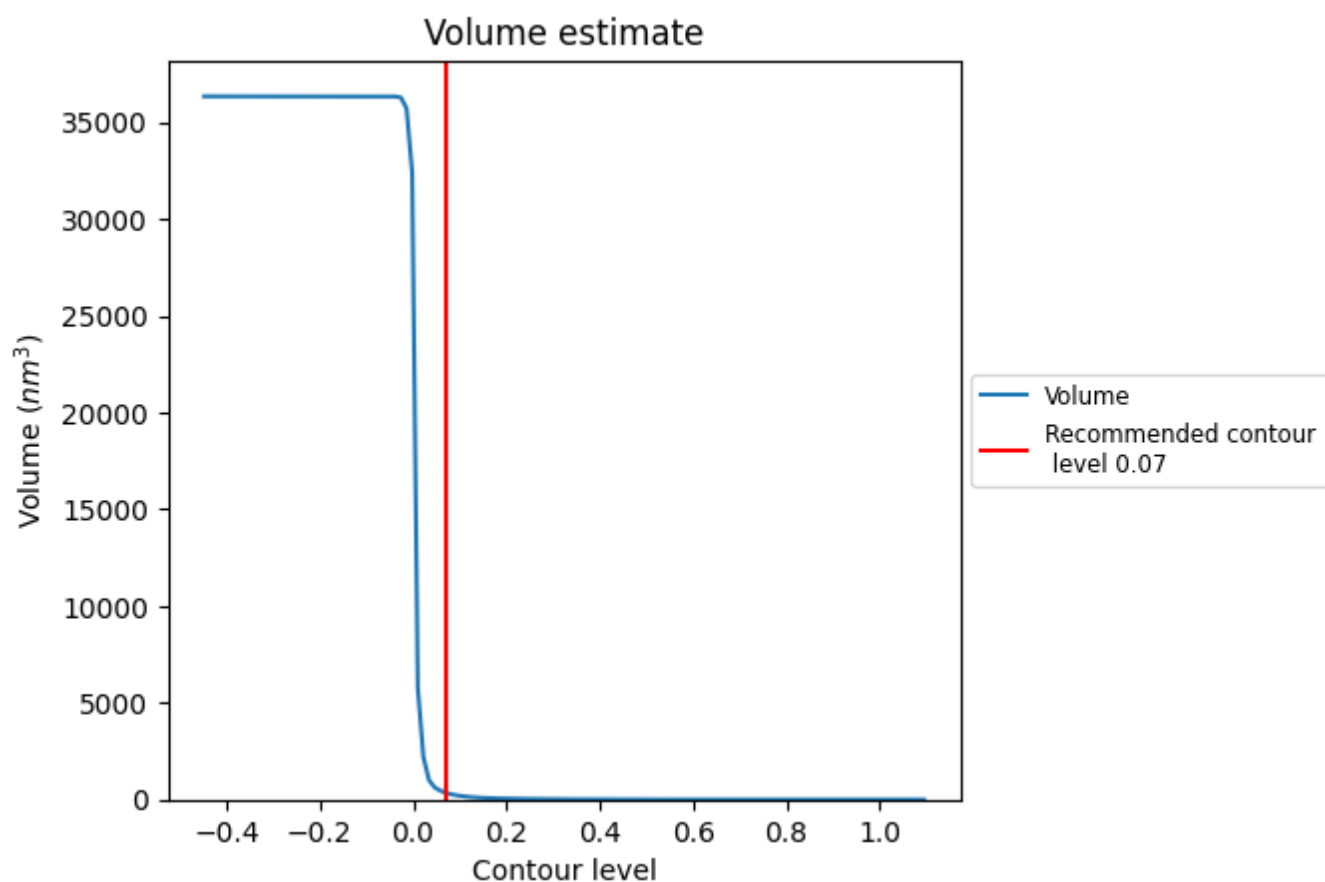
This section contains the results of statistical analysis of the map.

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.

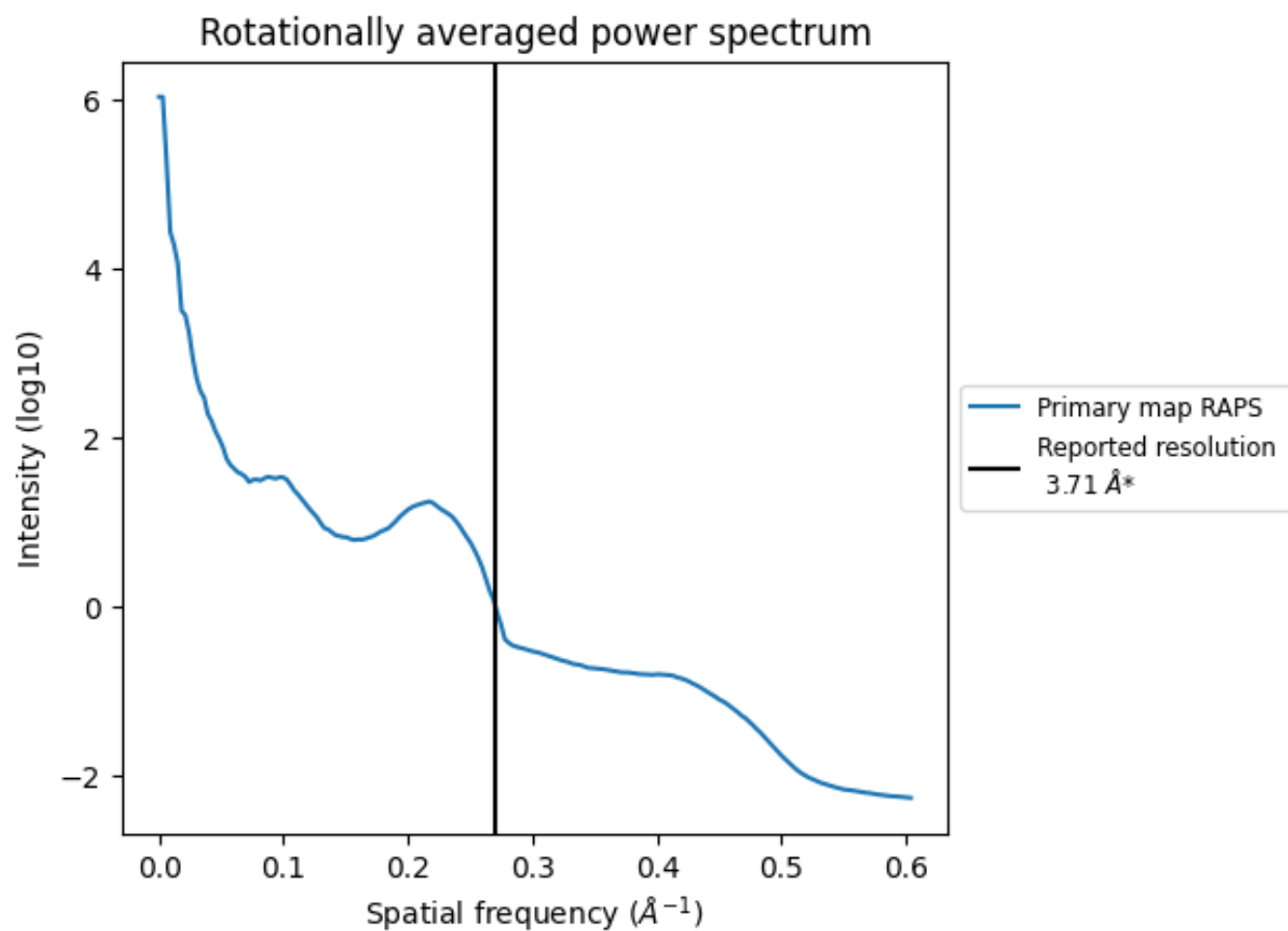
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 351 nm^3 ; this corresponds to an approximate mass of 317 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

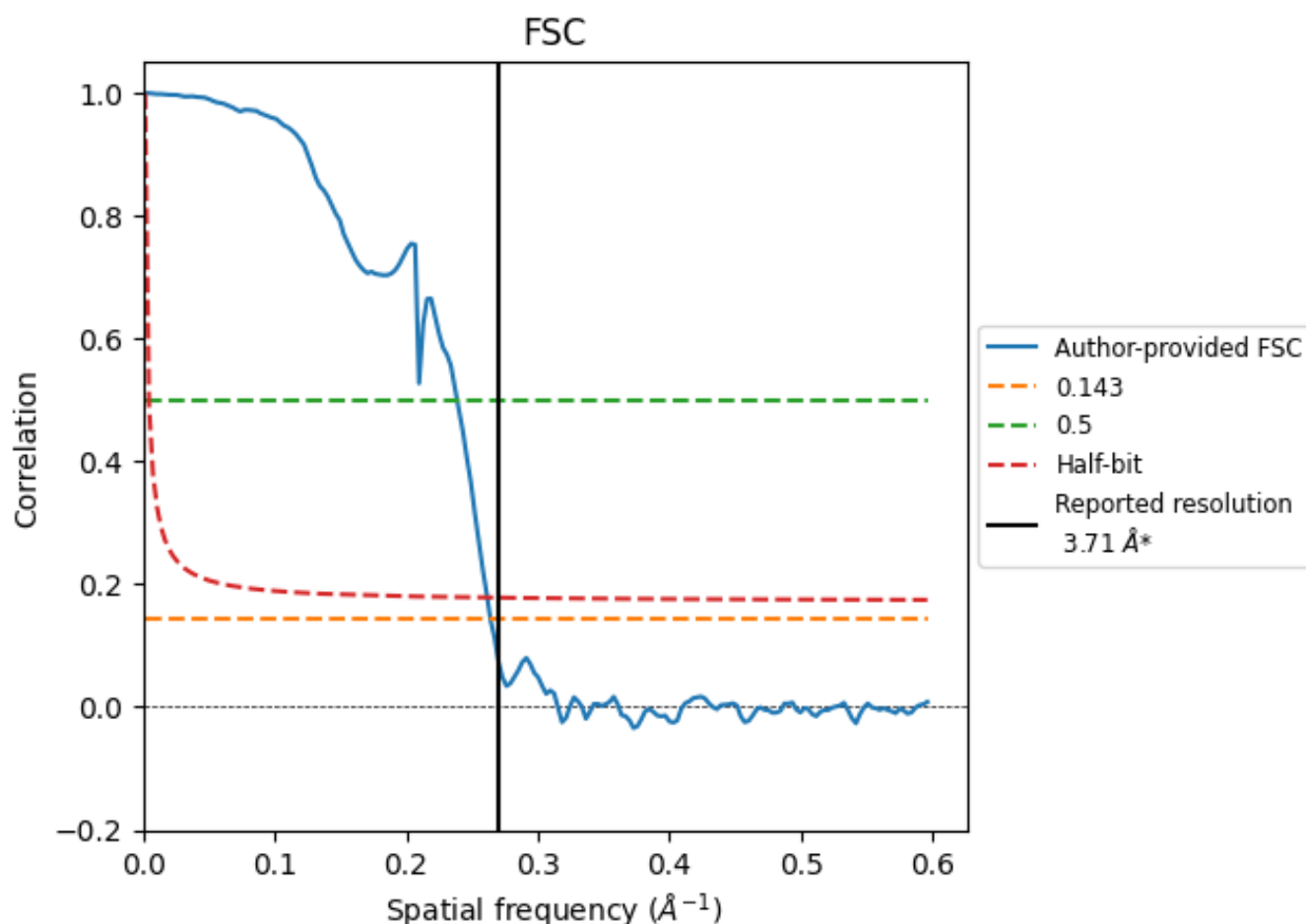


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

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 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

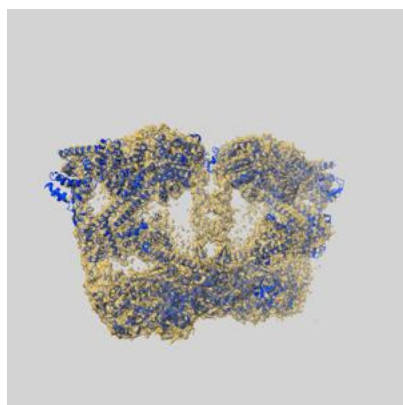
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.71	-	-
Author-provided FSC curve	3.79	4.19	3.82
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

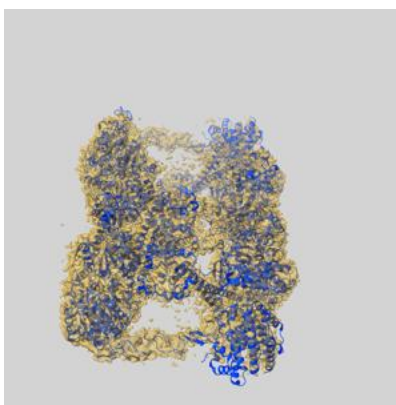
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-75702 and PDB model 11HT. Per-residue inclusion information can be found in section [3](#) on page [6](#).

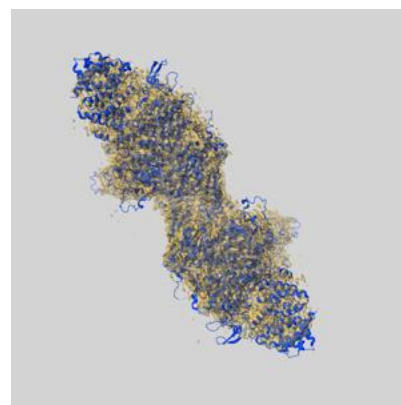
9.1 Map-model overlay [i](#)



X



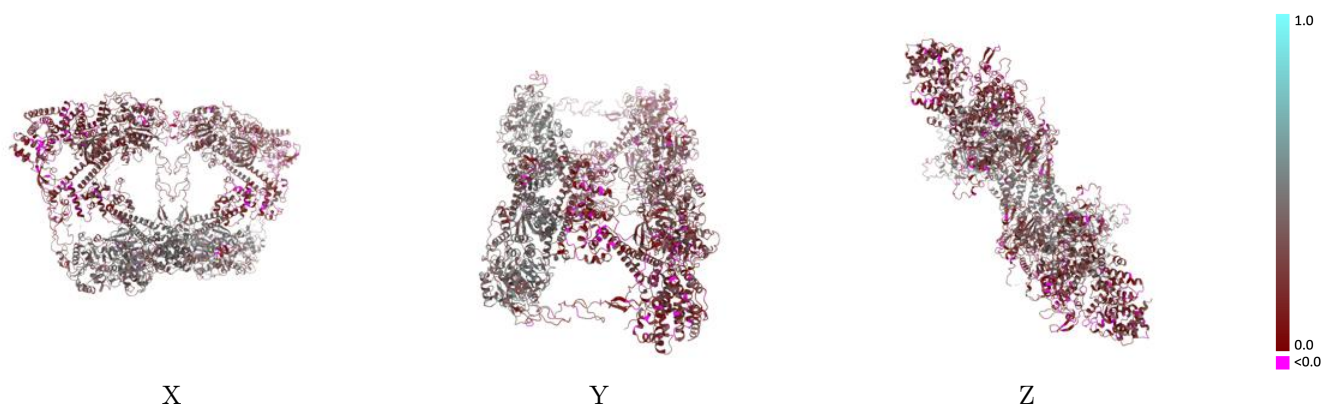
Y



Z

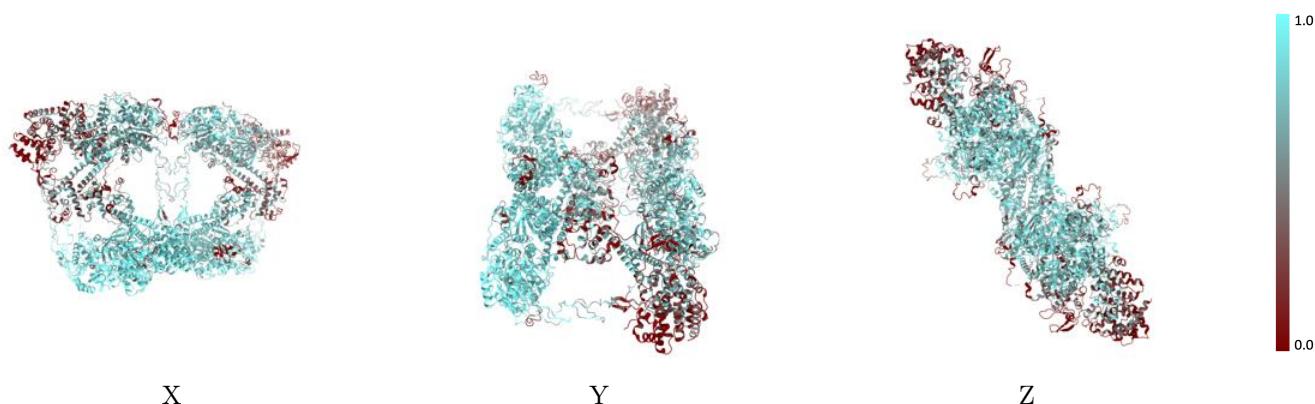
The images above show the 3D surface view of the map at the recommended contour level 0.07 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



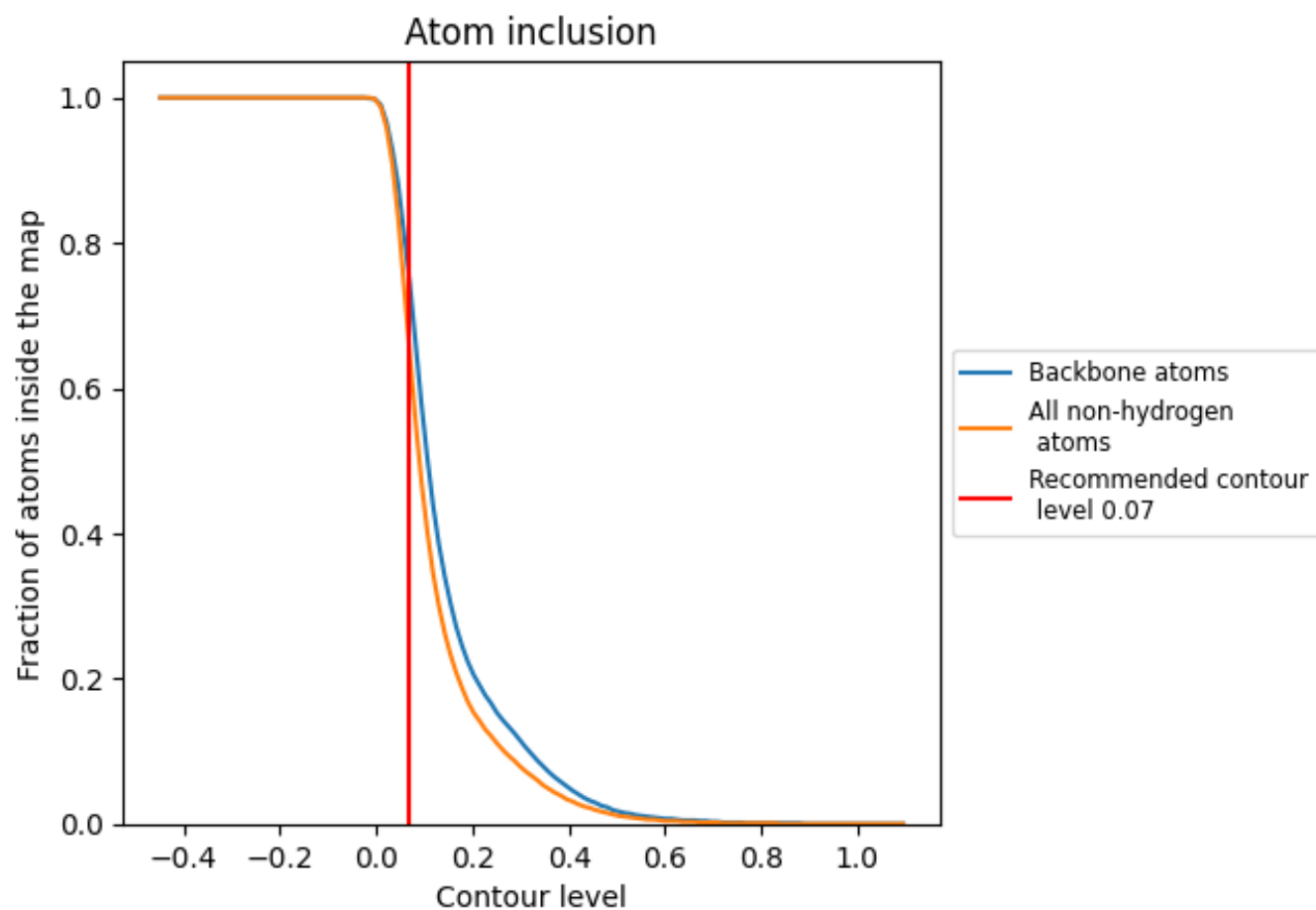
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.07).

9.4 Atom inclusion ⓘ



At the recommended contour level, 75% of all backbone atoms, 65% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6480	0.2930
A	0.7720	0.3580
B	0.5880	0.2450
C	0.7710	0.3560
D	0.5720	0.2360
E	0.2280	0.1950
F	0.2340	0.2060

1.0

0.0

<0.0