



wwPDB EM Validation Summary Report ⓘ

Mar 23, 2026 – 02:37 PM UTC

PDB ID : 4CRN / pdb_00004crn
EMDB ID : EMD-2597
Title : Cryo-EM of a pretermination complex with eRF1 and eRF3
Authors : Preis, A.; Heuer, A.; Barrio-Garcia, C.; Hauser, A.; Eyler, D.; Berninghausen, O.; Green, R.; Becker, T.; Beckmann, R.
Deposited on : 2014-02-28
Resolution : 9.10 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
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) : 2.49

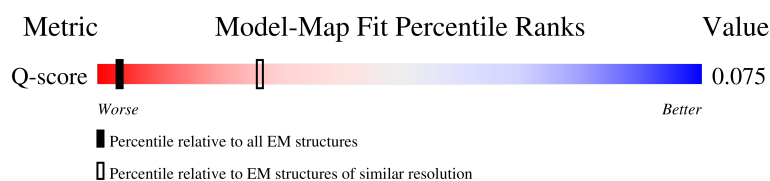
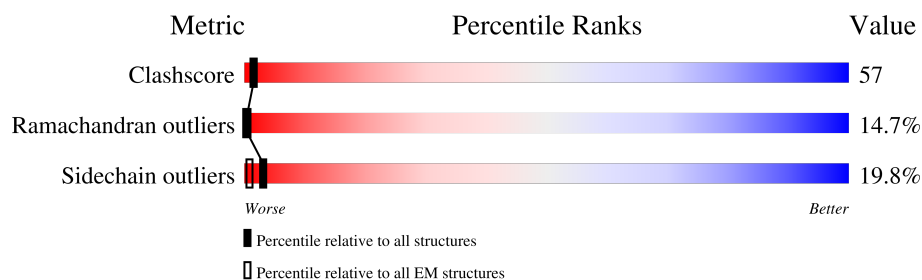
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 9.10 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	225 (8.70 - 9.60)

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	P	430	
2	X	437	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GNP	P	1685	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6693 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 ERF3 IN RIBOSOME BOUND ERF1-ERF3-GDPNP COMPLEX.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P	430	Total	C	N	O	S	0	0
			3351	2119	577	634	21		

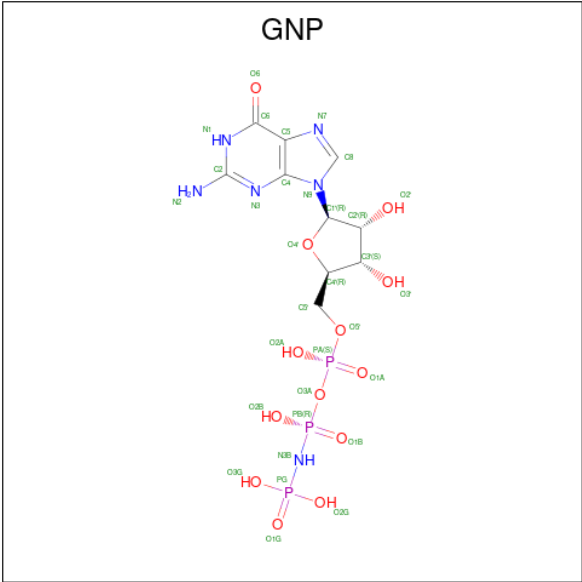
- Molecule 2 is a protein called ERF1 IN RIBOSOME-BOUND ERF1-ERF3-GDPNP COMPLEX.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	422	Total	C	N	O	S	0	1
			3310	2110	548	642	10		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	41	LEU	GLN	conflict	UNP P12385
X	300	PHE	TYR	conflict	UNP P12385

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (CCD ID: GNP) (formula: $C_{10}H_{17}N_6O_{13}P_3$).

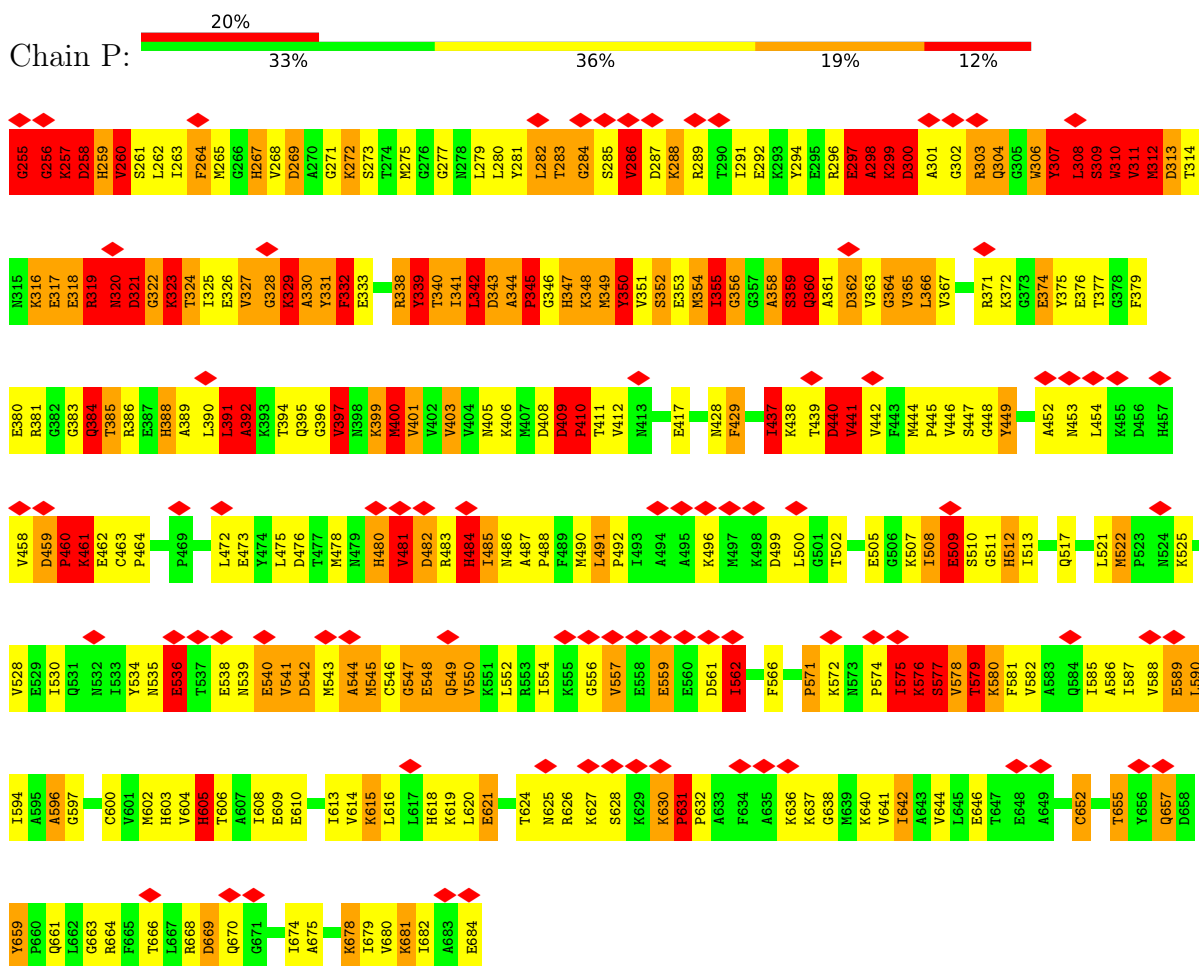


Mol	Chain	Residues	Atoms					AltConf
3	P	1	Total	C	N	O	P	0
			32	10	6	13	3	

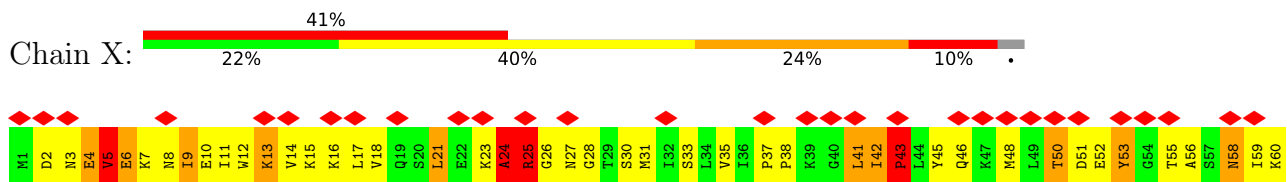
3 Residue-property plots

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: ERF3 IN RIBOSOME BOUND ERF1-ERF3-GDPNP COMPLEX



• Molecule 2: ERF1 IN RIBOSOME-BOUND ERF1-ERF3-GDPNP COMPLEX



ASP	V664	D304	A244	S183	Y122	S61
GLU	S365	T306	C245	A184	L123	R62
ASP	E366	L306	K246	L185	C124	V63
GLU	E367	K307	V247	R186	D125	R64
GLY	A308	A309	I248	F187	N126	R65
SER	P368	L309	S249	A188	K127	L66
ASP	L369	D310	I250	R189	F128	S67
ASP	T370	L311	V251	L190	H129	V68
ASP	E371	G312	D252	R191	T130	L69
ASP	W372	A313	V253	E192	E131	S70
PHE	L373	V314	S254	F193	V132	A71
ILE	A374	E315	Y255	K194	L136	I72
	A376	K316	G256	R195	Q138	T73
	N376	L317	G257	H196	A139	Q76
	Y377	T318	E258	N197	D140	Q77
	K378	V319	N259	Y198	D141	K78
	N379	F320	G260	V199	K142	L79
	F380	E321	F261	K200	F143	K80
		N322	N262	K201	G144	L81
		L323	Q263	V202	F145	Y82
	T383	E324	A264	A203	V147	N83
	L384	T325	I265	E204	M148	T84
	E385	L326	E266	V205	D149	L85
	F386	R327	L267	A206	G151	K87
	L387	Y328	S268	V207	T153	N88
	T388	T329	A269	Q208	L154	L90
	D389	F330	E270	N209	F155	V91
	K390	K331	A271	N210	C94	L92
	S391	D332	L272	I211	V158	Y93
	S392	A333	N274	T212	G95	G94
	G394	E334	K275	N213	D96	D96
	A395	D335	K276	D214	I97	I97
	Q396	D336	Y277	K215	I98	I98
	F397	N336	V278	V216	T99	E100
	V398	E337	Q279	V217	E101	D101
	T399	V338	E280	N218	G102	G102
	G400	T339	K281	V218	K103	K103
	F401	K340	K282	K219	E104	E104
	G402	F341	L283	G220	K105	K105
	G403	A342	L284	G221	K106	K106
	I404	E343	E285	L221	T107	T107
	G405	F344	A286	I222	T108	T108
	A406	E345	Y287	L223	F109	F109
	M407	A346	F289	D226	D110	D110
	L408	K347	D289	A227	P174	P174
	R409	D348	I291	D228	K175	K175
	Y410	K349	E290	D229	K176	K176
	K411	S350	Q292	F229	H177	H177
	V412	A352	D294	K230	K168	K168
	Q416	T353	T295	T231	F169	F169
	L417	D354	G296	L233	T170	T170
	V418	K355	K297	A234	V171	V171
	V419	A356	F298	K235	D172	D172
	E420	T357	C299	S236	L173	L173
	S421	G358	F300	E237	P176	P176
	E422	Q359	G301	L238	K177	K177
ASP		E360	I302	F239	H178	H178
GLU		K361	D240	D241	G178	G178
TYR		D362	P241	R242	R179	R179
TYR		V363	L243		G180	G180

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	39309	Depositor
Resolution determination method	Not provided	
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	0.02	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	147136	Depositor
Image detector	TVIPS TEMCAM-F416 (4k x 4k)	Depositor
Maximum map value	0.922	Depositor
Minimum map value	-0.456	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.183	Depositor
Map size ($\text{\AA}$)	455.4, 455.4, 455.4	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.2375, 1.2375, 1.2375	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: GNP

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	P	1.26	19/3412 (0.6%)	2.17	159/4600 (3.5%)
2	X	2.57	70/3363 (2.1%)	3.06	285/4532 (6.3%)
All	All	2.02	89/6775 (1.3%)	2.65	444/9132 (4.9%)

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	P	0	95
2	X	1	25
All	All	1	120

The worst 5 of 89 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	379	ASN	CG-ND2	97.10	3.37	1.33
2	X	183	SER	C-N	37.41	1.86	1.33
2	X	182	GLN	C-N	29.27	1.71	1.33
2	X	421	SER	C-N	-23.48	1.00	1.33
1	P	330	ALA	C-N	23.23	1.66	1.33

The worst 5 of 444 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	379	ASN	OD1-CG-ND2	-103.21	19.39	122.60
2	X	183	SER	O-C-N	31.26	159.49	122.92
2	X	269	ALA	O-C-N	-29.58	83.25	122.59
1	P	320	ASN	CA-C-N	18.20	156.31	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	320	ASN	C-N-CA	18.20	156.31	121.54

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	X	142	LYS	CA

5 of 120 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	P	255	GLY	Mainchain
1	P	256	GLY	Peptide
1	P	257	LYS	Mainchain
1	P	260	VAL	Peptide
1	P	264	PHE	Mainchain

5.2 Too-close contacts

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	P	3351	0	3391	346	0
2	X	3310	0	3338	440	0
3	P	32	0	12	56	0
All	All	6693	0	6741	769	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 57.

The worst 5 of 769 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:P:331:TYR:CZ	1:P:536:GLU:HG3	1.34	1.59
1:P:304:GLN:NE2	3:P:1685:GNP:H3'	1.15	1.47
2:X:182:GLN:C	2:X:183:SER:N	1.71	1.45
2:X:352:ALA:CB	2:X:361:MET:HG3	1.46	1.44
2:X:343:GLU:HB3	2:X:344:PRO:CD	1.45	1.43

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	P	428/430 (100%)	299 (70%)	69 (16%)	60 (14%)	0	3
2	X	420/437 (96%)	297 (71%)	58 (14%)	65 (16%)	0	3
All	All	848/867 (98%)	596 (70%)	127 (15%)	125 (15%)	0	3

5 of 125 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	258	ASP
1	P	260	VAL
1	P	285	SER
1	P	298	ALA
1	P	300	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	P	365/365 (100%)	299 (82%)	66 (18%)	2	9
2	X	362/377 (96%)	284 (78%)	78 (22%)	1	6
All	All	727/742 (98%)	583 (80%)	144 (20%)	3	7

5 of 144 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	X	280	GLU
2	X	412	VAL
2	X	284	LEU
2	X	330	PHE
1	P	549	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
2	X	177	HIS
2	X	196	HIS
2	X	396	GLN
2	X	279	GLN
2	X	376	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](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GNP	P	1685	-	34,34,34	1.62	5 (14%)	47,54,54	1.12	4 (8%)

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
3	GNP	P	1685	-	-	4/18/38/38	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1685	GNP	PA-O3A	-5.40	1.53	1.59
3	P	1685	GNP	PB-O3A	-4.43	1.53	1.59
3	P	1685	GNP	PB-O2B	-3.21	1.48	1.56
3	P	1685	GNP	PG-O2G	-3.18	1.48	1.56
3	P	1685	GNP	PG-O1G	2.31	1.49	1.46

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	1685	GNP	O2B-PB-O1B	3.46	117.29	109.87
3	P	1685	GNP	O2G-PG-O3G	3.40	116.73	107.59
3	P	1685	GNP	O3G-PG-O1G	-3.15	105.56	113.45
3	P	1685	GNP	O1G-PG-N3B	-2.64	107.89	111.77

There are no chirality outliers.

All (4) torsion outliers are listed below:

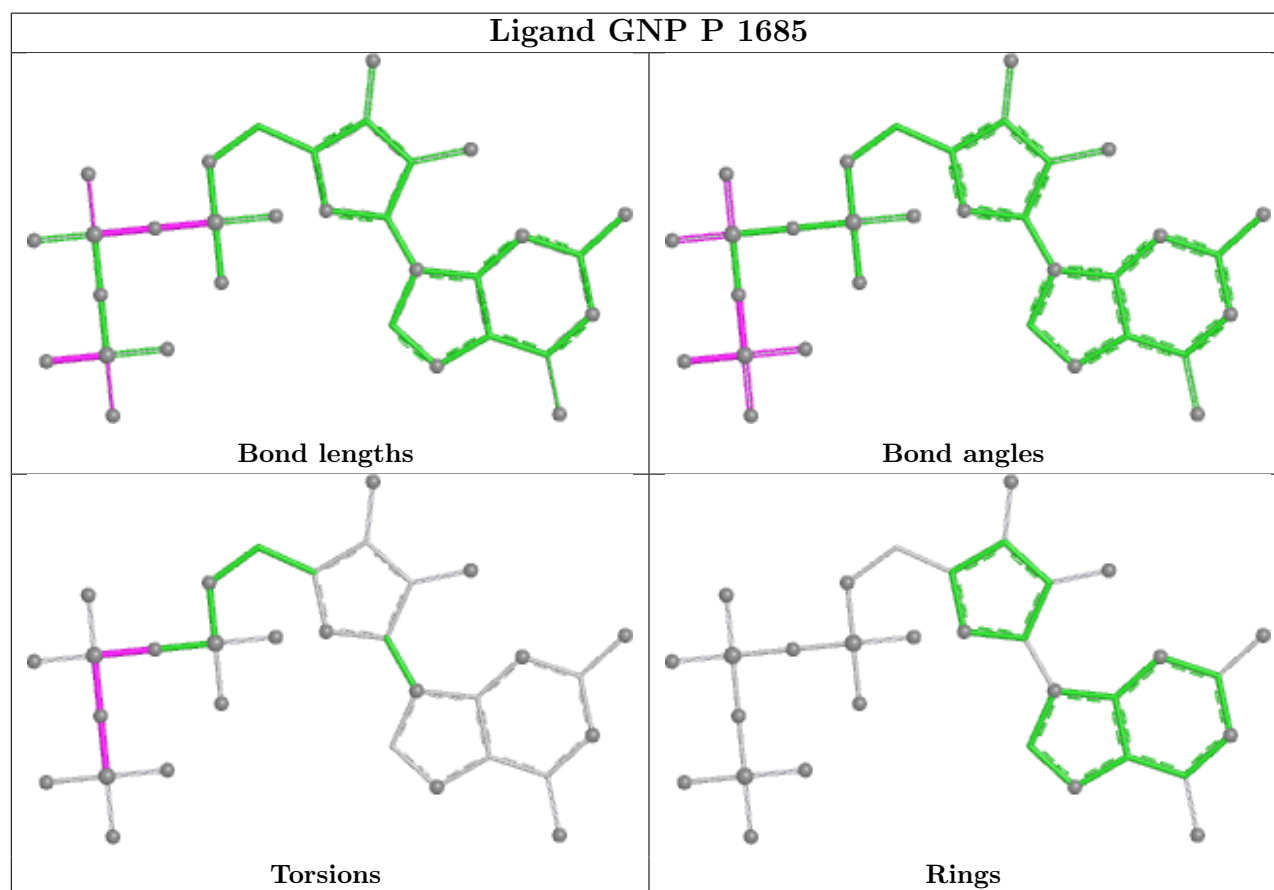
Mol	Chain	Res	Type	Atoms
3	P	1685	GNP	PB-N3B-PG-O1G
3	P	1685	GNP	PG-N3B-PB-O1B
3	P	1685	GNP	PG-N3B-PB-O3A
3	P	1685	GNP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 56 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	P	1685	GNP	56	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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	X	4
1	P	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	183:SER	C	184:ALA	N	1.86
1	X	182:GLN	C	183:SER	N	1.71
1	P	330:ALA	C	331:TYR	N	1.66
1	X	269:ALA	C	270:GLU	N	1.10
1	X	421:SER	C	422:GLU	N	1.00

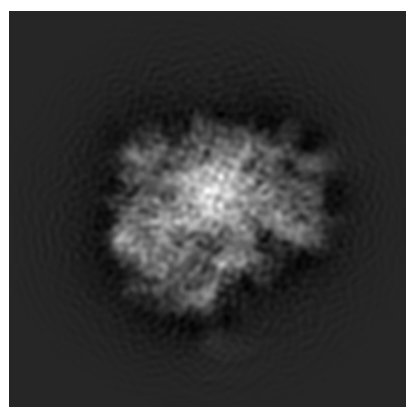
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-2597. These allow visual inspection of the internal detail of the map and identification of artifacts.

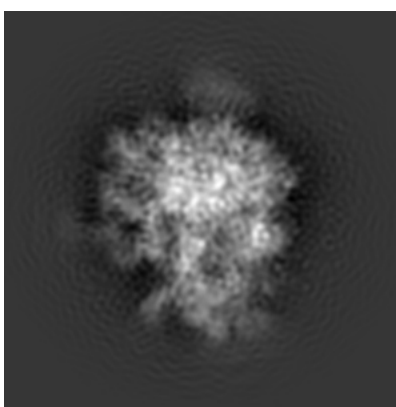
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

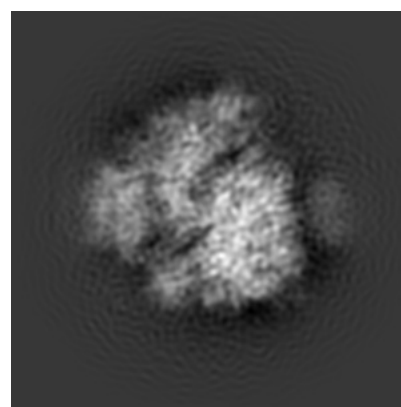
6.1.1 Primary map



X



Y

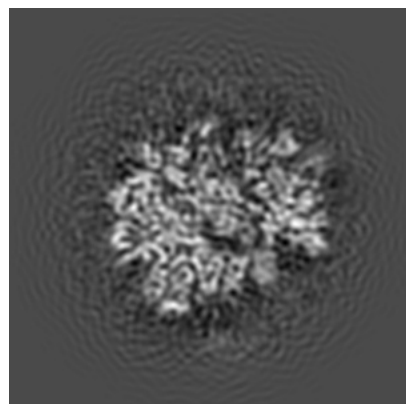


Z

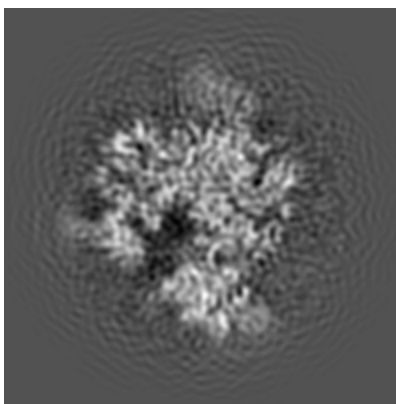
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

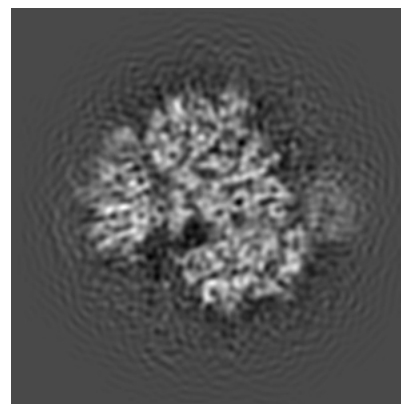
6.2.1 Primary map



X Index: 184



Y Index: 184

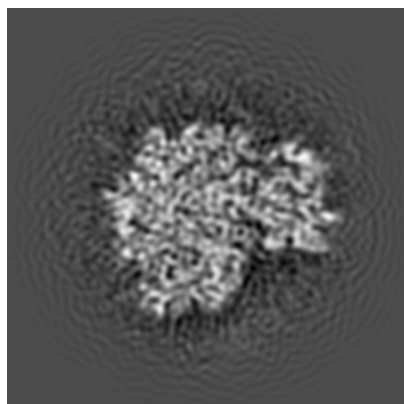


Z Index: 184

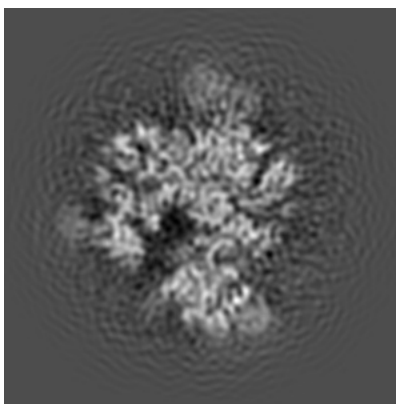
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

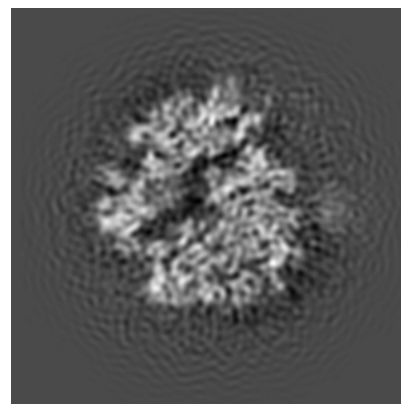
6.3.1 Primary map



X Index: 194



Y Index: 186

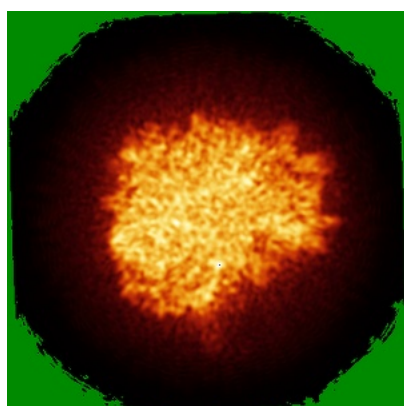


Z Index: 168

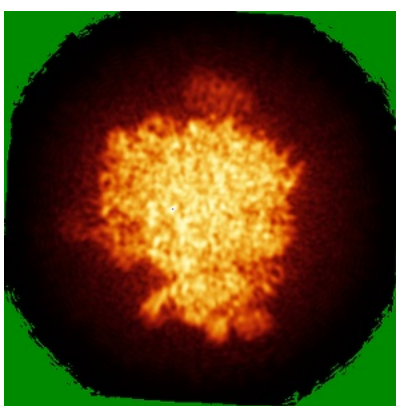
The images above show the largest variance slices of the map in three orthogonal directions.

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

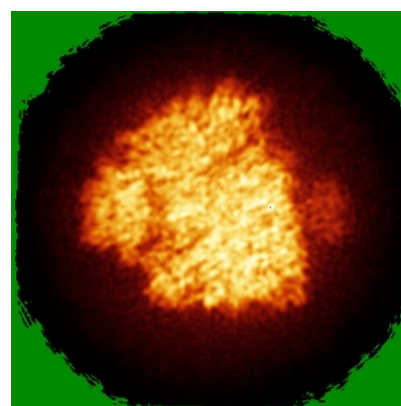
6.4.1 Primary map



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 0.183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

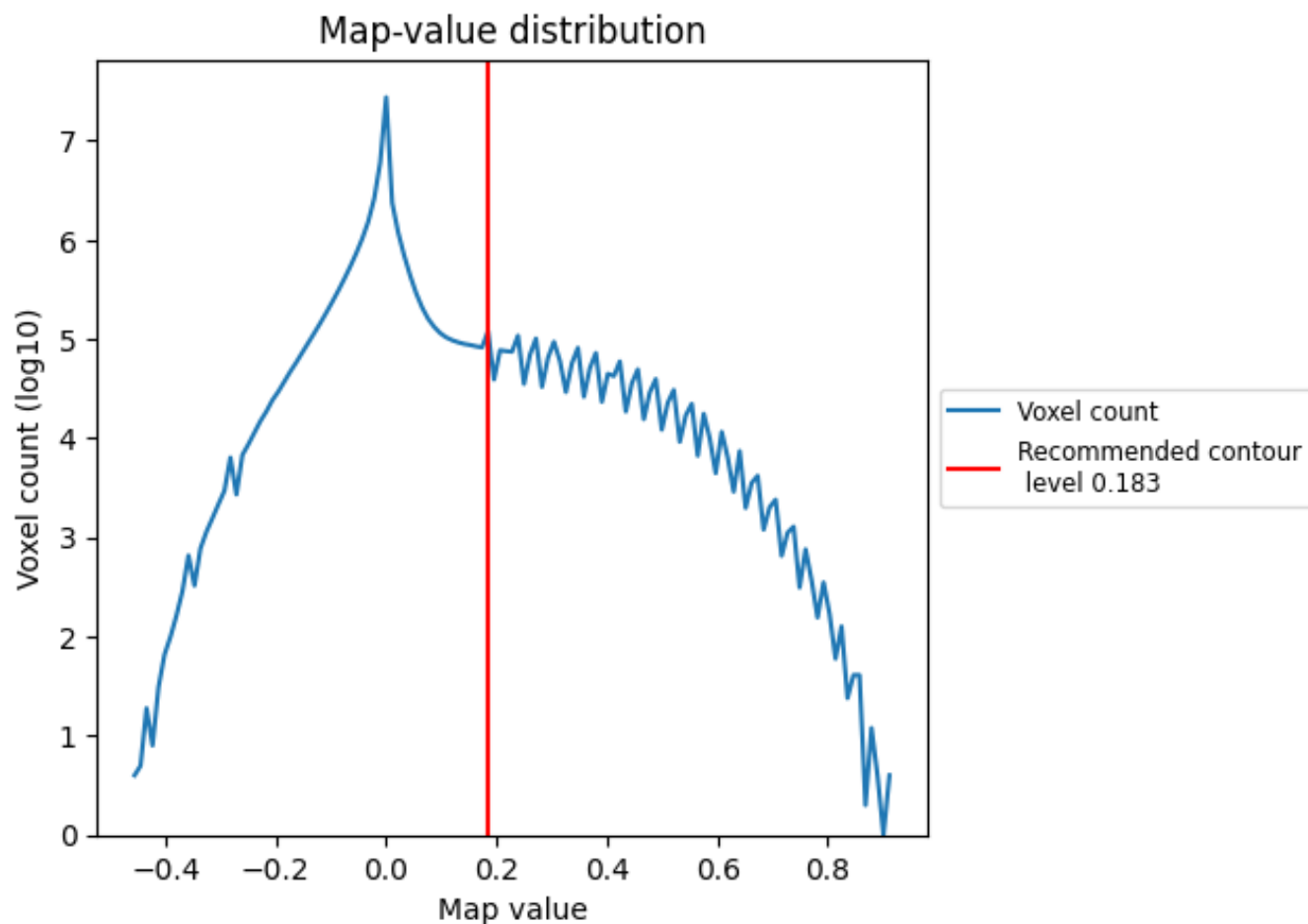
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

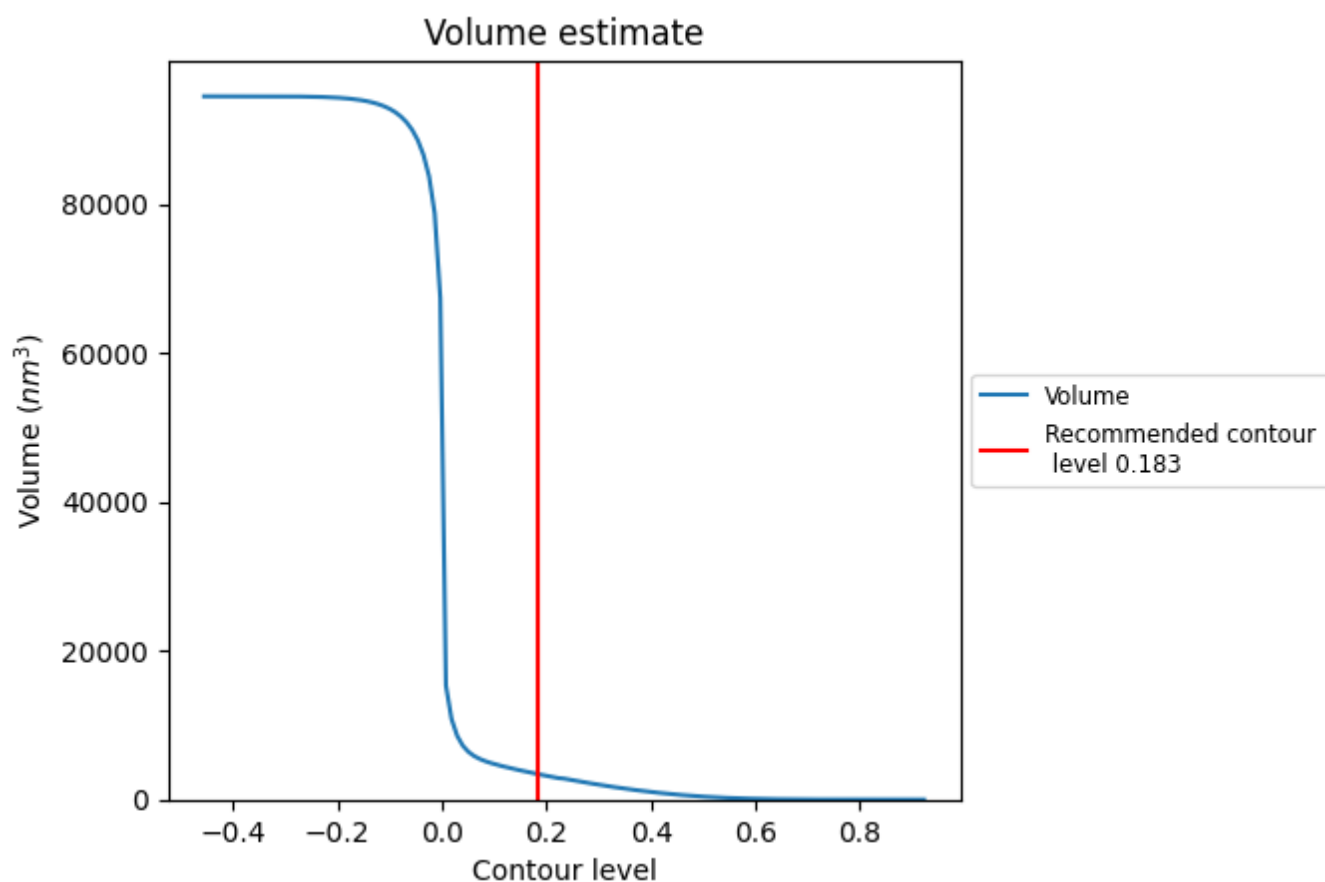
This section contains the results of statistical analysis of the map.

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.

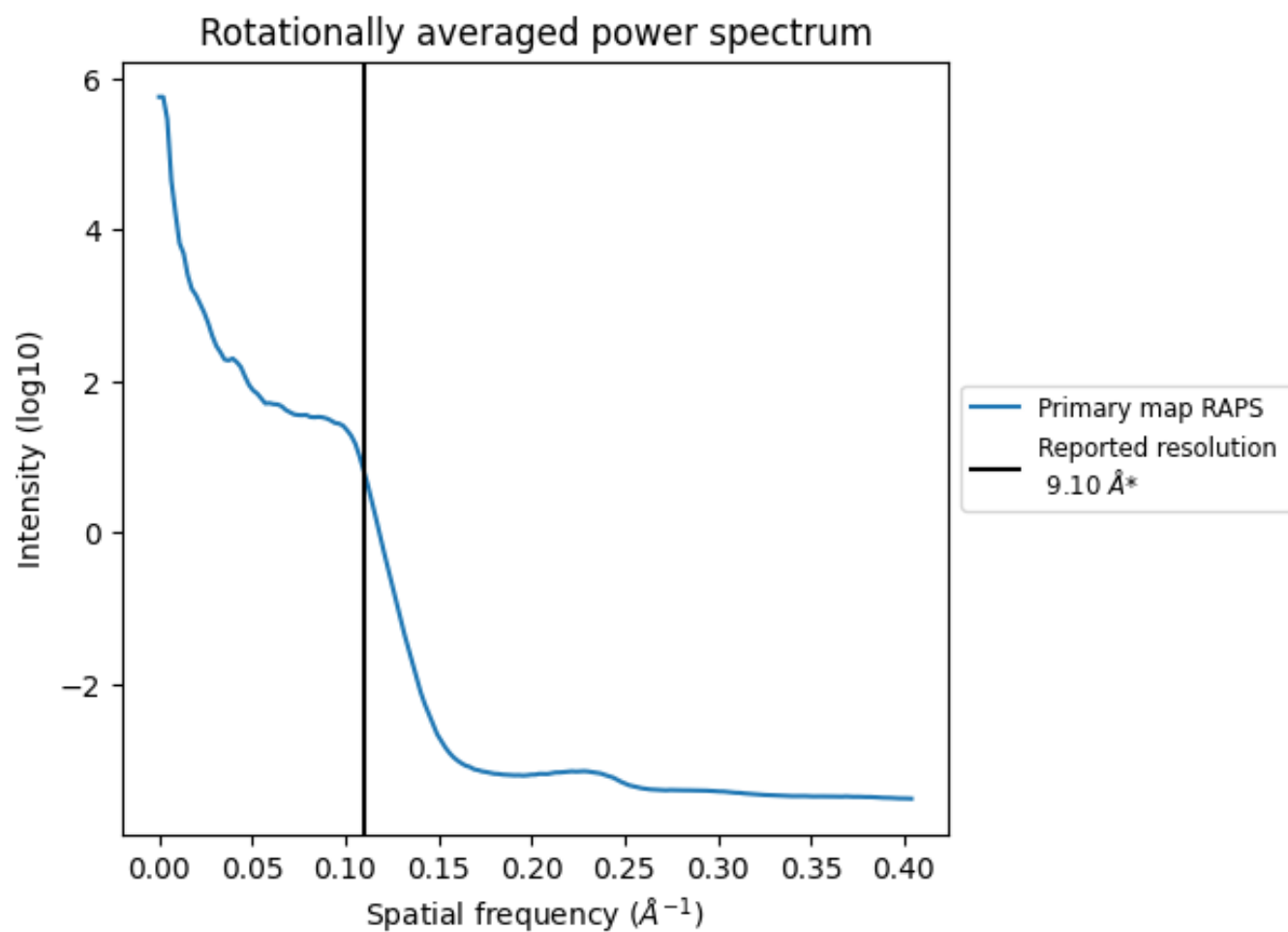
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 3424 nm³; this corresponds to an approximate mass of 3093 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 0.110 Å⁻¹

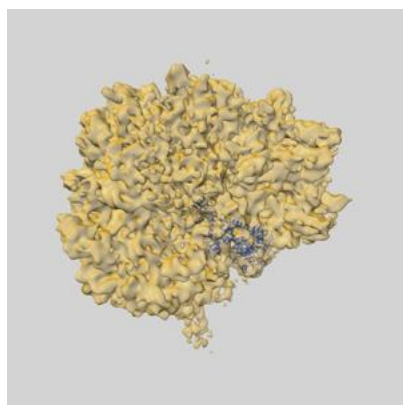
8 Fourier-Shell correlation

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

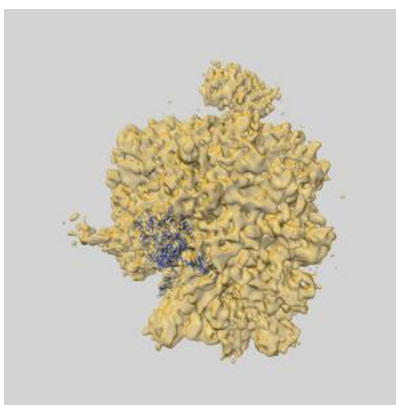
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-2597 and PDB model 4CRN. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

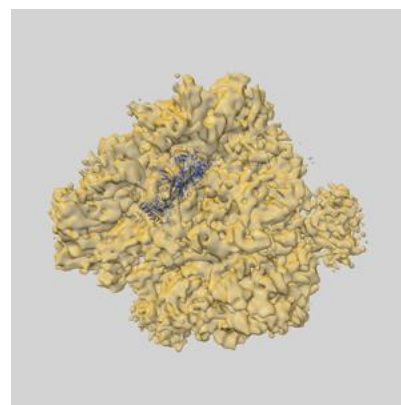
9.1 Map-model overlay [i](#)



X



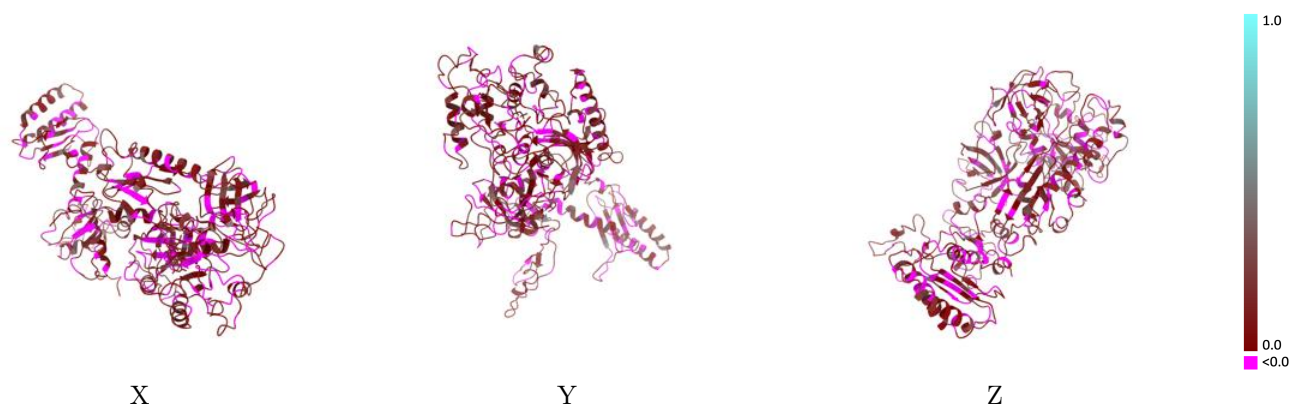
Y



Z

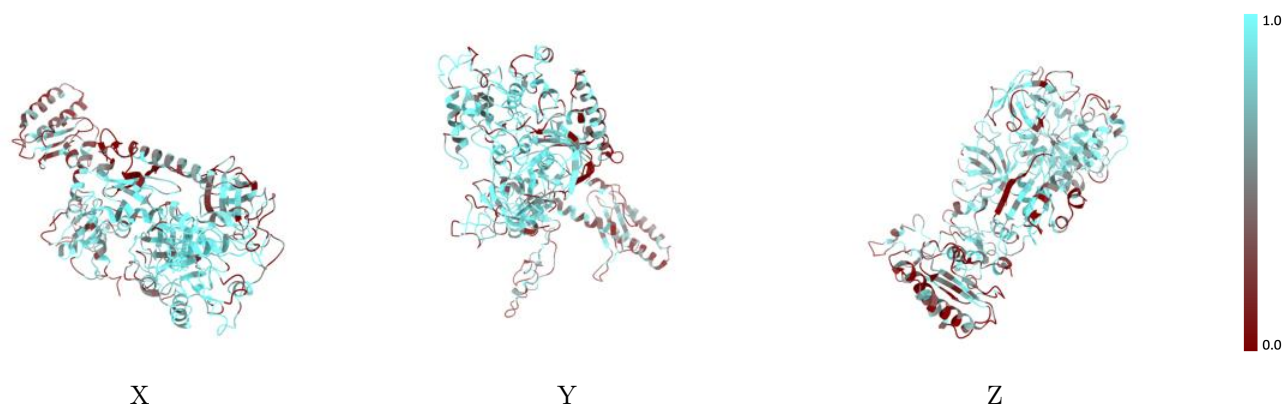
The images above show the 3D surface view of the map at the recommended contour level 0.183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



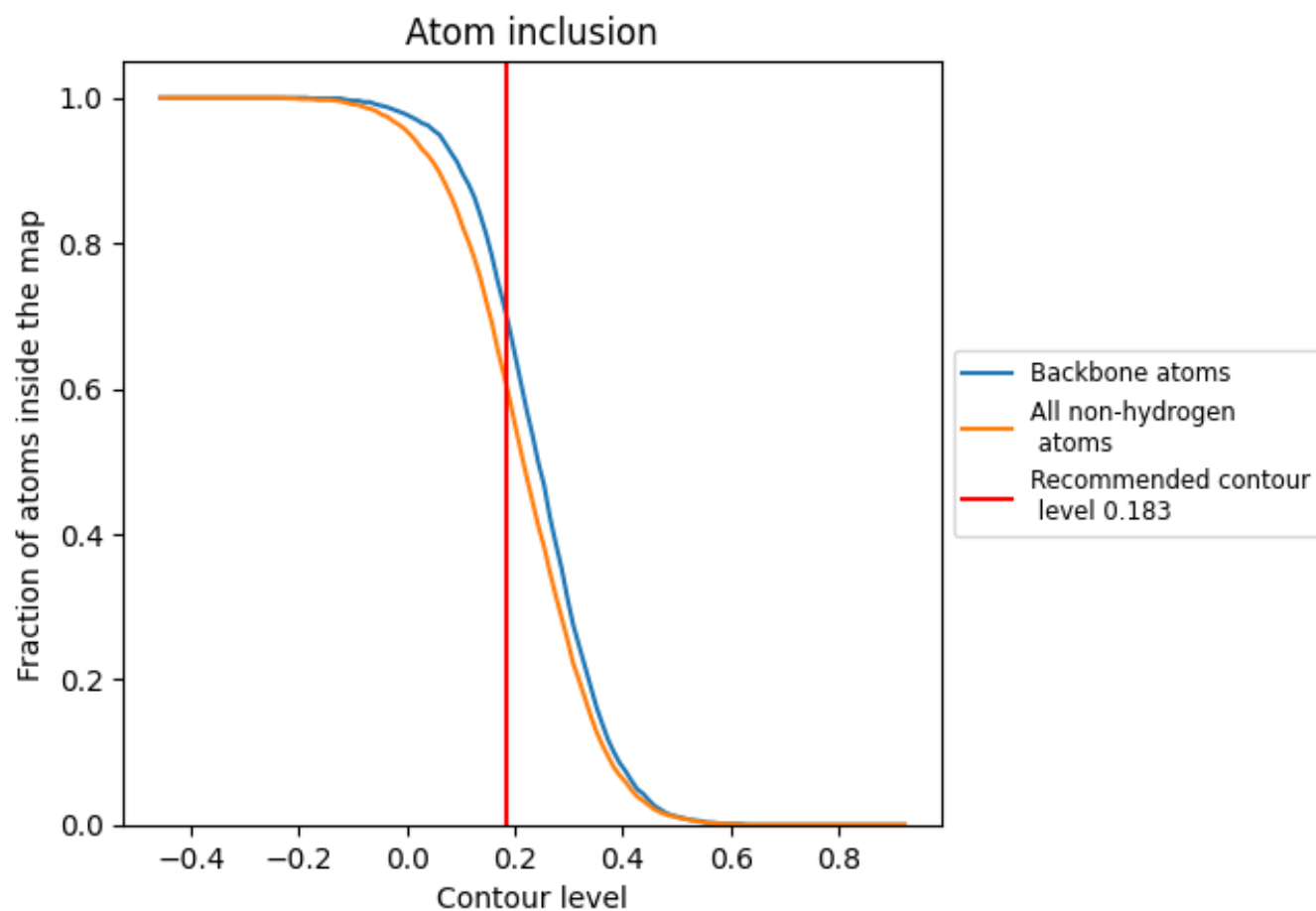
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.183).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 61% 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 (0.183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6100	0.0750
P	0.7140	0.0740
X	0.5040	0.0750

