wwPDB EM Validation Summary Report (i)

Aug 6, 2026 – 11:07 AM JST

PDB ID	:	7V5C / pdb_00007v5c
EMDB ID	:	EMD-31722
Title	:	Cryo-EM structure of the mouse ABCB9 (ADP.BeF3-bound)
Authors	:	Park, J.G.; Kim, S.; Jang, E.; Choi, S.H.; Han, H.; Kim, J.W.; Ju, S.; Min, D.S.; Jin, M.S.
Deposited on	:	2021-08-17
Resolution	:	3.20 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 (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:

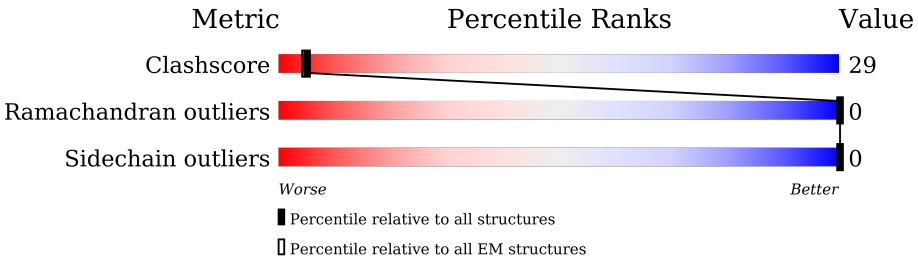
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using 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

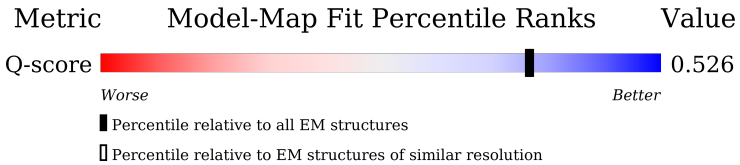
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	15020 (2.70 - 3.70)

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	A	762	43% 32% 25%
1	B	762	45% 30% 25%

2 Entry composition (i)

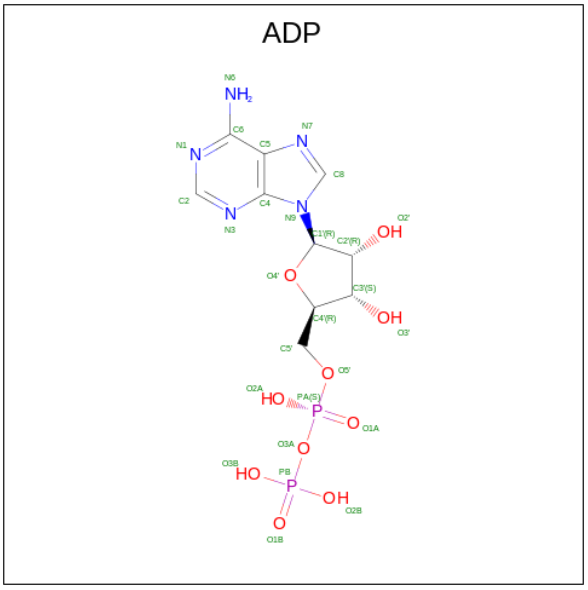
There are 4 unique types of molecules in this entry. The entry contains 8940 atoms, of which 24 are hydrogens and 0 are deuteriums.

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 ABC-type oligopeptide transporter ABCB9.

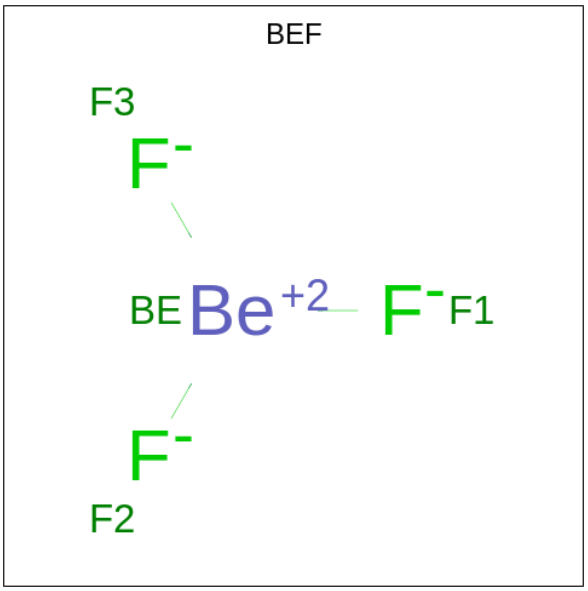
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	572	4425	2828	756	821	20	0	0
1	B	572	4427	2832	756	819	20	0	0

- Molecule 2 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
			Total	C	H	N	O	P	
2	A	1	39	10	12	5	10	2	0
2	B	1	39	10	12	5	10	2	0

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

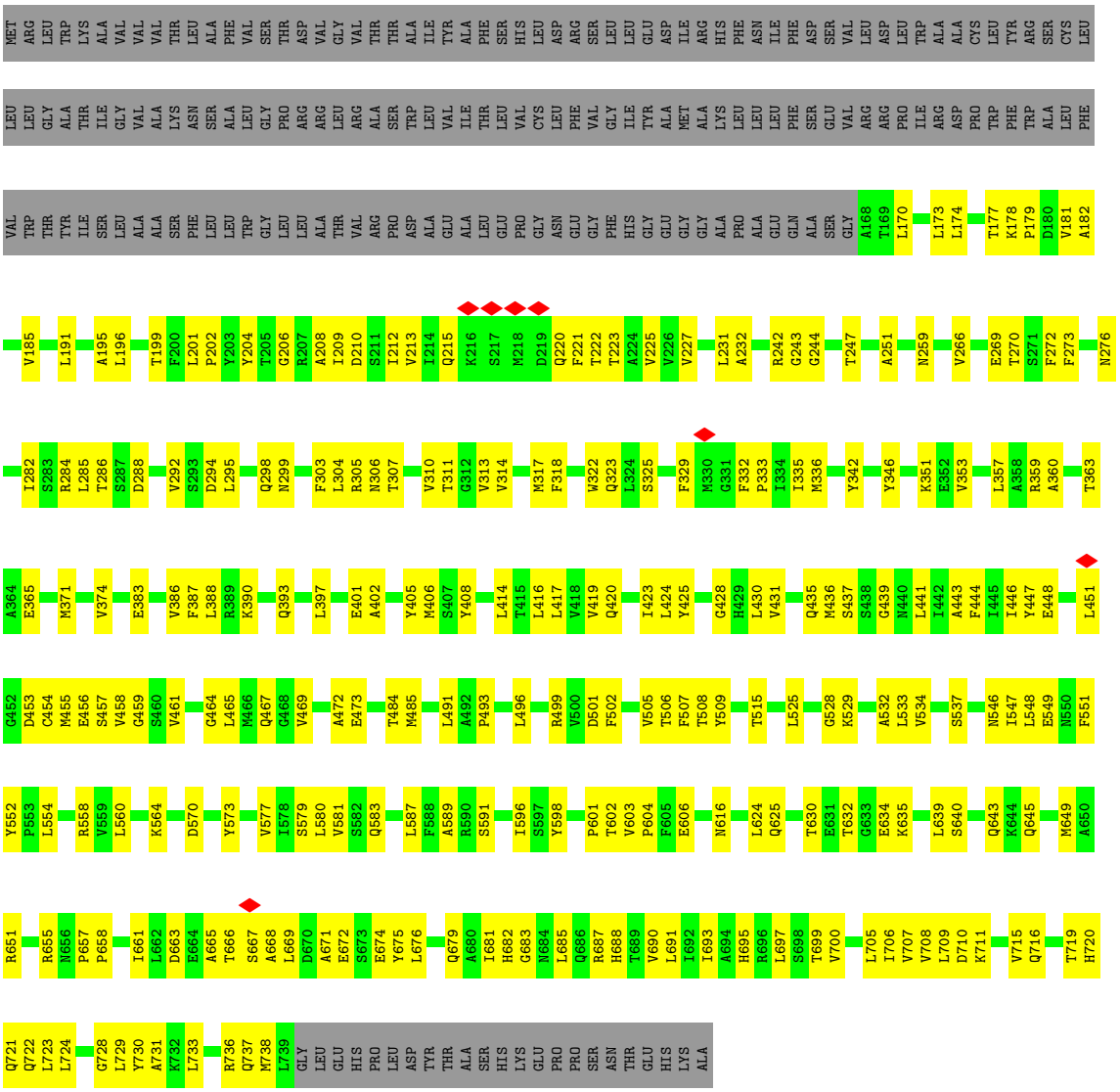
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
4	A	1	1	1	0
4	B	1	1	1	0

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: ABC-type oligopeptide transporter ABCB9

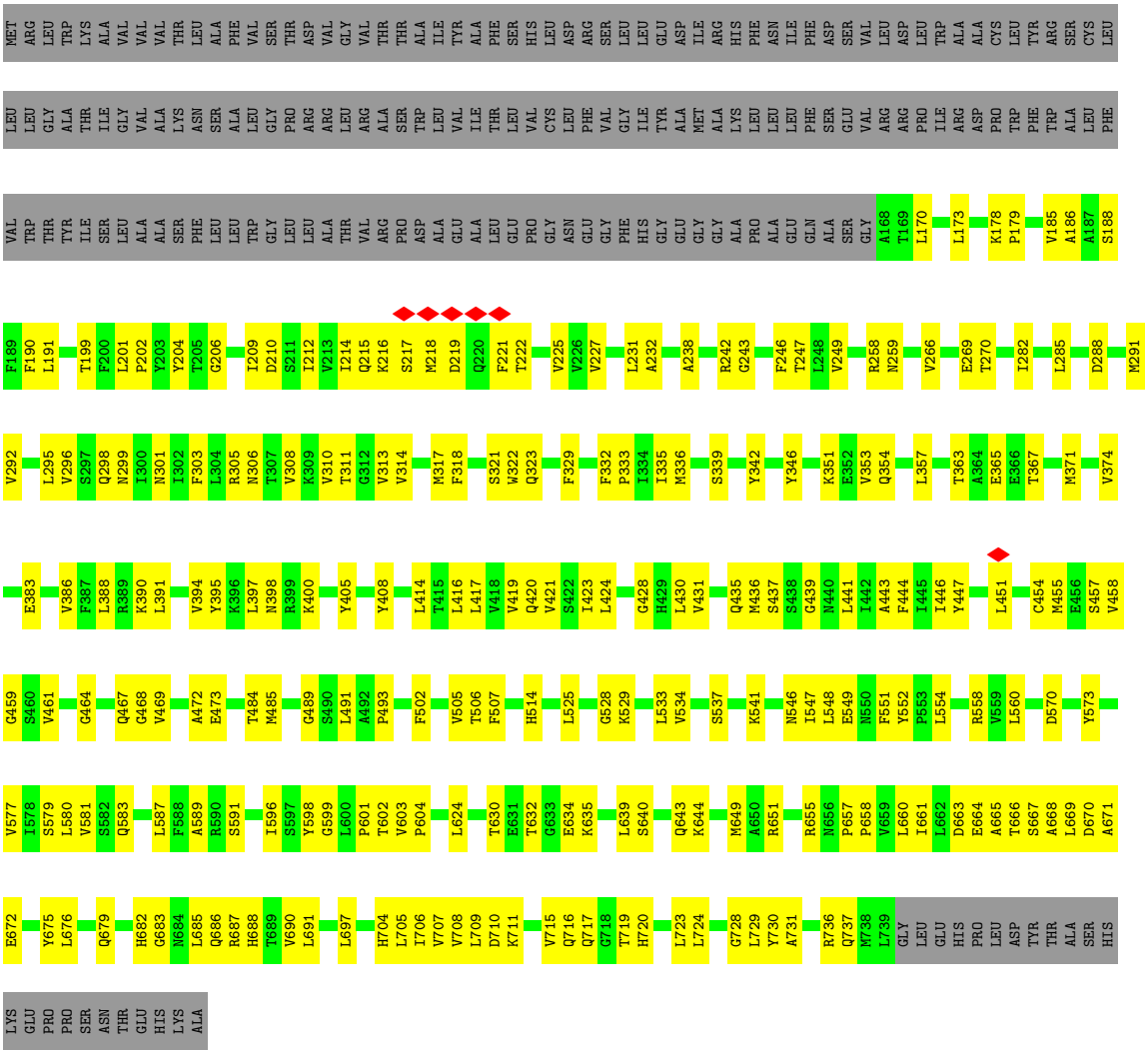
Chain A: 43% 32% 25%



- Molecule 1: ABC-type oligopeptide transporter ABCB9

Chain B:

45%
30%
25%


MET ARG LEU TRP LYS ALA VAL VAL VAL THR LEU ALA PHE VAL SER THR ASP VAL GLY VAL THR THR ALA ILE TYR ALA PHE SER HIS LEU ASP ARG SER LEU LEU GLU ASP ILE ARG HIS PHE ASN ILE PHE ASP SER VAL LEU ASP LEU TRP ALA ALA CYS LEU TYR ARG SER CYS LEU
LEU LEU GLY ALA THR ILE GLY VAL VAL ALA LYS ASN SER ALA LEU GLY PRO ARG ARG LEU ARG ALA SER TRP LEU VAL ILE THR LEU VAL CYS LEU PHE VAL GLY ILE TYR ALA MET ALA LYS LEU LEU LEU PHE SER GLU VAL ARG ARG PRO ILE ARG ASP PRO TRP PHE TRP ALA ALA LEU PHE
VAL TRP THR TYR ILE SER LEU ALA ALA SER PHE LEU LEU TRP GLY LEU LEU ALA THR VAL ARG PRO ASP ALA GLU ALA LEU GLU PRO GLY ASN GLU GLY PHE HIS GLY GLU GLY GLY ALA PRO ALA GLU GLN ALA SER GLY A168 T169 L170 L173 K178 P179 V185 A186 A187 S188
F189 F190 L191 T199 F200 L201 P202 Y203 Y204 T205 G206 I209 D210 S211 I212 V213 I214 Q215 K216 S217 M218 D219 Q220 F221 T222 V225 V226 V227 L231 A232 A238 R242 G243 F246 T247 L248 V249 R258 N259 V266 E269 T270 I282 L285 D288 M291
V292 L295 V296 S297 Q298 N299 I300 N301 I302 F303 L304 R305 N306 T307 V308 K309 V310 T311 G312 V313 V314 M317 F318 S321 W322 Q323 F329 F332 P333 I334 I335 M336 S339 Y342 Y346 K351 E352 V353 Q354 L357 T363 A364 E365 E366 T367 M371 V374
E383 V386 F387 L388 R389 K390 L391 V394 Y395 K396 L397 N398 R399 K400 Y405 Y408 L414 T415 L416 L417 V418 V419 Q420 V421 S422 I423 L424 G428 H429 L430 V431 Q435 M436 S437 S438 G439 N440 L441 I442 A443 F444 I445 I446 Y447 L451 C454 M455 E456 S457 V458
G459 S460 V461 G464 Q467 G468 V469 A472 E473 T484 M485 G489 S490 L491 A492 P493 F502 V505 T506 F507 H514 L525 G528 K529 L533 V534 S537 K541 N546 I547 L548 E549 N550 F551 Y552 P553 L554 R558 V559 L560 D570 Y573
V577 I578 S579 L580 V581 S582 Q583 L587 F588 A589 R590 S591 I596 S597 Y598 G599 L600 P601 T602 V603 P604 L624 T630 E631 T632 G633 E634 K635 L639 S640 Q643 K644 M649 A650 R651 R655 N656 P657 P658 V659 L660 I661 L662 D663 E664 A665 T666 S667 A668 L669 D670 A671
E672 Y675 L676 Q679 H682 G683 N684 L685 Q686 R687 H688 T689 V690 L691 L697 H704 L705 I706 V707 V708 L709 D710 K711 V715 Q716 Q717 G718 T719 H720 L723 L724 G728 L729 Y730 A731 R736 Q737 M738 L739 GLY LEU GLU HIS PRO LEU ASP TYR THR ALA SER HIS
LYS GLU PRO PRO SER ASN THR GLU HIS LYS ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	212390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.134	Depositor
Minimum map value	-1.313	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.071	Depositor
Recommended contour level	0.3	Depositor
Map size (Å)	215.8, 215.8, 215.8	wwPDB
Map dimensions	260, 260, 260	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	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: BEF, 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	A	0.20	0/4503	0.36	0/6100
1	B	0.20	0/4506	0.39	0/6104
All	All	0.20	0/9009	0.38	0/12204

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	4425	0	4501	290	0
1	B	4427	0	4504	274	0
2	A	27	12	12	0	0
2	B	27	12	12	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8916	24	9029	521	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

The worst 5 of 521 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:292:VAL:HG21	1:B:472:ALA:HB2	1.39	1.05
1:A:292:VAL:HG21	1:A:472:ALA:HB2	1.41	1.03
1:A:416:LEU:HB3	1:A:451:LEU:HD13	1.41	0.98
1:B:416:LEU:HB3	1:B:451:LEU:HD23	1.49	0.93
1:A:209:ILE:HD12	1:A:212:ILE:HD11	1.50	0.92

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	570/762 (75%)	531 (93%)	39 (7%)	0	100	100
1	B	570/762 (75%)	533 (94%)	37 (6%)	0	100	100
All	All	1140/1524 (75%)	1064 (93%)	76 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	483/638 (76%)	483 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	483/638 (76%)	483 (100%)	0	100	100
All	All	966/1276 (76%)	966 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	520	ASN
1	B	679	GLN
1	B	686	GLN
1	B	618	HIS
1	A	618	HIS

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)

Of 6 ligands modelled in this entry, 2 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	$\#\|Z\| > 2$
2	ADP	A	801	-	27,29,29	1.43	5 (18%)	42,45,45	2.04	12 (28%)
3	BEF	B	802	-	0,3,3	-	-	-		
3	BEF	A	802	-	0,3,3	-	-	-		
2	ADP	B	801	-	27,29,29	1.44	4 (14%)	42,45,45	2.04	12 (28%)

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	ADP	A	801	-	-	0/16/32/32	0/3/3/3
2	ADP	B	801	-	-	0/16/32/32	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ADP	C5-C4	3.50	1.45	1.39
2	A	801	ADP	C5-C4	3.49	1.45	1.39
2	A	801	ADP	C5-N7	-2.89	1.33	1.39
2	B	801	ADP	C5-N7	-2.86	1.33	1.39
2	B	801	ADP	C4-N9	-2.57	1.32	1.37

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	ADP	C5-C4-N3	-6.26	118.58	126.75
2	B	801	ADP	C5-C4-N3	-6.21	118.65	126.75
2	A	801	ADP	N3-C4-N9	4.36	134.26	127.08
2	B	801	ADP	N3-C4-N9	4.35	134.25	127.08
2	A	801	ADP	C2-N3-C4	4.14	121.54	111.75

There are no chirality outliers.

There are no torsion outliers.

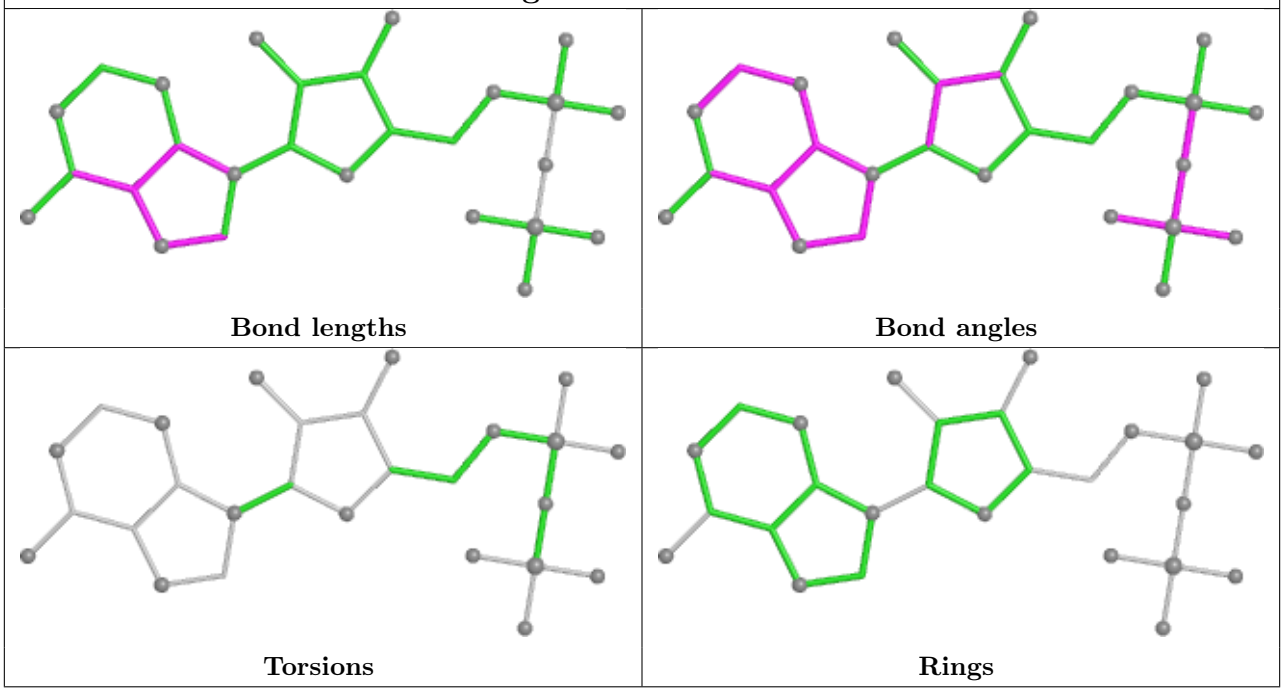
There are no ring outliers.

No monomer is involved in short contacts.

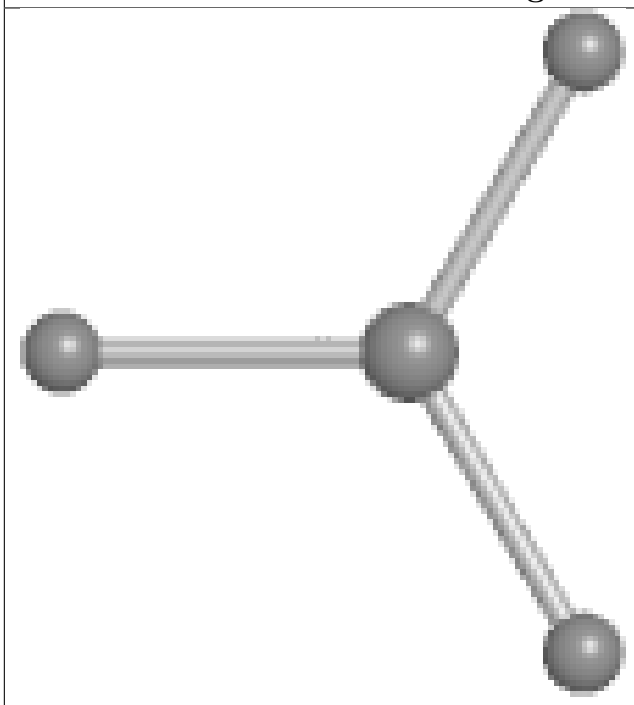
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

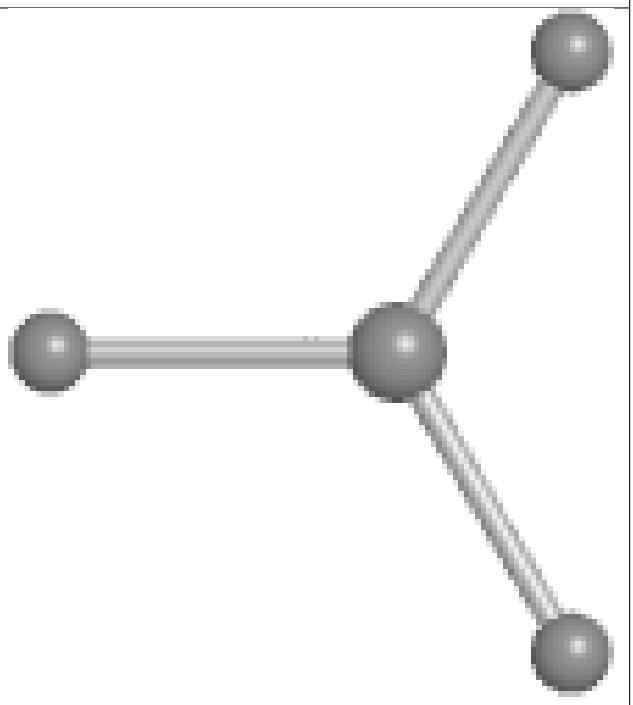
Ligand ADP A 801



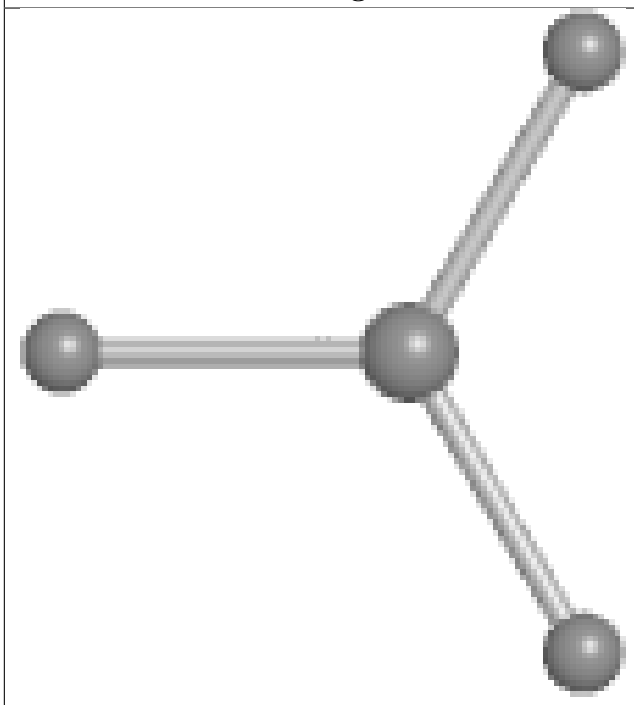
Ligand BEF B 802



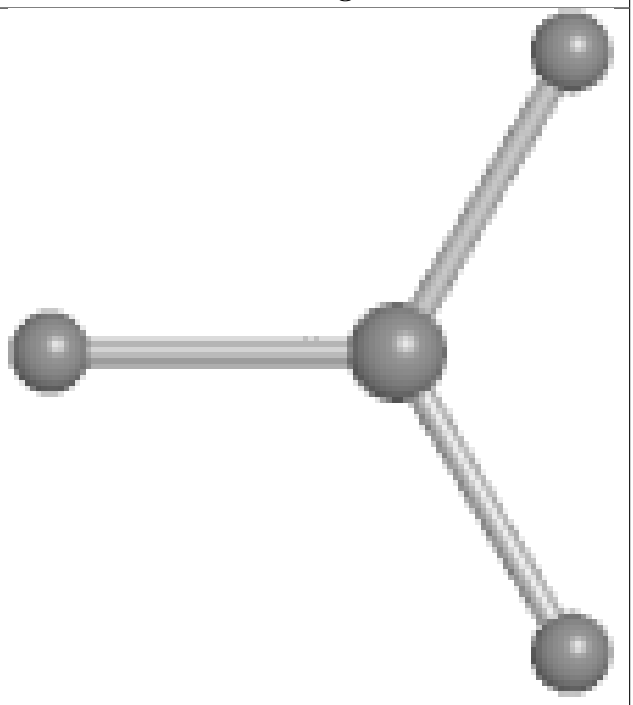
Bond lengths



Bond angles

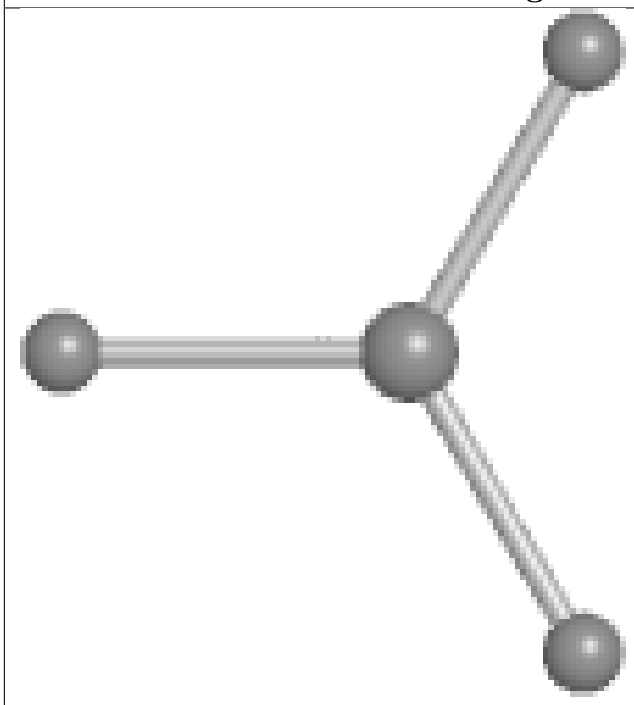


Torsions

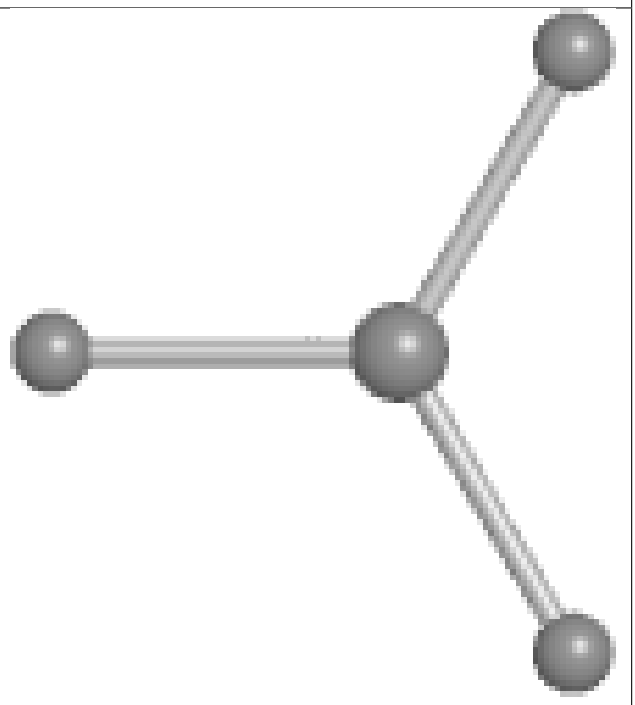


Rings

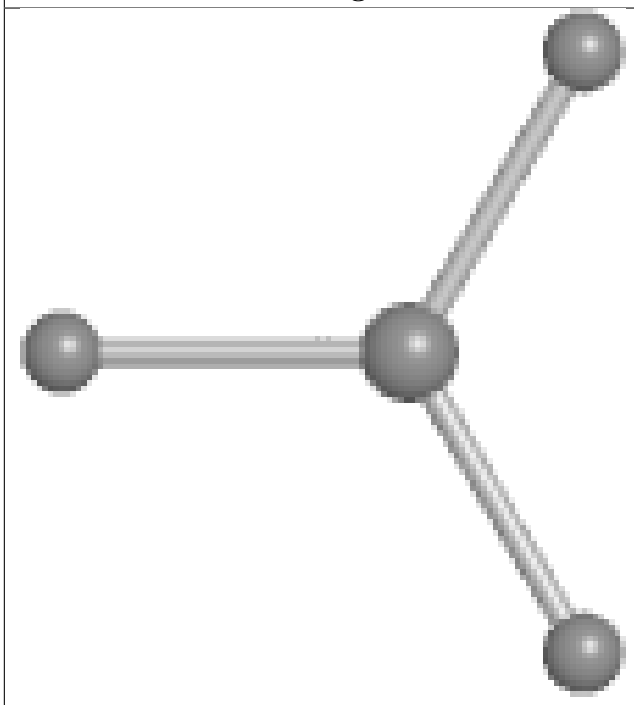
Ligand BEF A 802



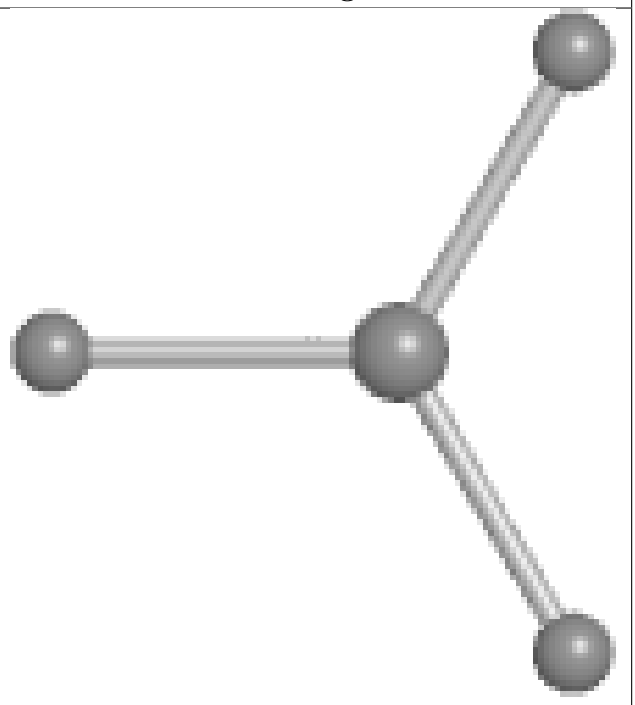
Bond lengths



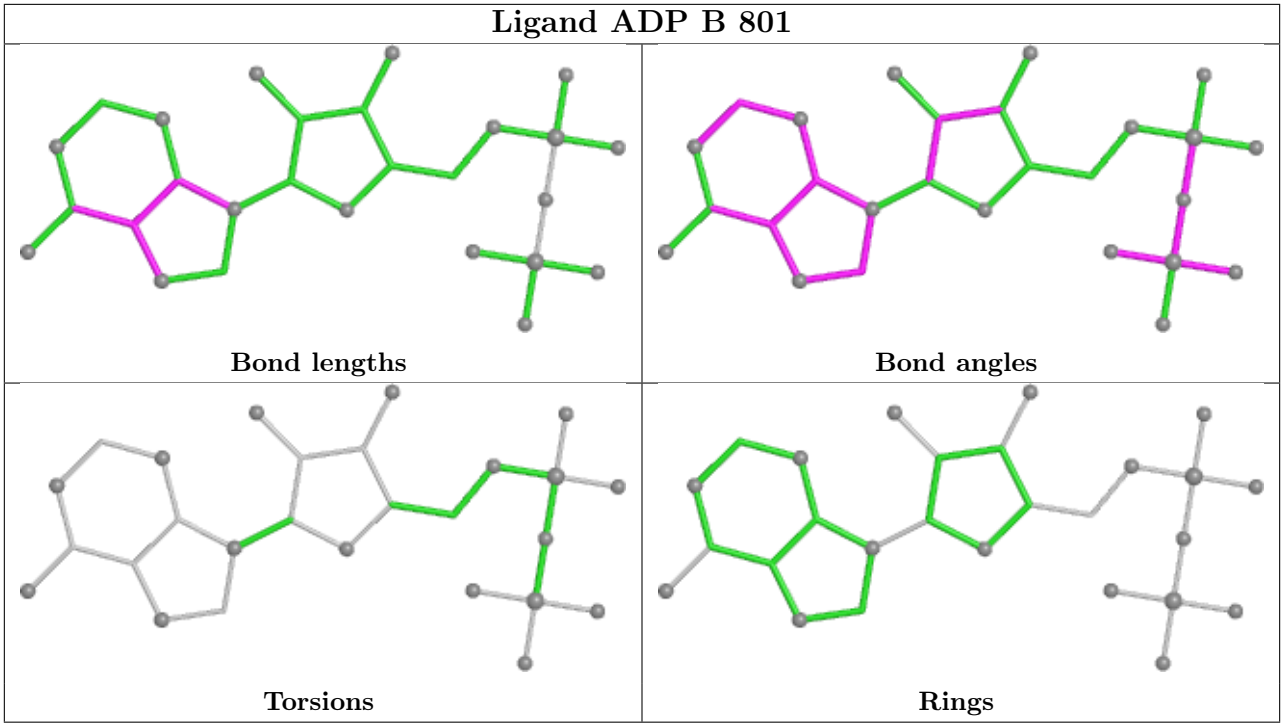
Bond angles



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.

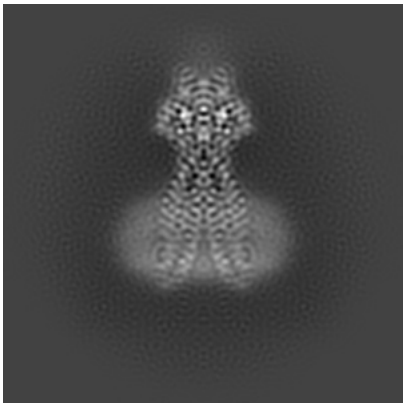
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-31722. These allow visual inspection of the internal detail of the map and identification of artifacts.

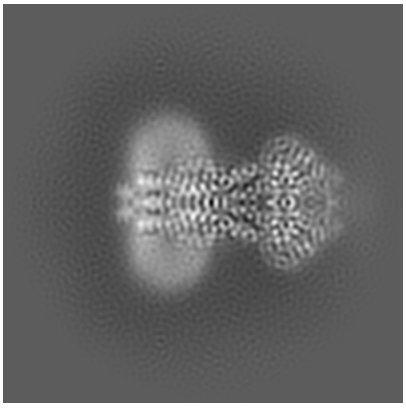
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

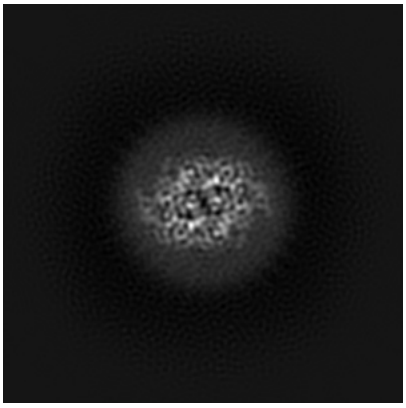
6.1.1 Primary map



X



Y



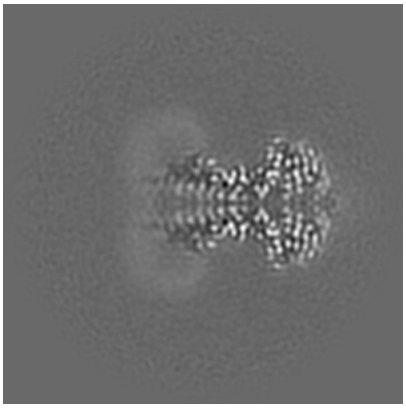
Z

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

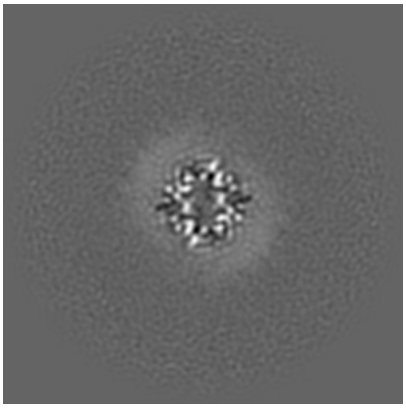
6.2 Central slices (i)

6.2.1 Primary map

X Index: 130



Y Index: 130

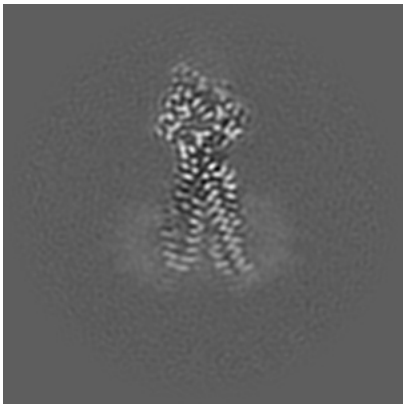


Z Index: 130

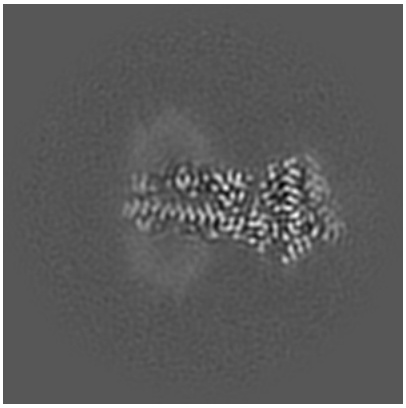
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

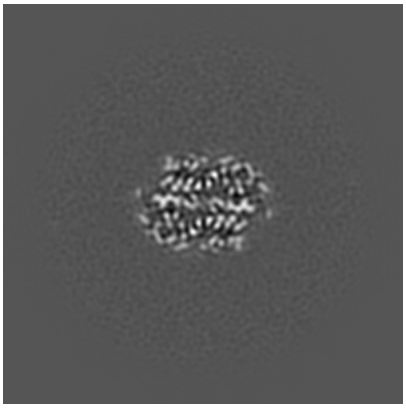
6.3.1 Primary map



X Index: 117



Y Index: 117

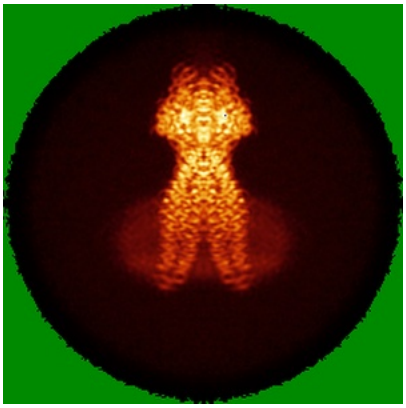


Z Index: 185

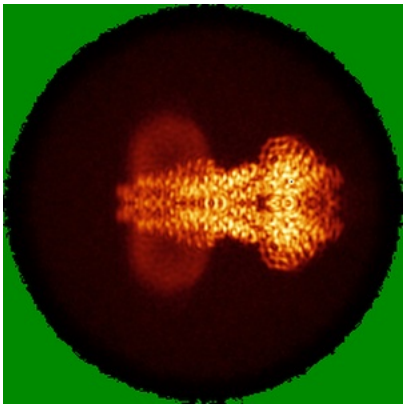
The images above show the largest variance slices of the map in three orthogonal directions.

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

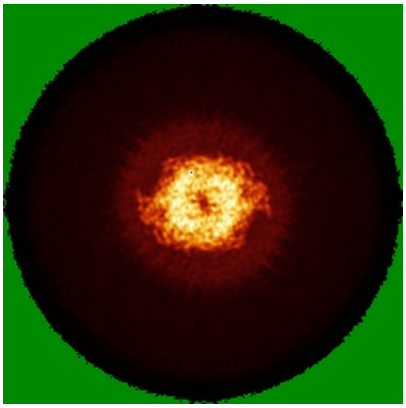
6.4.1 Primary map



X



Y



Z

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.

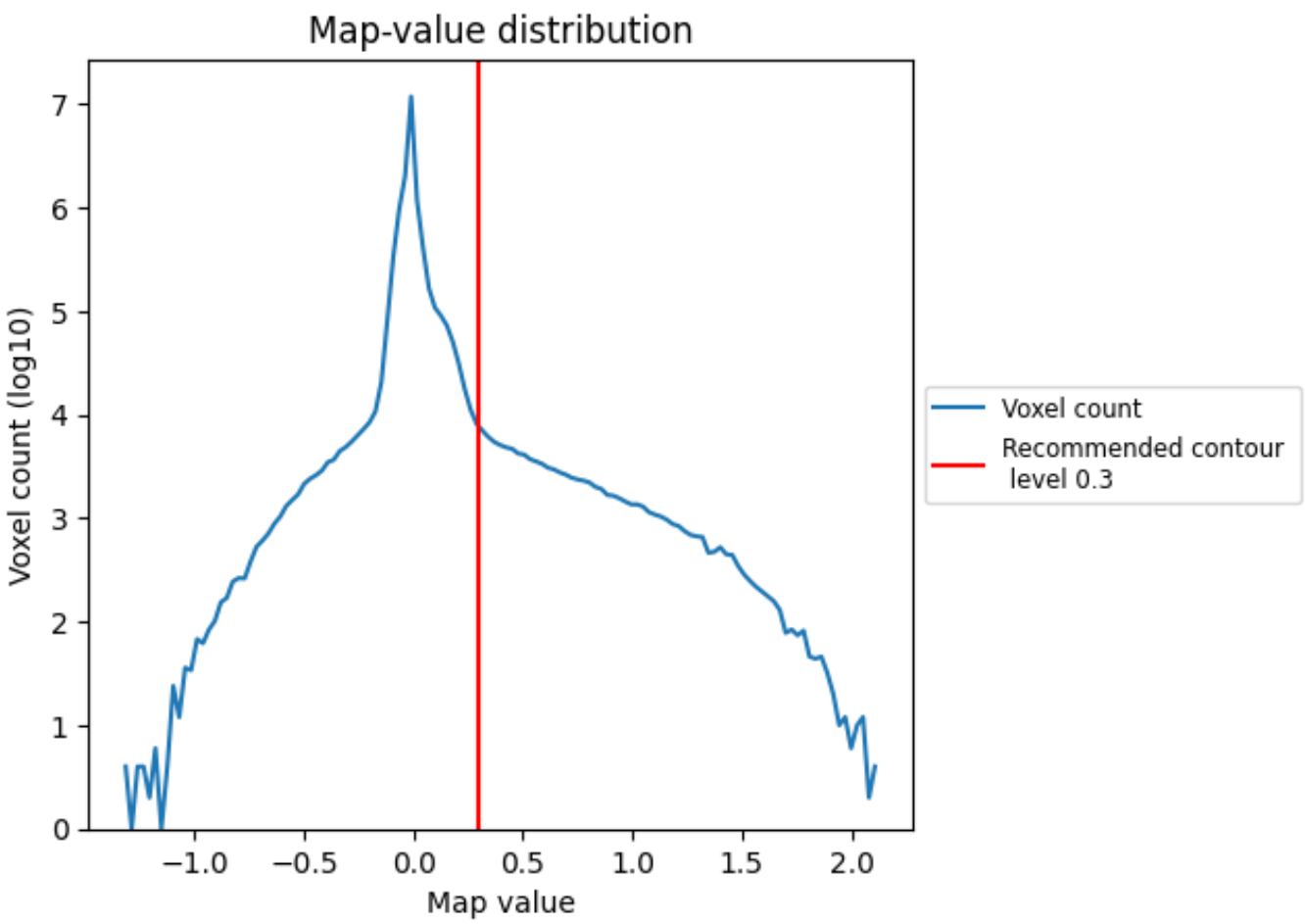
6.6 Mask visualisation (i)

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

7 Map analysis (i)

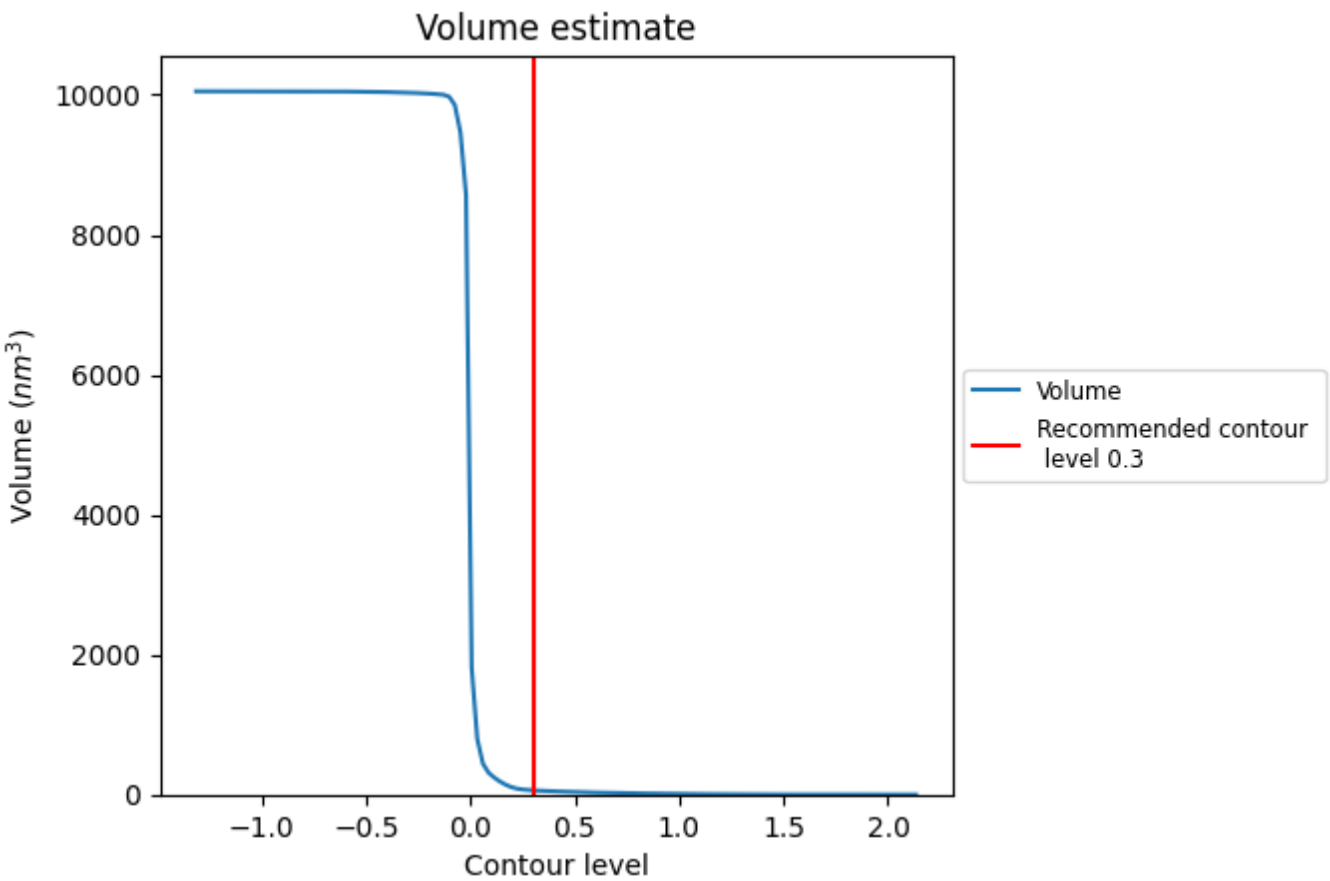
This section contains the results of statistical analysis of the map.

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.

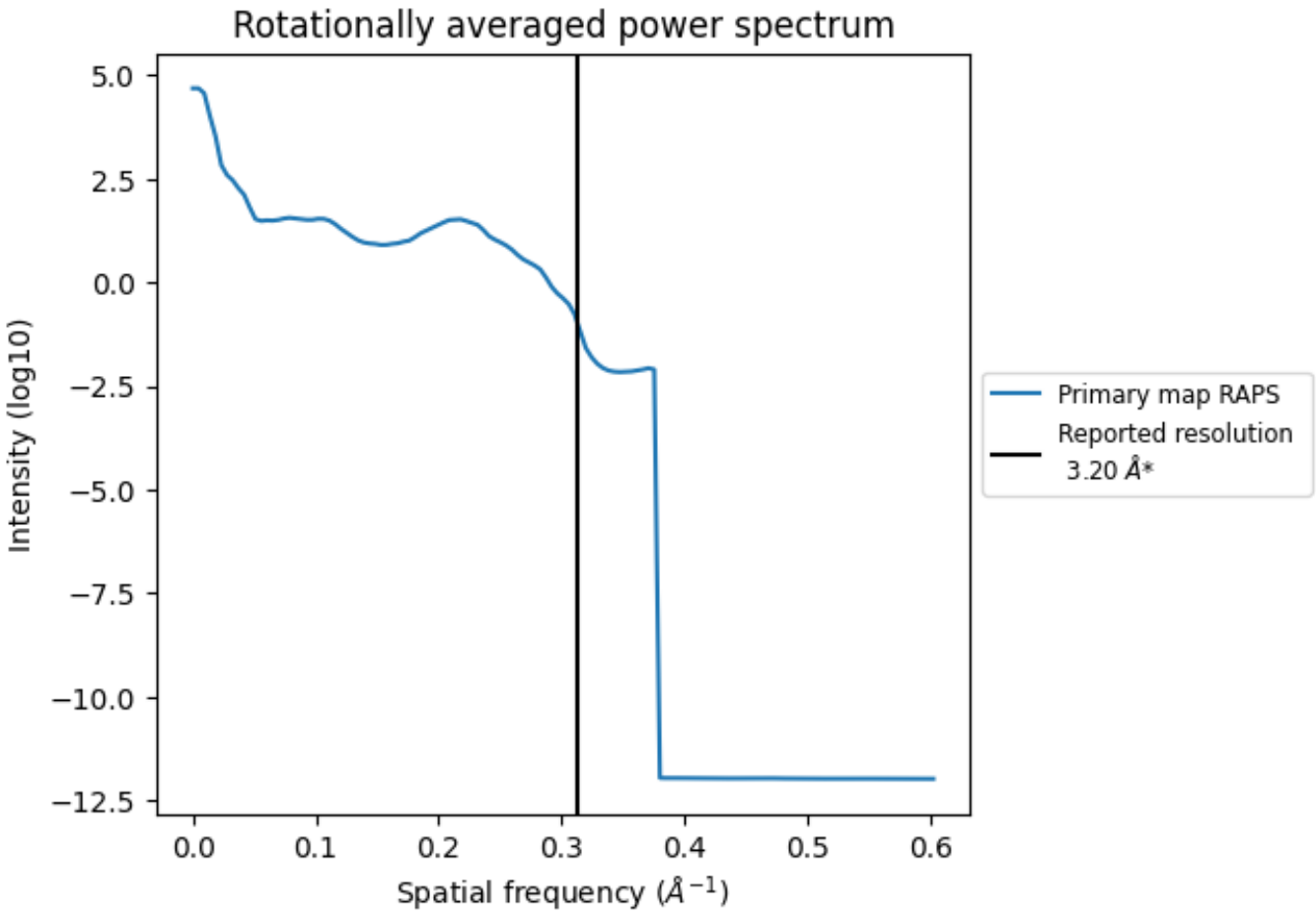
7.2 Volume estimate (i)



The volume at the recommended contour level is 60 nm^3; this corresponds to an approximate mass of 54 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 0.312 Å^{-1}

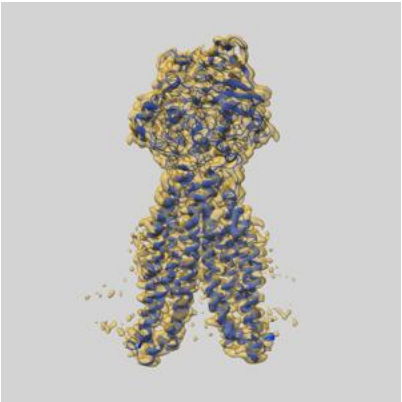
8 Fourier-Shell correlation (i)

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

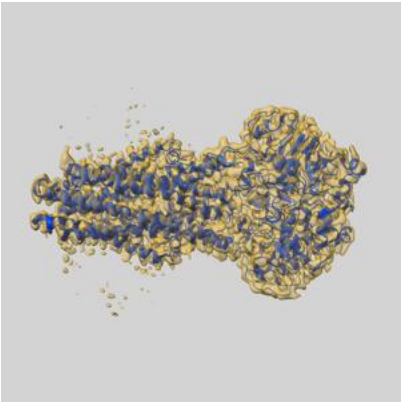
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-31722 and PDB model 7V5C. Per-residue inclusion information can be found in section 3 on page 5.

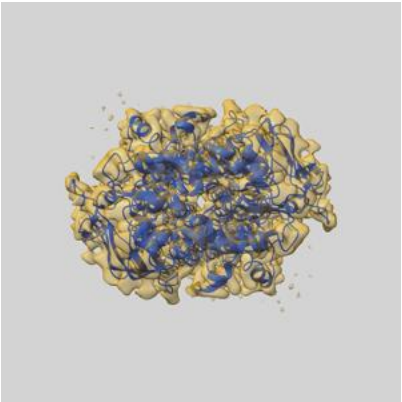
9.1 Map-model overlay (i)



X



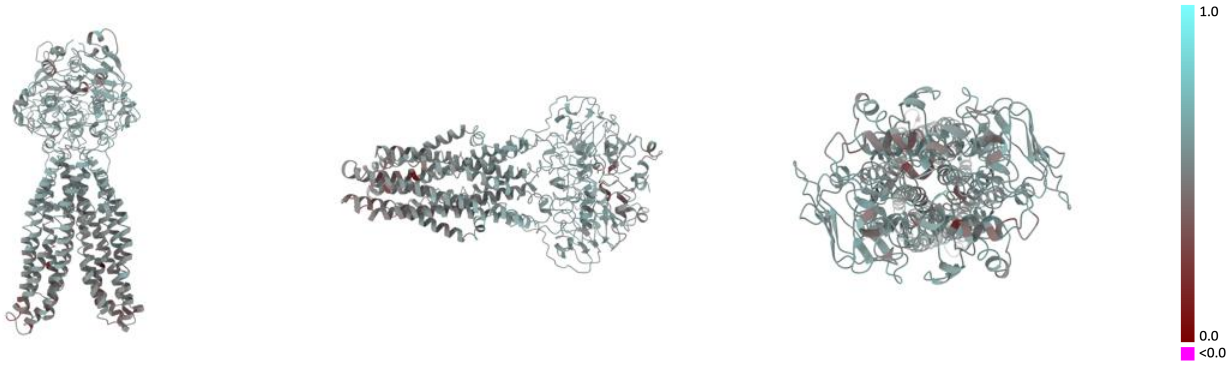
Y



Z

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

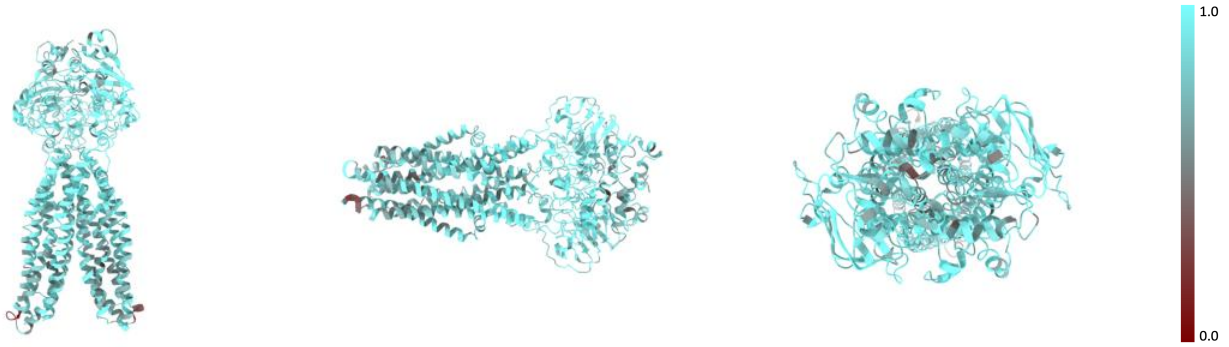
9.2 Q-score mapped to coordinate model (i)



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.

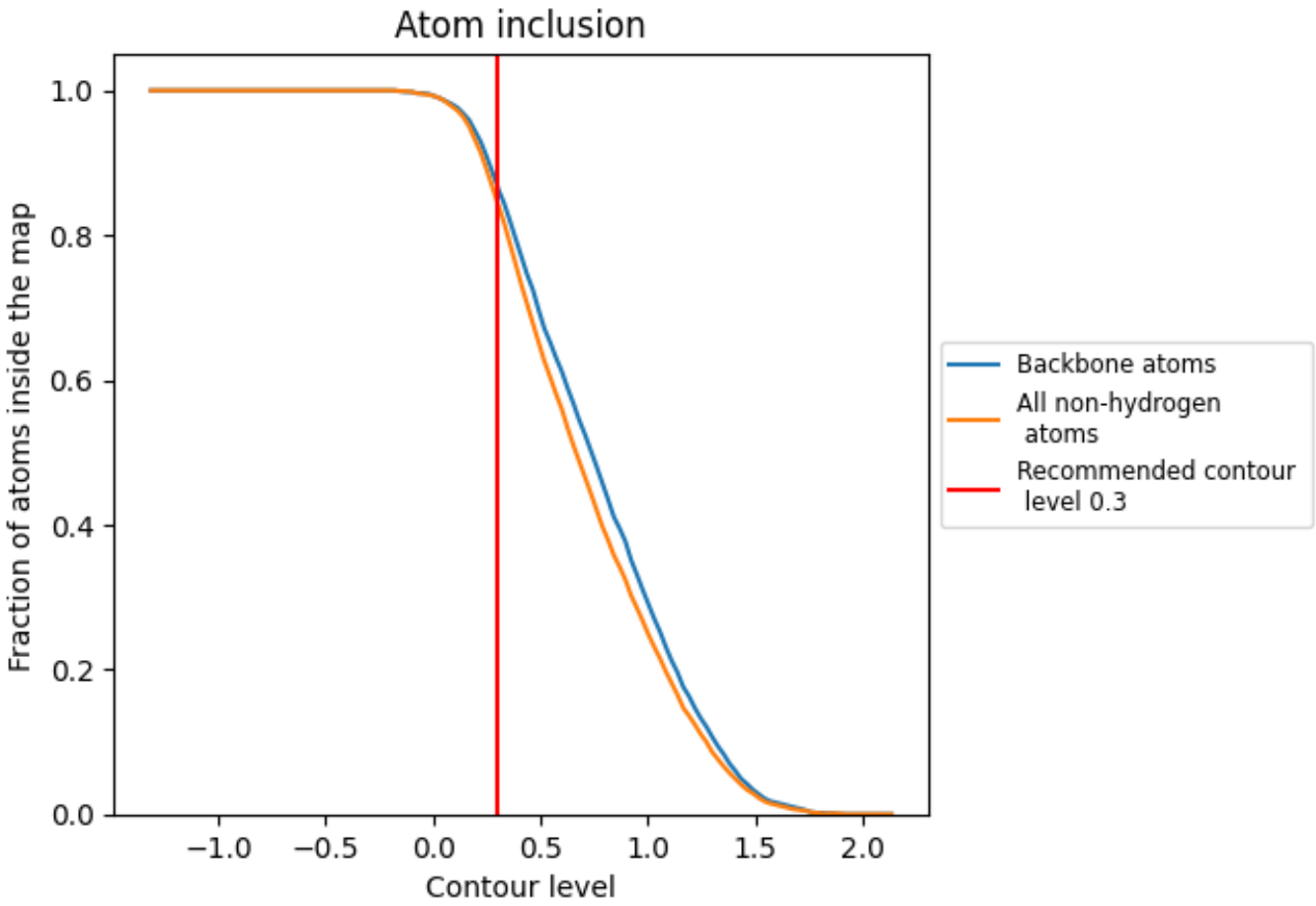
9.3 Atom inclusion mapped to coordinate model (i)



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, 87% of all backbone atoms, 84% 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	0.8450	0.5260
A	0.8440	0.5230
B	0.8510	0.5280