wwPDB EM Validation Summary Report (i)

Dec 12, 2022 – 03:51 am GMT

PDB ID	:	4UMM
EMDB ID	:	EMD-2631
Title	:	The Cryo-EM structure of the palindromic DNA-bound USP-EcR nuclear receptor reveals an asymmetric organization with allosteric domain positioning
Authors	:	Maletta, M.; Orlov, I.; Moras, D.; Billas, I.M.L.; Klaholz, B.P.
Deposited on	:	2014-05-19
Resolution	:	11.60 Å(reported)
Based on initial model	:	1R1K

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 (1)) were used in the production of this report:

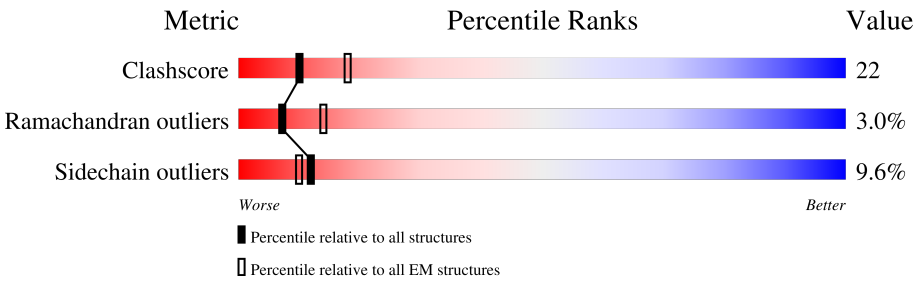
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 11.60 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	78	5% 92% 8%
2	C	20	45% 55%
3	D	20	15% 75% 10%
4	E	87	• 87% 10% •
5	F	264	• 41% 43% 7% 9%
6	G	266	• 43% 39% 6% 11%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 6030 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 ECR-USP.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	78	639	386	129	113	11	0	0

- Molecule 2 is a DNA chain called 5'-D(*CP*AP*AP*GP*GP*GP*TP*TP*CP*AP*AP*TP*GP*CP *AP*CP*TP*TP*GP*TP)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	C	20	407	196	74	118	19	0	0

- Molecule 3 is a DNA chain called 5'-D(*DGP*AP*CP*AP*AP*GP*TP*GP*CP*AP*TP*TP*GP*DAP *AP*CP*CP*CP*TP*T)-3'.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	D	20	405	195	75	116	19	0	0

- Molecule 4 is a protein called ECDYSONE RECEPTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	87	692	424	132	120	16	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	193	MET	ILE	conflict	UNP O18473

- Molecule 5 is a protein called GENE REGULATION PROTEIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	F	241	1925	1233	335	345	12	0	0

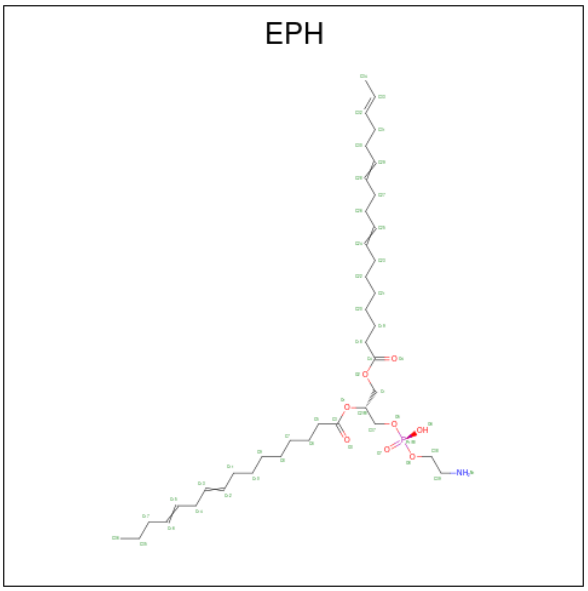
- Molecule 6 is a protein called ECDYSONE RECEPTOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	G	236	1872	1194	316	346	16	0	0

There are 22 discrepancies between the modelled and reference sequences:

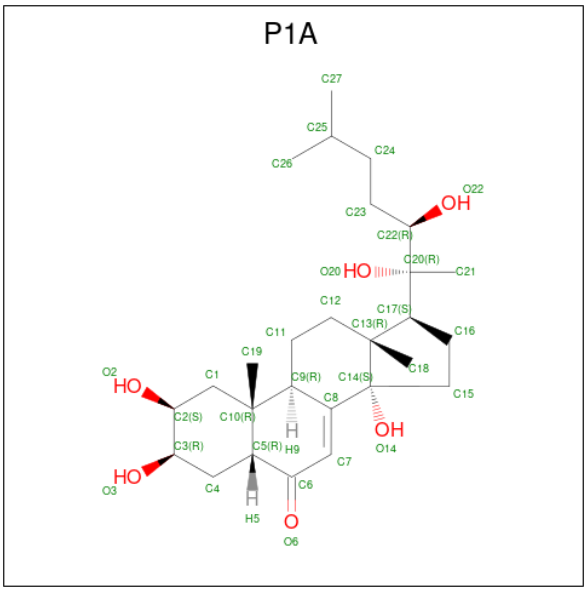
Chain	Residue	Modelled	Actual	Comment	Reference
G	267	GLY	-	expression tag	UNP O18473
G	268	SER	-	expression tag	UNP O18473
G	269	HIS	-	expression tag	UNP O18473
G	270	MET	-	expression tag	UNP O18473
G	271	ALA	-	expression tag	UNP O18473
G	272	SER	-	expression tag	UNP O18473
G	273	MET	-	expression tag	UNP O18473
G	274	THR	-	expression tag	UNP O18473
G	275	GLY	-	expression tag	UNP O18473
G	276	GLY	-	expression tag	UNP O18473
G	277	GLN	-	expression tag	UNP O18473
G	278	GLN	-	expression tag	UNP O18473
G	279	MET	-	expression tag	UNP O18473
G	280	GLY	-	expression tag	UNP O18473
G	281	ARG	-	expression tag	UNP O18473
G	282	ASP	-	expression tag	UNP O18473
G	283	PRO	-	expression tag	UNP O18473
G	322	THR	-	insertion	UNP O18473
G	323	TRP	-	insertion	UNP O18473
G	324	GLN	-	insertion	UNP O18473
G	483	CYS	GLY	conflict	UNP O18473
G	489	LYS	GLU	conflict	UNP O18473

- Molecule 7 is L-ALPHA-PHOSPHATIDYL-BETA-OLEOYL-GAMMA-PALMITOYL-PHOSPHATIDYLETHANOLAMINE (three-letter code: EPH) (formula: $C_{39}H_{68}NO_8P$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	F	1	49	39	1	8	1	0

- Molecule 8 is 2,3,14,20,22-PENTAHYDROXYCHOLEST-7-EN-6-ONE (three-letter code: P1A) (formula: $C_{27}H_{44}O_6$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
8	G	1	33	27	6	0

- Molecule 9 is water.

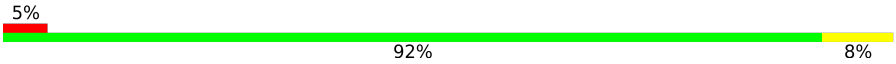
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
9	F	1	5	5	0
			Total	O	
9	F	2	5	5	0
			Total	O	
9	F	2	5	5	0
			Total	O	
9	G	2	3	3	0
			Total	O	
9	G	1	3	3	0

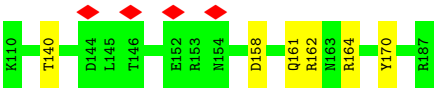
3 Residue-property plots (i)

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: ECR-USP

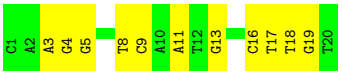
Chain A:





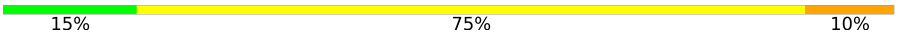
• Molecule 2: 5'-D(*CP*AP*AP*GP*GP*GP*TP*TP*CP*AP*AP*TP*GP*CP *AP*CP*TP*TP*GP*TP)-3'

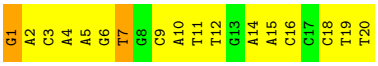
Chain C:



• Molecule 3: 5'-D(*DGP*AP*CP*AP*AP*GP*TP*GP*CP*AP*TP*TP*GP*DAP *AP*CP*CP*CP*TP*T)-3'

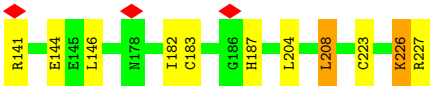
Chain D:





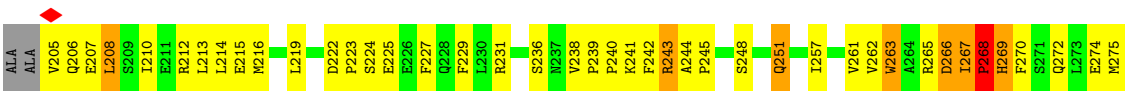
• Molecule 4: ECDYSONE RECEPTOR

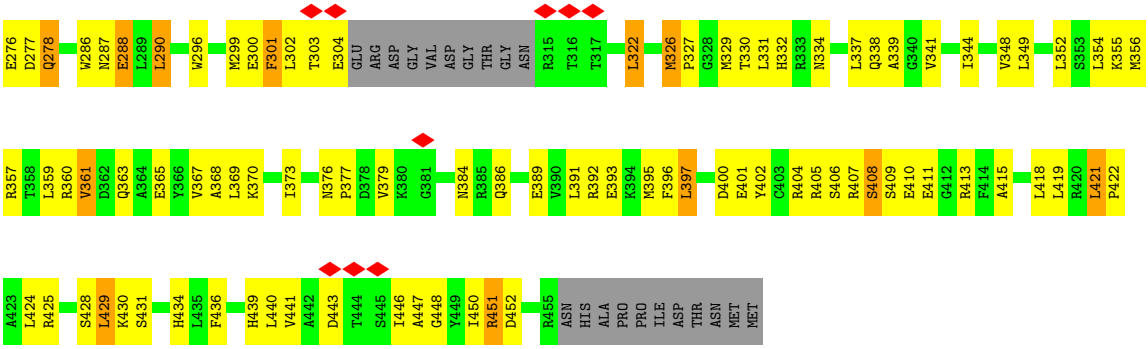
Chain E:



• Molecule 5: GENE REGULATION PROTEIN

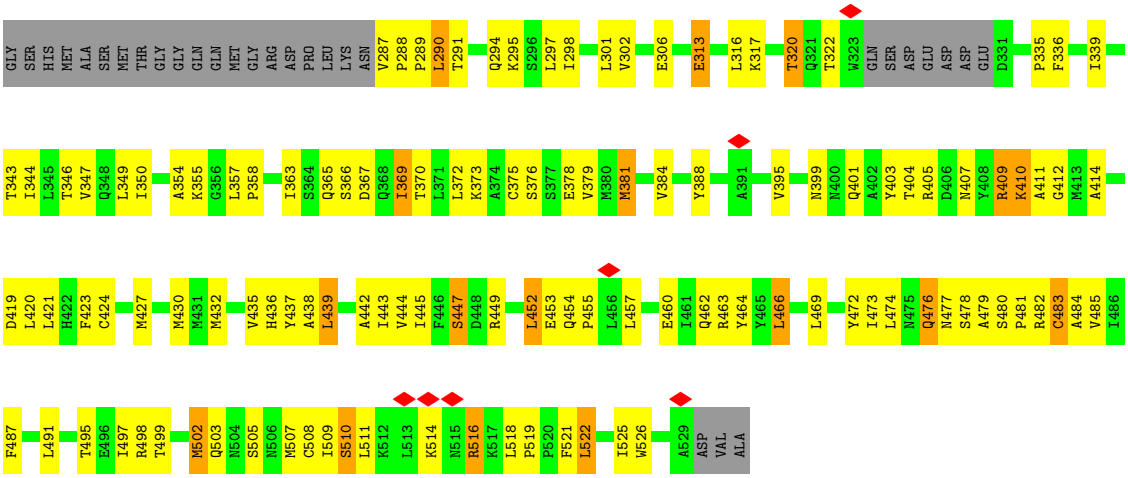
Chain F:





• Molecule 6: ECDYSONE RECEPTOR

Chain G:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	50000	Depositor
Resolution determination method	Not provided	
CTF correction method	CCD IMAGES 4096X4096	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	100	Depositor
Electron dose ($e^-/Å^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	64244	Depositor
Image detector	FEI EAGLE (4k x 4k)	Depositor
Maximum map value	13.818	Depositor
Minimum map value	-2.772	Depositor
Average map value	0.123	Depositor
Map value standard deviation	0.867	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	163.20001, 163.20001, 163.20001	wwPDB
Map dimensions	96, 96, 96	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.7000002, 1.7000002, 1.7000002	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: EPH, P1A

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	0.61	0/647	0.84	0/854
2	C	1.49	2/456 (0.4%)	2.02	15/703 (2.1%)
3	D	1.47	2/454 (0.4%)	2.13	26/699 (3.7%)
4	E	0.61	0/702	0.85	0/933
5	F	58.15	3/1960 (0.2%)	2.48	7/2646 (0.3%)
6	G	0.55	0/1905	0.72	0/2579
All	All	32.91	7/6124 (0.1%)	1.72	48/8414 (0.6%)

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
5	F	1	2

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	268	PRO	N-CA	1657.13	29.64	1.47
5	F	268	PRO	CA-C	1434.96	30.22	1.52
5	F	268	PRO	CA-CB	1349.91	28.53	1.53
3	D	11	DT	C5-C7	6.85	1.54	1.50
3	D	4	DA	C3'-O3'	-6.70	1.35	1.44

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	268	PRO	N-CA-CB	-82.73	4.02	103.30
5	F	268	PRO	CA-N-CD	-52.78	37.60	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	268	PRO	CB-CA-C	-43.34	3.64	112.00
5	F	268	PRO	N-CA-C	-41.33	4.65	112.10
5	F	268	PRO	CA-C-O	-30.72	46.47	120.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	F	268	PRO	CA

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	F	267	ILE	Peptide
5	F	268	PRO	Mainchain

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	639	0	634	3	0
2	C	407	0	225	0	0
3	D	405	0	224	2	0
4	E	692	0	690	7	0
5	F	1925	0	1969	120	0
6	G	1872	0	1880	129	0
7	F	49	0	67	6	0
8	G	33	0	43	3	0
9	F	5	0	0	1	0
9	G	3	0	0	0	0
All	All	6030	0	5732	255	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 22.

The worst 5 of 255 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:268:PRO:C	5:F:268:PRO:HB3	1.65	1.15
6:G:480:SER:HB2	6:G:481:PRO:HD2	1.51	0.91
6:G:403:TYR:HA	6:G:407:ASN:HD22	1.35	0.91
6:G:453:GLU:C	6:G:455:PRO:HD3	1.95	0.87
5:F:262:VAL:HG23	5:F:265:ARG:NH2	1.92	0.84

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	76/78 (97%)	74 (97%)	2 (3%)	0	100	100
4	E	85/87 (98%)	79 (93%)	5 (6%)	1 (1%)	13	50
5	F	237/264 (90%)	196 (83%)	33 (14%)	8 (3%)	3	26
6	G	232/266 (87%)	193 (83%)	29 (12%)	10 (4%)	2	22
All	All	630/695 (91%)	542 (86%)	69 (11%)	19 (3%)	7	28

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	F	268	PRO
5	F	301	PHE
6	G	322	THR
6	G	479	ALA
5	F	408	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	68/68 (100%)	68 (100%)	0	100	100
4	E	75/75 (100%)	73 (97%)	2 (3%)	44	65
5	F	212/231 (92%)	185 (87%)	27 (13%)	4	18
6	G	205/235 (87%)	180 (88%)	25 (12%)	5	20
All	All	560/609 (92%)	506 (90%)	54 (10%)	12	27

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	440	LEU
6	G	369	ILE
6	G	495	THR
6	G	290	LEU
6	G	316	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	386	GLN
6	G	305	GLN
6	G	294	GLN
6	G	348	GLN
5	F	251	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 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	$\#\|Z\| > 2$
7	EPH	F	1456	-	48,48,48	1.61	8 (16%)	51,53,53	1.58	7 (13%)
8	P1A	G	1530	-	36,36,36	3.58	17 (47%)	59,60,60	2.30	19 (32%)

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
7	EPH	F	1456	-	-	17/52/52/52	-
8	P1A	G	1530	-	-	2/17/87/87	0/4/4/4

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	G	1530	P1A	C20-C22	8.67	1.68	1.55
8	G	1530	P1A	C9-C8	6.92	1.65	1.52
8	G	1530	P1A	C1-C10	6.70	1.64	1.54
8	G	1530	P1A	O3-C3	-6.17	1.30	1.43
8	G	1530	P1A	C21-C20	6.05	1.63	1.52

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	1530	P1A	C21-C20-C22	7.91	114.99	110.28
8	G	1530	P1A	C20-C17-C13	5.63	126.67	120.52
7	F	1456	EPH	O8-P1-O7	-4.89	89.97	109.07
8	G	1530	P1A	C18-C13-C14	4.88	114.95	109.14
7	F	1456	EPH	O5-P1-O7	-4.87	90.06	109.07

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

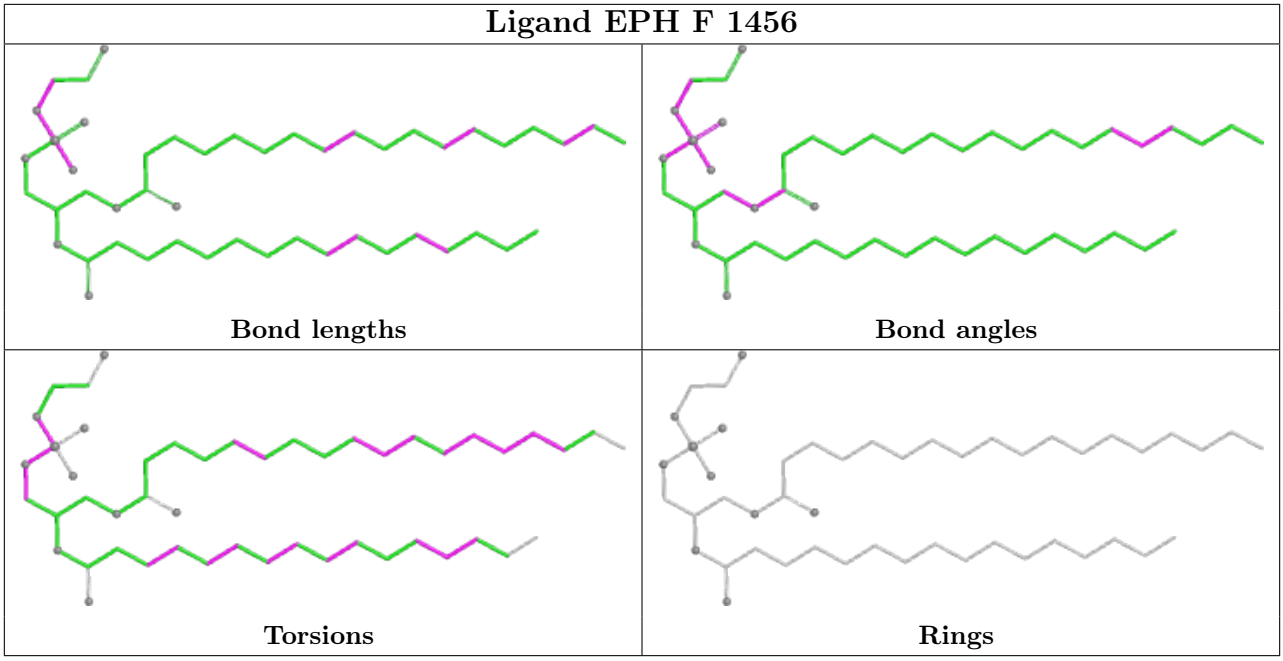
Mol	Chain	Res	Type	Atoms
7	F	1456	EPH	C29-C30-C31-C32
7	F	1456	EPH	C27-C28-C29-C30
7	F	1456	EPH	C14-C15-C16-C17
7	F	1456	EPH	C11-C12-C13-C14
7	F	1456	EPH	C37-O5-P1-O8

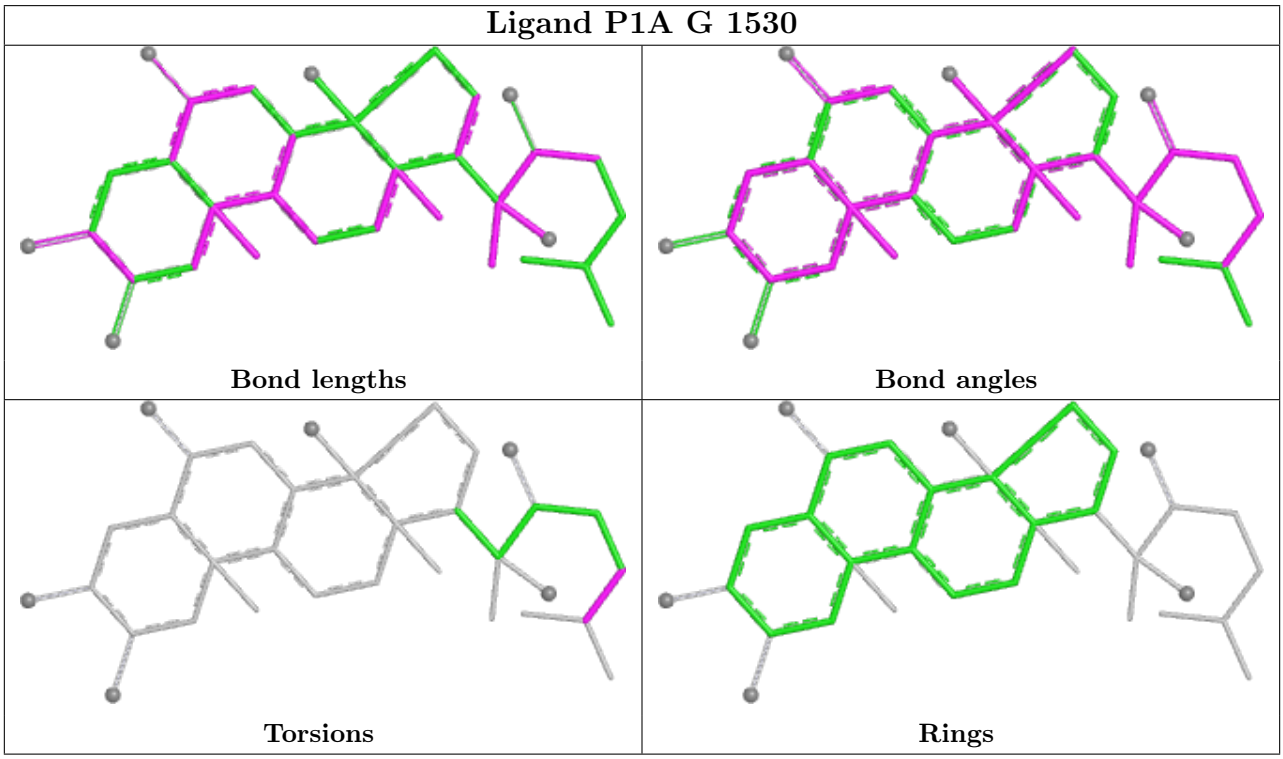
There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	1456	EPH	6	0
8	G	1530	P1A	3	0

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





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-2631. 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: 48

Y Index: 48

Z Index: 48

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: 69

Y Index: 47

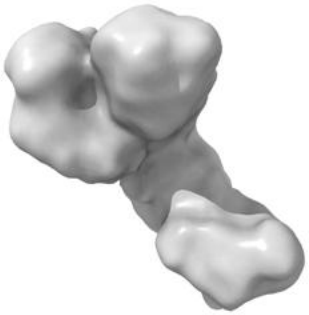
Z Index: 50

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

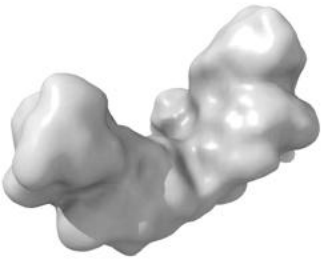
6.4 Orthogonal surface views (i)

6.4.1 Primary map

X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

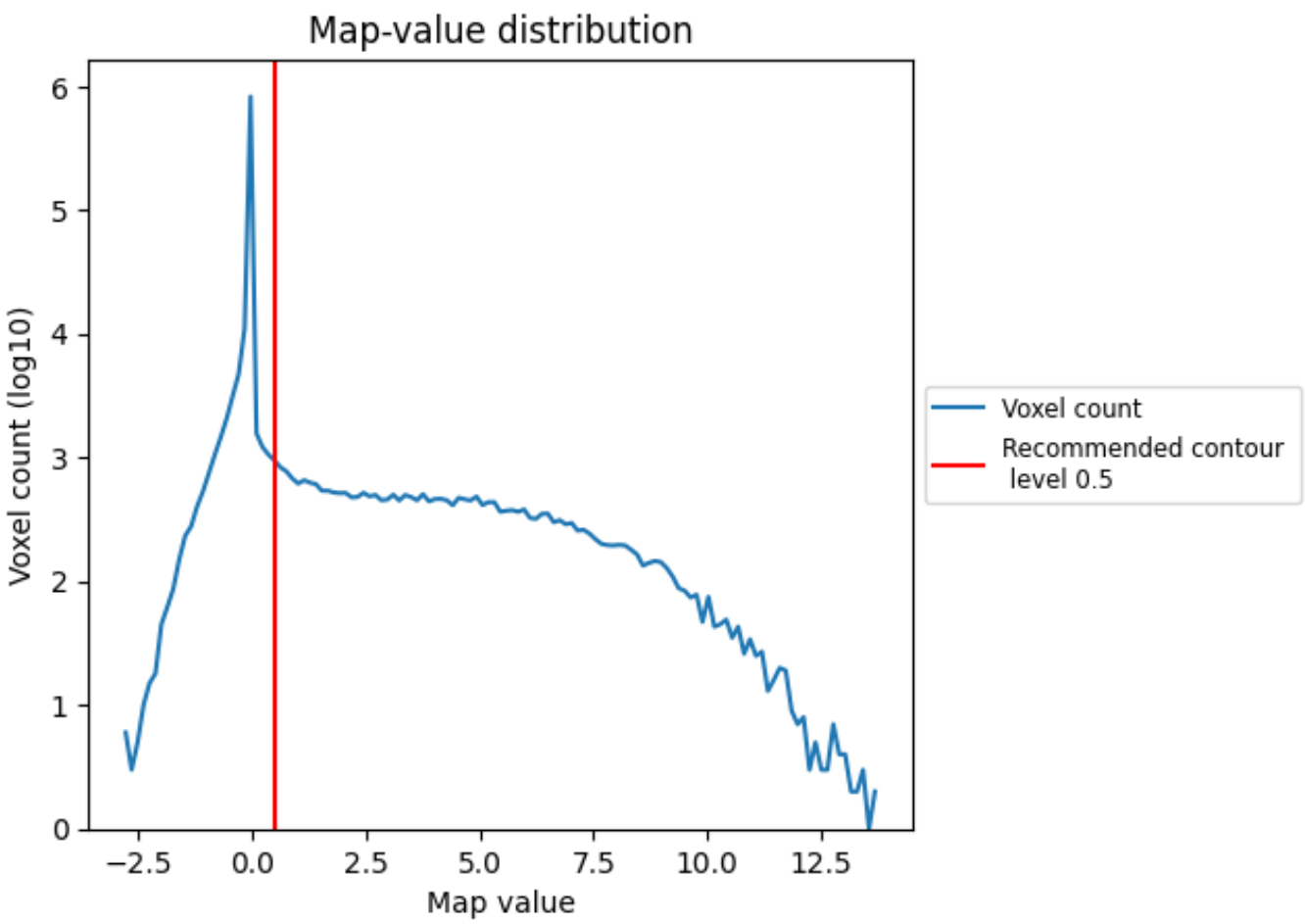
6.5 Mask visualisation (i)

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

7 Map analysis (i)

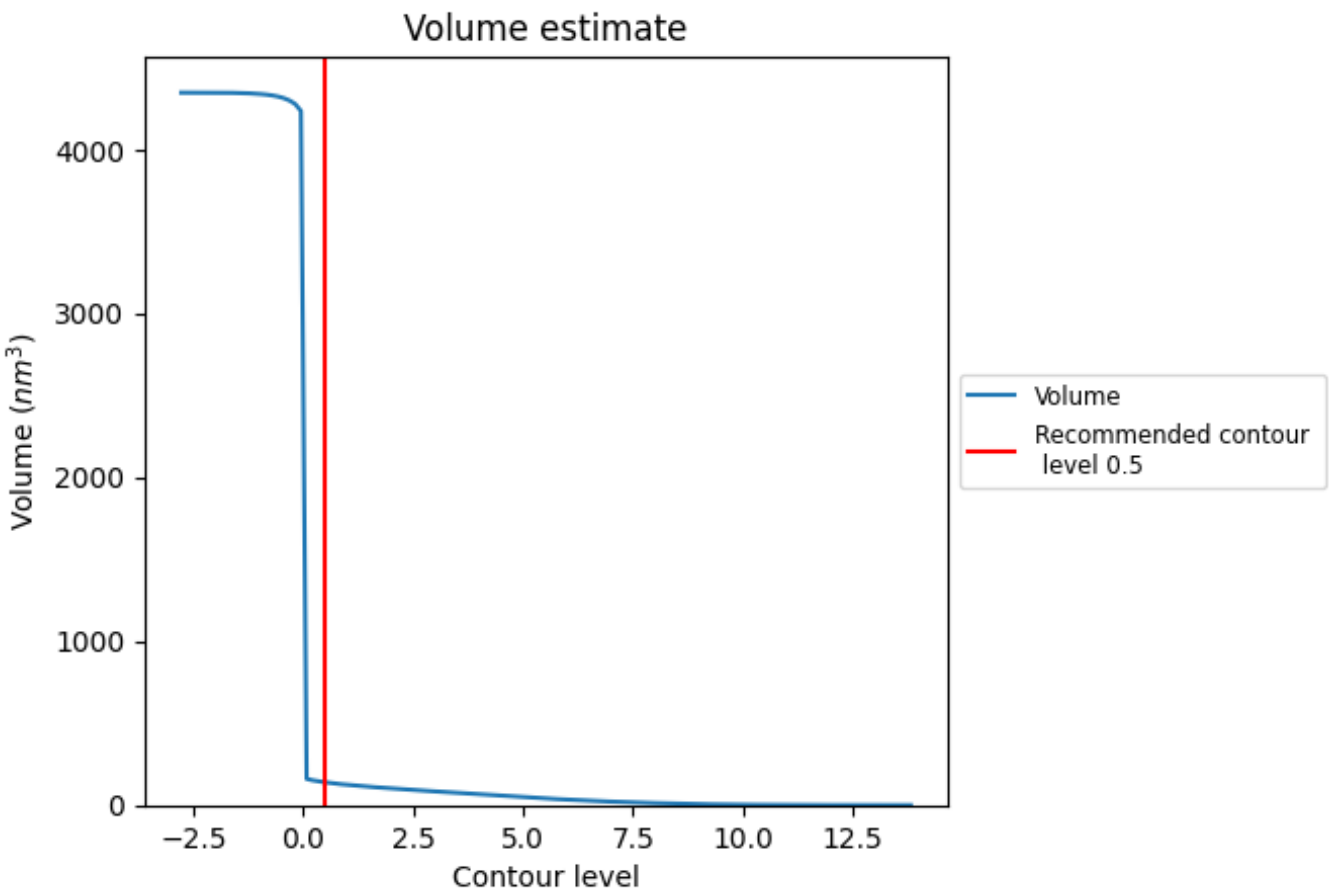
This section contains the results of statistical analysis of the map.

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.

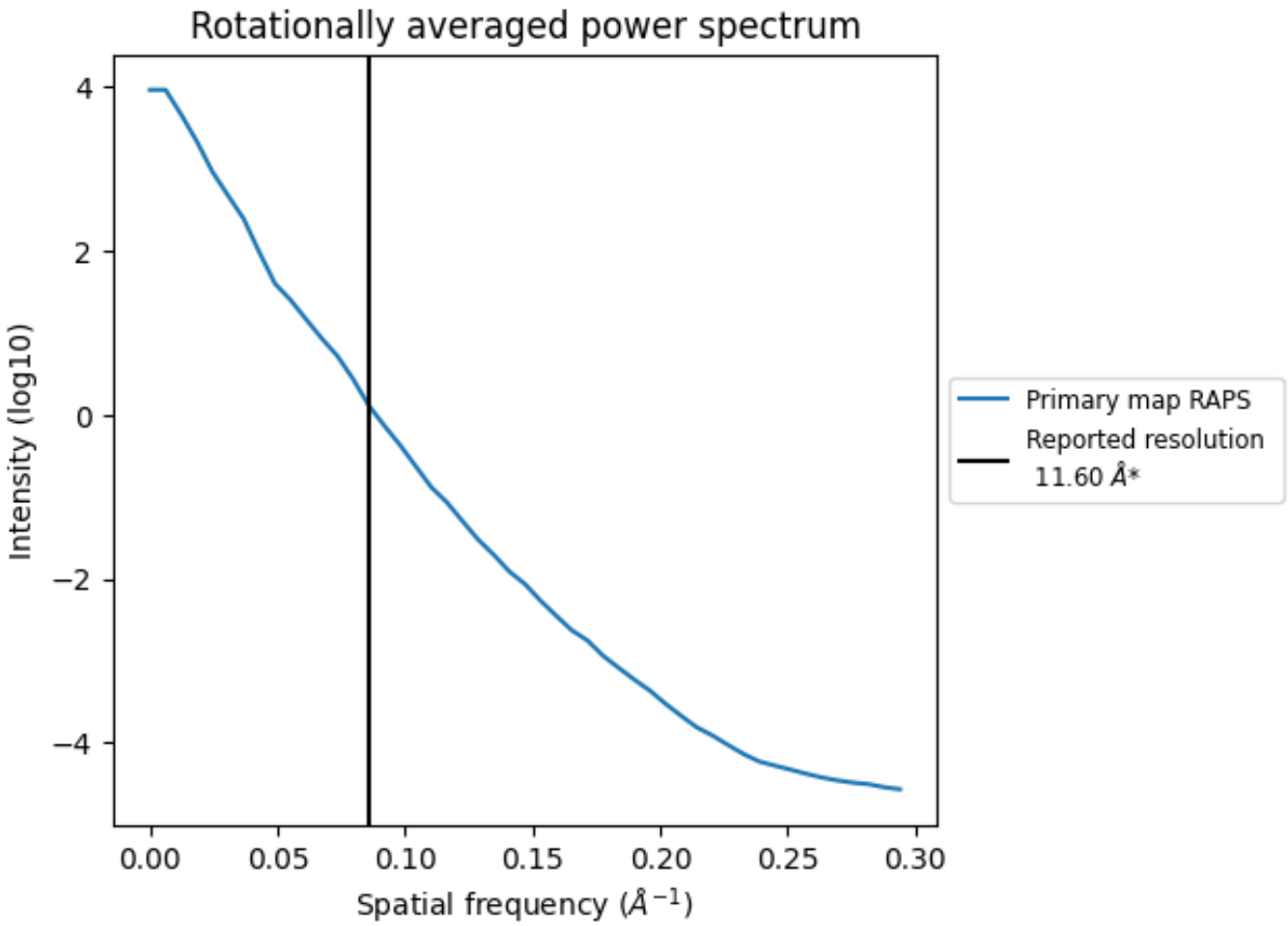
7.2 Volume estimate (i)



The volume at the recommended contour level is 140 nm^3; this corresponds to an approximate mass of 126 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 0.086 Å^{-1}

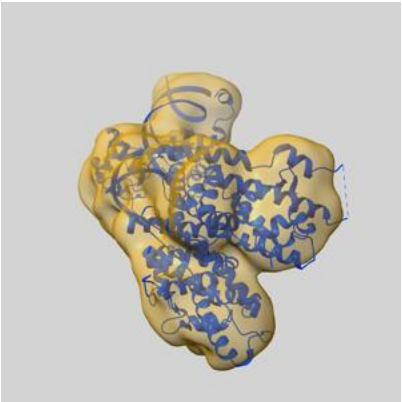
8 Fourier-Shell correlation (i)

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

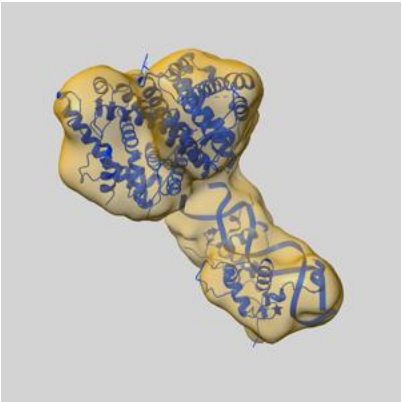
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-2631 and PDB model 4UMM. Per-residue inclusion information can be found in section 3 on page 7.

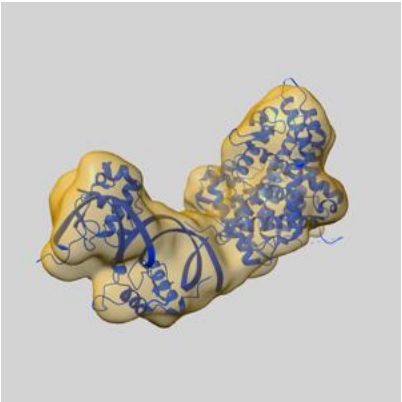
9.1 Map-model overlay (i)



X



Y



Z

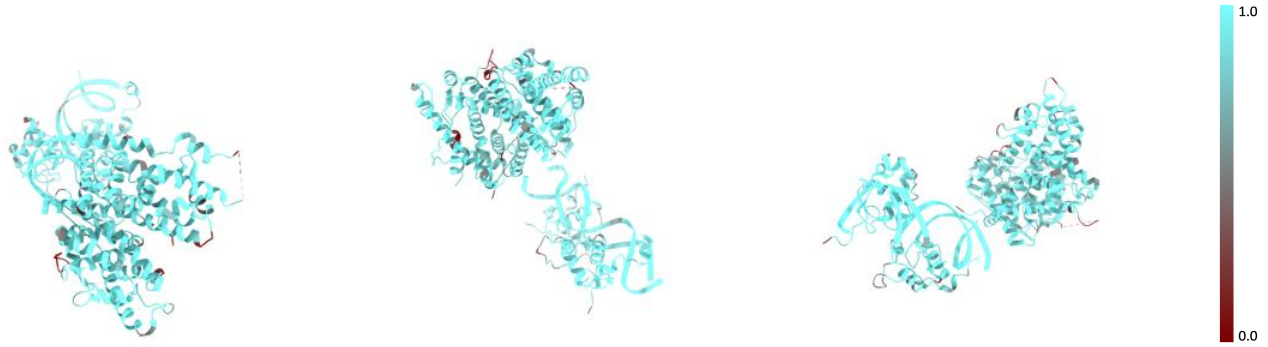
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

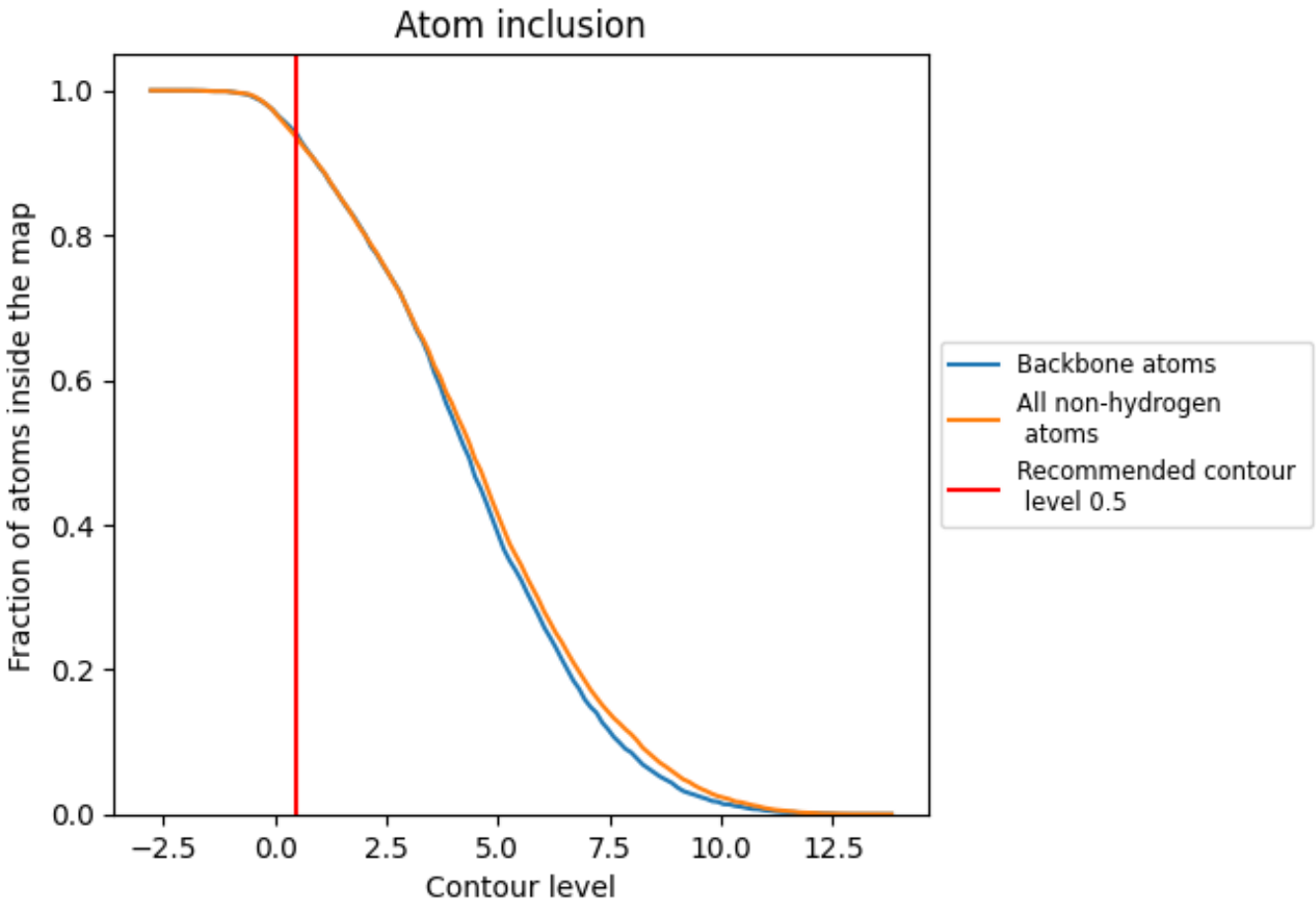
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.5).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 93% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9341	0.0710
A	0.8905	0.0640
C	0.9926	0.0760
D	0.9778	0.1160
E	0.9119	0.0720
F	0.9373	0.0670
G	0.9351	0.0660