Full wwPDB EM Validation Report (i)

Sep 28, 2024 – 11:32 AM EDT

PDB ID	:	6VWG
EMDB ID	:	EMD-21415
Title	:	Head region of the open conformation of the human type 1 insulin-like growth factor receptor ectodomain in complex with human insulin-like growth factor II.
Authors	:	Xu, Y.; Kirk, N.S.; Lawrence, M.C.; Croll, T.I.
Deposited on	:	2020-02-19
Resolution	:	3.21 Å(reported)
Based on initial model	:	5U8R

This is a Full wwPDB EM Validation 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:

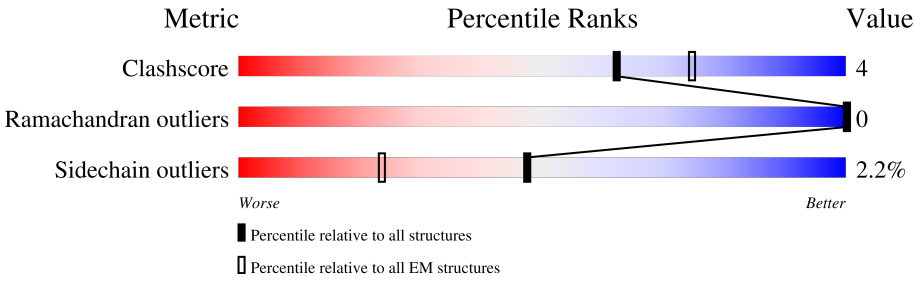
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 3.21 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=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	952	40% 6% 54%
1	B	952	29% 68%
2	I	67	75% 6% 19%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 12807 atoms, of which 6338 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 Leucine-zippered human type 1 insulin-like growth factor receptor ectodomain.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	439	6916	2201	3418	607	654	36	0	0
1	B	307	4980	1589	2478	434	469	10	0	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	939	SER	-	expression tag	UNP P03069
A	940	SER	-	expression tag	UNP P03069
A	941	SER	-	expression tag	UNP P03069
A	942	GLU	-	expression tag	UNP P03069
A	943	GLN	-	expression tag	UNP P03069
A	944	LYS	-	expression tag	UNP P03069
A	945	LEU	-	expression tag	UNP P03069
A	946	ILE	-	expression tag	UNP P03069
A	947	SER	-	expression tag	UNP P03069
A	948	GLU	-	expression tag	UNP P03069
A	949	GLU	-	expression tag	UNP P03069
A	950	ASP	-	expression tag	UNP P03069
A	951	LEU	-	expression tag	UNP P03069
A	952	ASN	-	expression tag	UNP P03069
B	939	SER	-	expression tag	UNP P03069
B	940	SER	-	expression tag	UNP P03069
B	941	SER	-	expression tag	UNP P03069
B	942	GLU	-	expression tag	UNP P03069
B	943	GLN	-	expression tag	UNP P03069
B	944	LYS	-	expression tag	UNP P03069
B	945	LEU	-	expression tag	UNP P03069
B	946	ILE	-	expression tag	UNP P03069
B	947	SER	-	expression tag	UNP P03069
B	948	GLU	-	expression tag	UNP P03069
B	949	GLU	-	expression tag	UNP P03069

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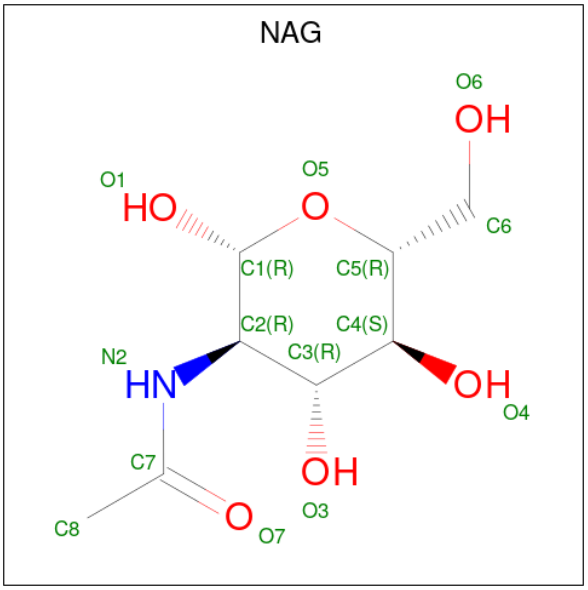
Chain	Residue	Modelled	Actual	Comment	Reference
B	950	ASP	-	expression tag	UNP P03069
B	951	LEU	-	expression tag	UNP P03069
B	952	ASN	-	expression tag	UNP P03069

- Molecule 2 is a protein called Insulin-like growth factor II.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
2	I	54	799	256	386	70	81	6	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



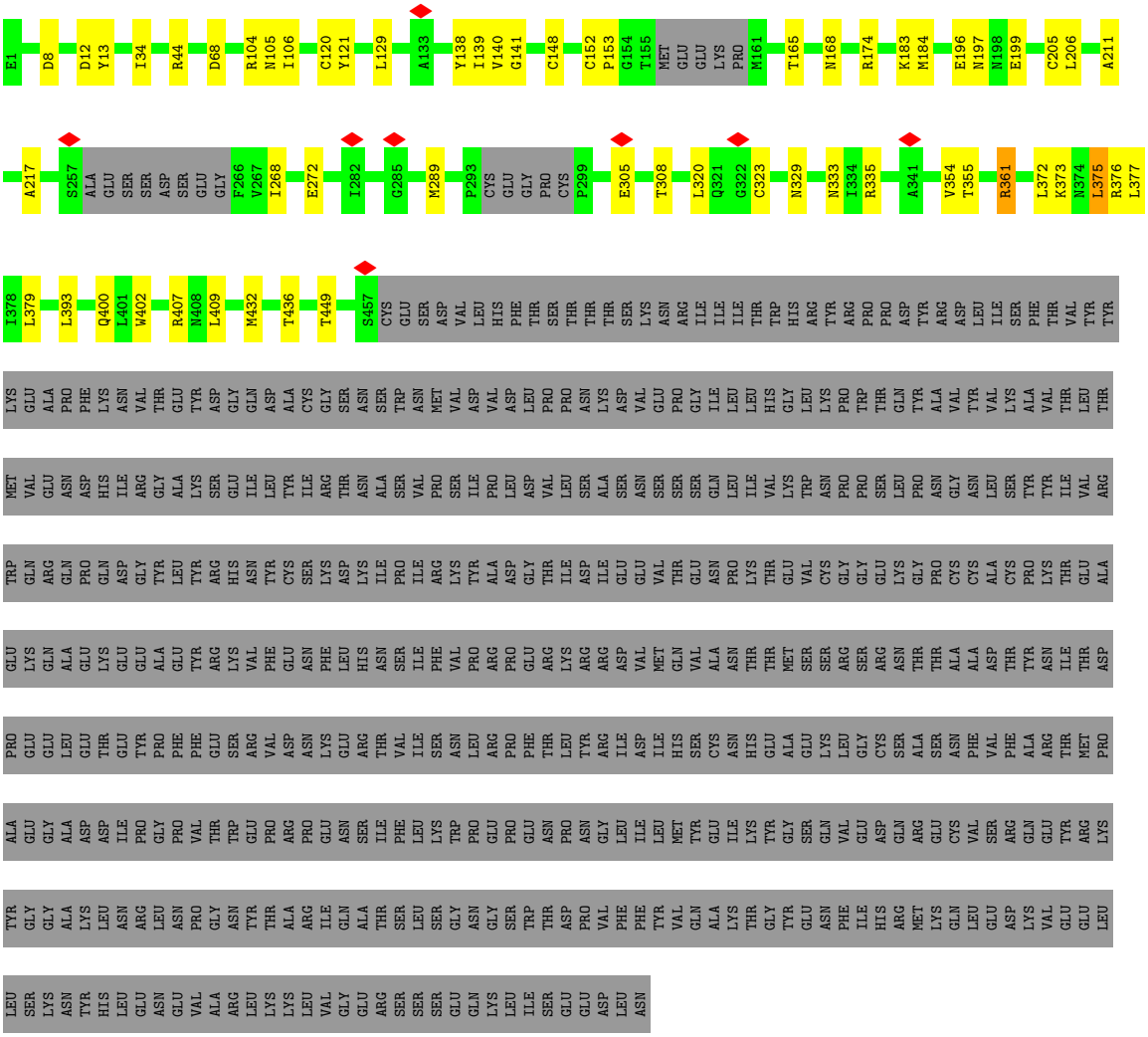
Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
3	A	1	28	8	14	1	5	0
			Total	C	H	N	O	
3	A	1	28	8	14	1	5	0
			Total	C	H	N	O	
3	A	1	28	8	14	1	5	0
			Total	C	H	N	O	
3	B	1	28	8	14	1	5	0

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.

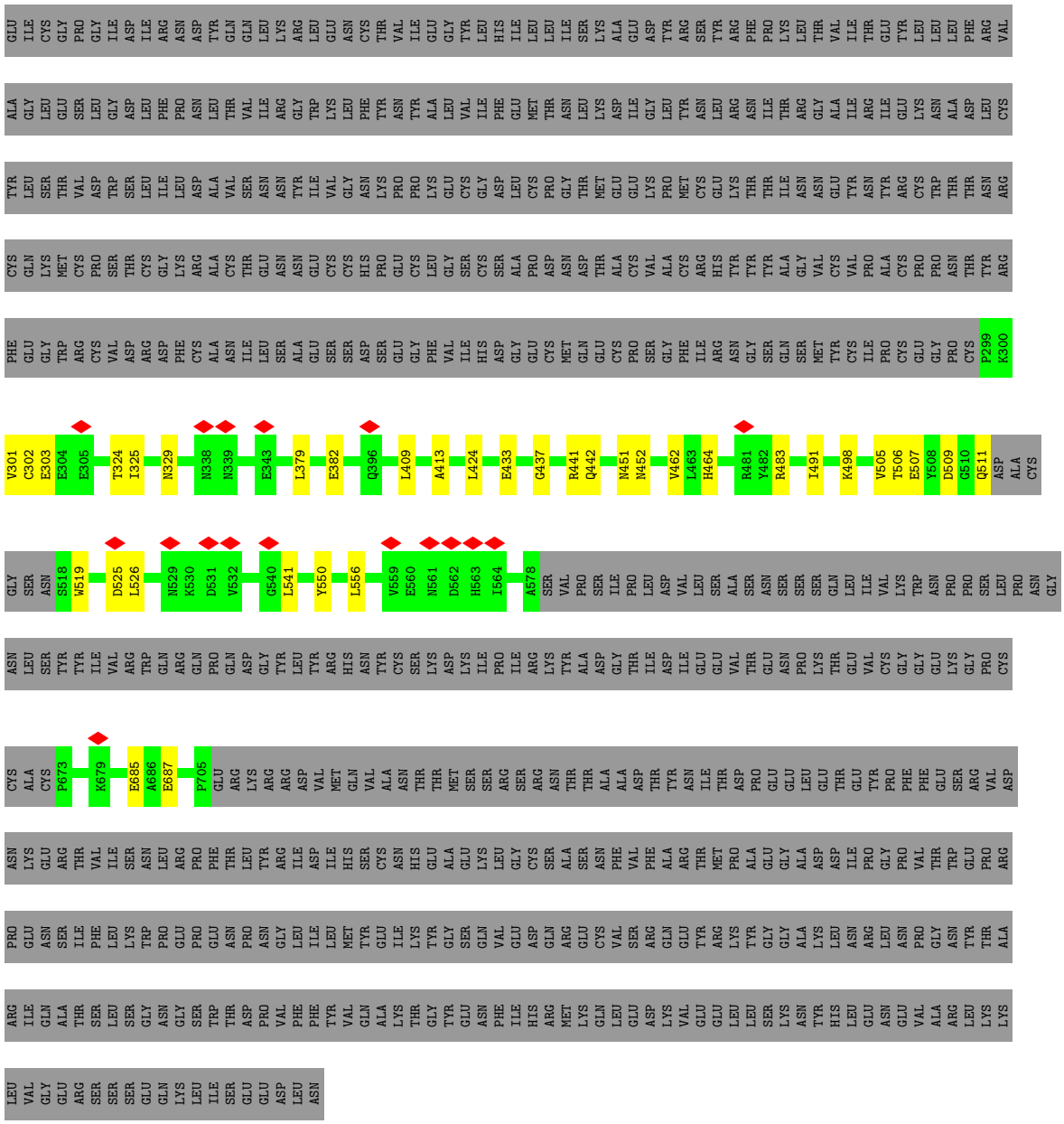
• Molecule 1: Leucine-zippered human type 1 insulin-like growth factor receptor ectodomain

Chain A: 40% 6% 54%



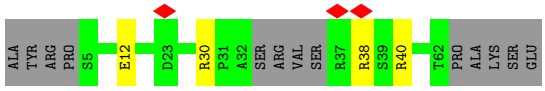
• Molecule 1: Leucine-zippered human type 1 insulin-like growth factor receptor ectodomain

Chain B: 29% 68%



- Molecule 2: Insulin-like growth factor II

Chain I:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	205471	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.541	Depositor
Minimum map value	-1.628	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	423.99997, 423.99997, 423.99997	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: NAG

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	0.35	0/3566	0.56	0/4819
1	B	0.35	0/2555	0.53	0/3452
2	I	0.34	0/418	0.55	0/561
All	All	0.35	0/6539	0.55	0/8832

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	3498	3418	3416	34	0
1	B	2502	2478	2477	18	0
2	I	413	386	382	2	0
3	A	42	42	39	2	0
3	B	14	14	13	0	0
All	All	6469	6338	6327	52	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 4.

All (52) 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:498:LYS:NZ	1:B:509:ASP:OD2	2.26	0.67
1:B:433:GLU:OE2	1:B:442:GLN:NE2	2.28	0.65
1:A:152:CYS:HB2	1:A:153:PRO:CD	2.30	0.61
1:A:335:ARG:NH2	1:B:687:GLU:OE2	2.38	0.56
1:B:483:ARG:NH2	2:I:12:GLU:OE2	2.39	0.55
1:A:104:ARG:NH1	1:A:183:LYS:O	2.41	0.54
1:A:120:CYS:SG	1:A:121:TYR:N	2.78	0.50
1:B:437:GLY:O	1:B:441:ARG:NH2	2.44	0.50
1:B:329:ASN:ND2	1:B:382:GLU:OE2	2.44	0.50
1:A:196:GLU:O	1:A:197:ASN:ND2	2.45	0.49
1:A:165:THR:OG1	1:A:174:ARG:NH1	2.46	0.49
1:A:152:CYS:HB2	1:A:153:PRO:HD2	1.94	0.49
3:A:1002:NAG:H3	3:A:1002:NAG:H83	1.94	0.48
1:A:44:ARG:NH2	1:A:68:ASP:O	2.47	0.47
1:A:449:THR:O	1:A:449:THR:HG22	2.13	0.47
1:B:424:LEU:O	1:B:452:ASN:ND2	2.39	0.47
1:A:373:LYS:O	1:A:407:ARG:NH2	2.45	0.47
1:B:541:LEU:HD12	1:B:541:LEU:N	2.30	0.47
1:A:354:VAL:HG12	1:A:355:THR:O	2.16	0.46
1:A:375:LEU:HD23	1:A:376:ARG:N	2.31	0.46
1:A:375:LEU:HD23	1:A:376:ARG:H	1.81	0.46
1:A:211:ALA:H	1:A:217:ALA:HB1	1.80	0.45
1:A:129:LEU:HD13	1:A:184:MET:HB3	1.99	0.45
1:B:525:ASP:OD1	1:B:526:LEU:N	2.50	0.45
1:B:301:VAL:HG12	1:B:303:GLU:H	1.83	0.44
1:A:140:VAL:HG23	1:A:141:GLY:N	2.33	0.44
3:A:1002:NAG:C1	3:A:1002:NAG:H82	2.47	0.44
1:A:12:ASP:OD1	1:A:13:TYR:N	2.50	0.44
1:A:268:ILE:HD12	1:A:289:MET:HA	1.99	0.44
1:A:197:ASN:OD1	1:A:199:GLU:HG2	2.19	0.43
1:B:324:THR:OG1	1:B:325:ILE:N	2.52	0.43
1:B:451:ASN:OD1	1:B:452:ASN:N	2.52	0.43
1:A:320:LEU:HA	1:A:323:CYS:SG	2.59	0.43
1:B:505:VAL:CG1	1:B:506:THR:N	2.82	0.42
1:A:13:TYR:CE2	1:A:34:ILE:HG21	2.55	0.42
1:A:138:TYR:OH	1:B:685:GLU:HG3	2.20	0.42
1:A:376:ARG:O	1:A:377:LEU:HD22	2.20	0.42
1:A:105:ASN:HD22	1:A:206:LEU:HD11	1.85	0.41
1:A:333:ASN:ND2	1:A:335:ARG:HH12	2.18	0.41
1:A:139:ILE:HG22	1:A:139:ILE:O	2.21	0.41
1:B:491:ILE:HD11	1:B:556:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:ASN:OD1	1:A:329:ASN:N	2.53	0.41
1:A:432:MET:HG3	1:A:436:THR:OG1	2.21	0.41
1:B:462:VAL:HG13	1:B:464:HIS:CE1	2.56	0.41
1:A:372:LEU:HB2	1:A:402:TRP:CH2	2.56	0.41
1:A:436:THR:HG22	1:A:436:THR:O	2.20	0.41
1:A:361:ARG:HA	1:A:393:LEU:O	2.21	0.40
1:B:379:LEU:O	1:B:413:ALA:HB3	2.21	0.40
1:A:105:ASN:OD1	1:A:106:ILE:N	2.54	0.40
1:B:507:GLU:O	1:B:519:TRP:NE1	2.54	0.40
1:A:308:THR:HG22	1:A:329:ASN:HB2	2.02	0.40
1:A:305:GLU:OE1	2:I:38:ARG:NH2	2.54	0.40

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	431/952 (45%)	384 (89%)	47 (11%)	0	100	100
1	B	301/952 (32%)	266 (88%)	35 (12%)	0	100	100
2	I	50/67 (75%)	43 (86%)	7 (14%)	0	100	100
All	All	782/1971 (40%)	693 (89%)	89 (11%)	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	390/852 (46%)	380 (97%)	10 (3%)	41	68
1	B	277/852 (32%)	273 (99%)	4 (1%)	62	80
2	I	45/57 (79%)	43 (96%)	2 (4%)	24	55
All	All	712/1761 (40%)	696 (98%)	16 (2%)	47	71

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASP
1	A	148	CYS
1	A	168	ASN
1	A	205	CYS
1	A	272	GLU
1	A	361	ARG
1	A	375	LEU
1	A	379	LEU
1	A	400	GLN
1	A	409	LEU
1	B	302	CYS
1	B	409	LEU
1	B	511	GLN
1	B	550	TYR
2	I	30	ARG
2	I	40	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	ASN
1	A	333	ASN
1	A	451	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)

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	$\#\|Z\| > 2$
3	NAG	A	1001	1	14,14,15	0.19	0	17,19,21	0.65	1 (5%)
3	NAG	B	1001	1	14,14,15	0.26	0	17,19,21	0.87	1 (5%)
3	NAG	A	1002	1	14,14,15	0.90	1 (7%)	17,19,21	1.25	2 (11%)
3	NAG	A	1003	1	14,14,15	0.26	0	17,19,21	0.68	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
3	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
3	NAG	A	1002	1	-	5/6/23/26	0/1/1/1
3	NAG	A	1003	1	-	3/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	NAG	C1-C2	2.98	1.56	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1002	NAG	C2-N2-C7	3.26	127.27	122.90
3	A	1002	NAG	C1-O5-C5	3.16	116.42	112.19
3	B	1001	NAG	C1-O5-C5	2.87	116.04	112.19
3	A	1001	NAG	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	NAG	C3-C2-N2-C7
3	A	1002	NAG	C8-C7-N2-C2
3	A	1002	NAG	O7-C7-N2-C2
3	A	1003	NAG	C4-C5-C6-O6
3	A	1003	NAG	O5-C5-C6-O6
3	A	1002	NAG	C1-C2-N2-C7
3	A	1002	NAG	O5-C5-C6-O6
3	B	1001	NAG	C3-C2-N2-C7
3	B	1001	NAG	C1-C2-N2-C7
3	A	1002	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1002	NAG	2	0

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.

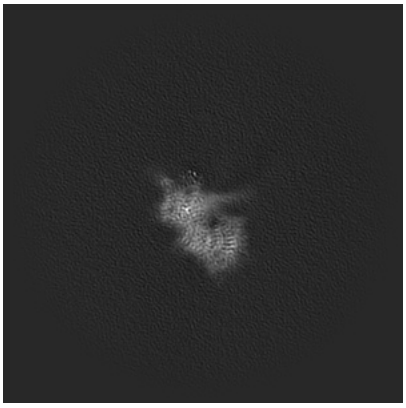
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-21415. These allow visual inspection of the internal detail of the map and identification of artifacts.

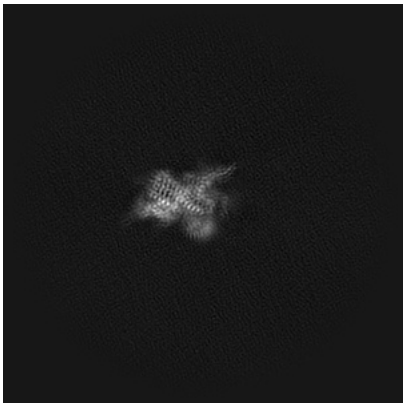
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

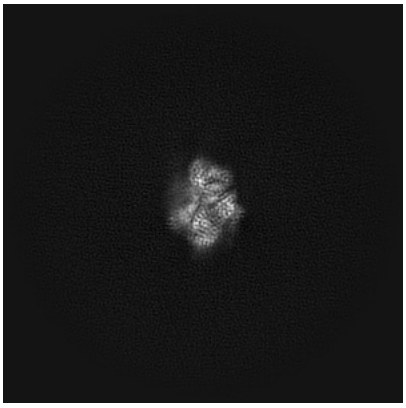
6.1.1 Primary map



X



Y

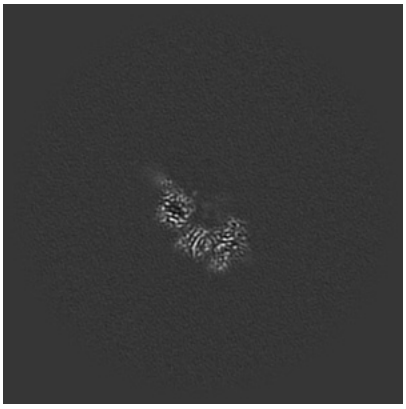


Z

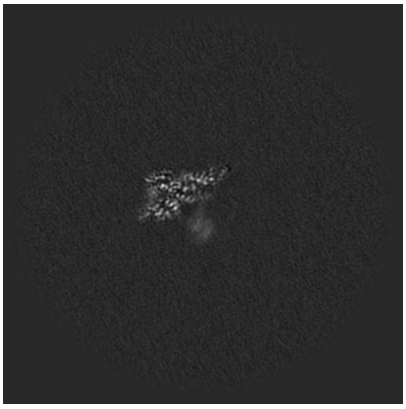
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

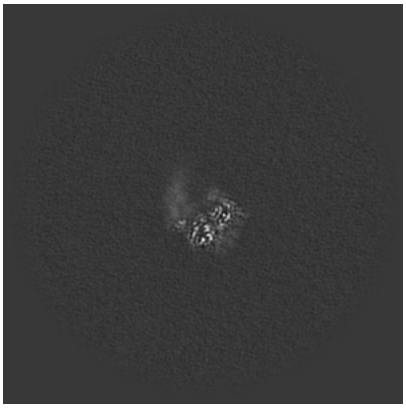
6.2.1 Primary map



X Index: 200



Y Index: 200

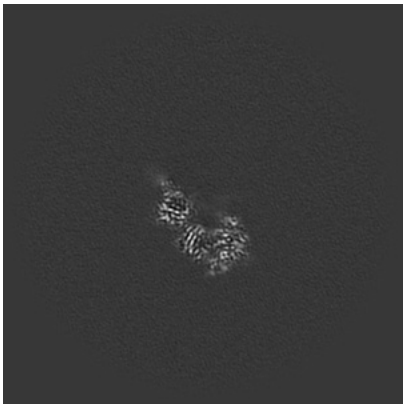


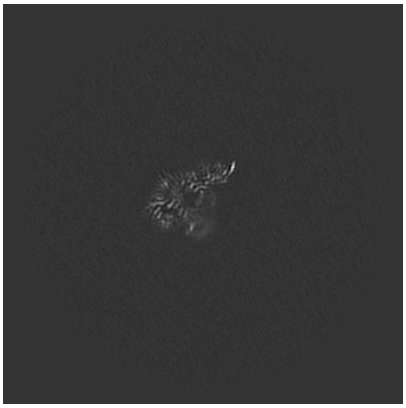
Z Index: 200

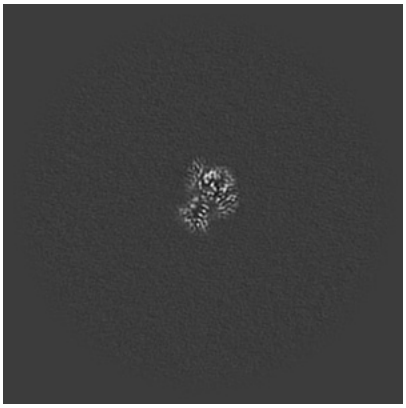
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 197

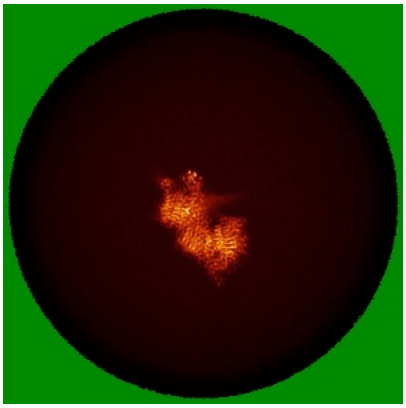

Y Index: 191

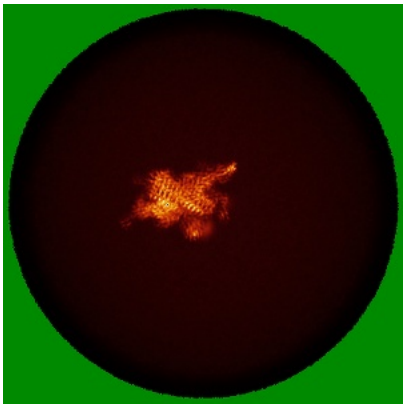

Z Index: 161

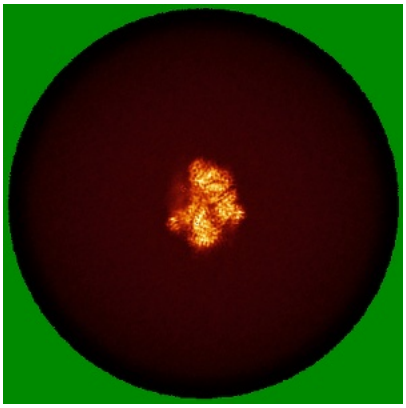
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

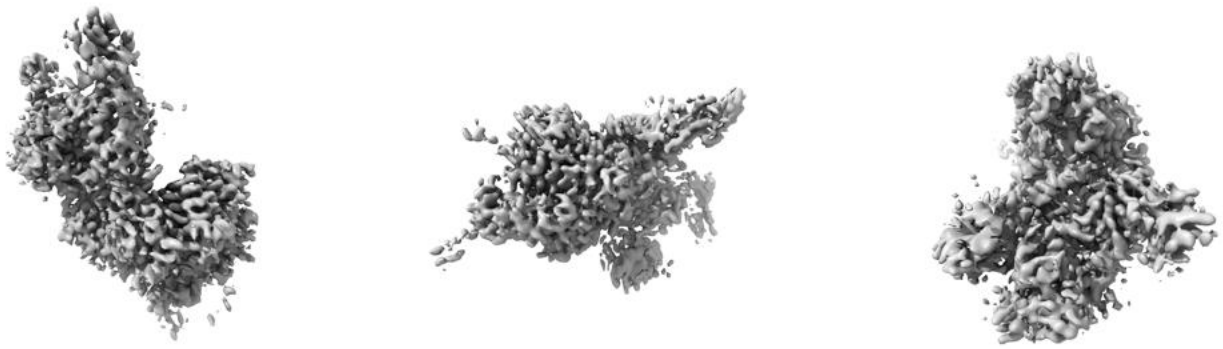

Y


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

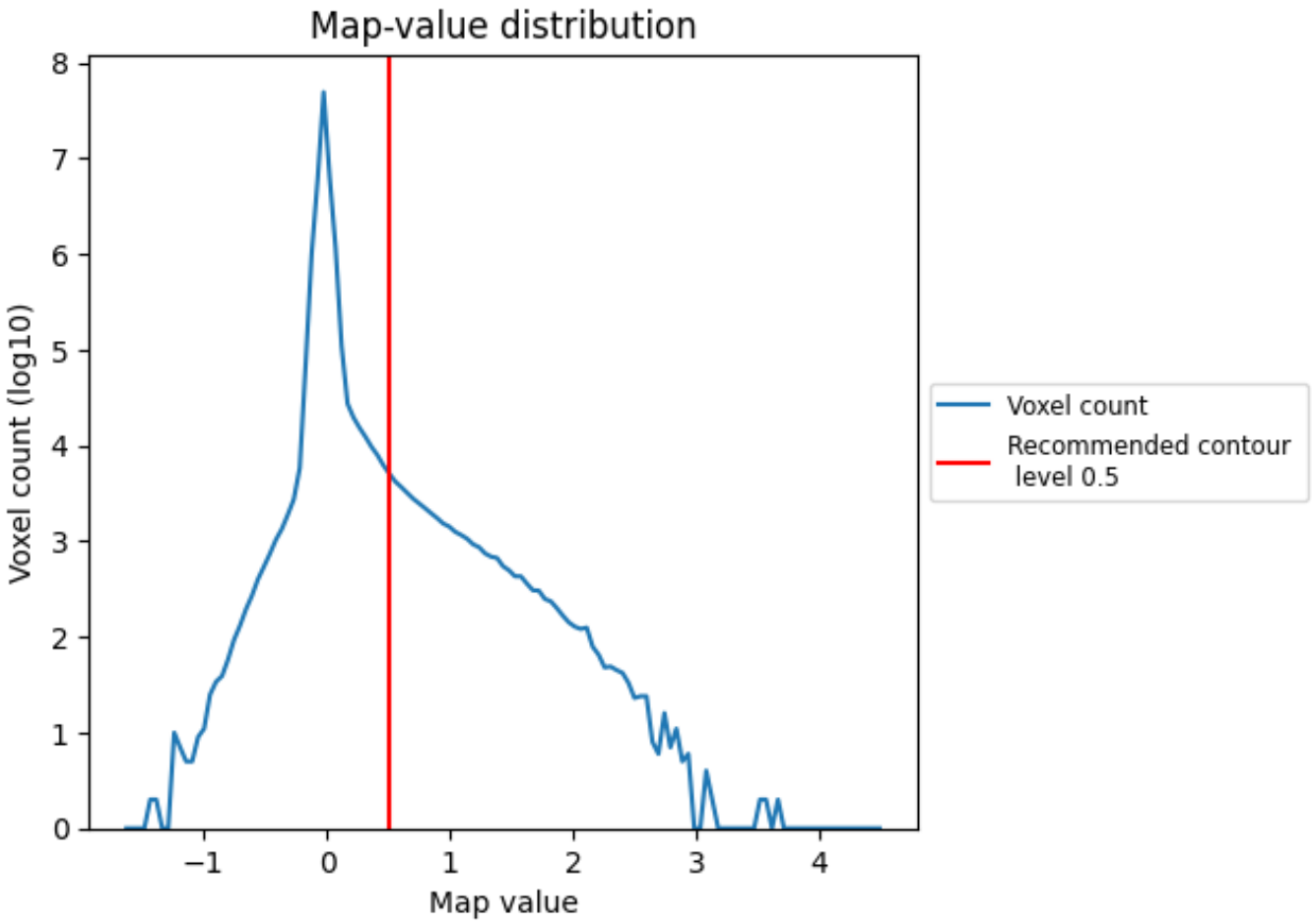
6.6 Mask visualisation (i)

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

7 Map analysis (i)

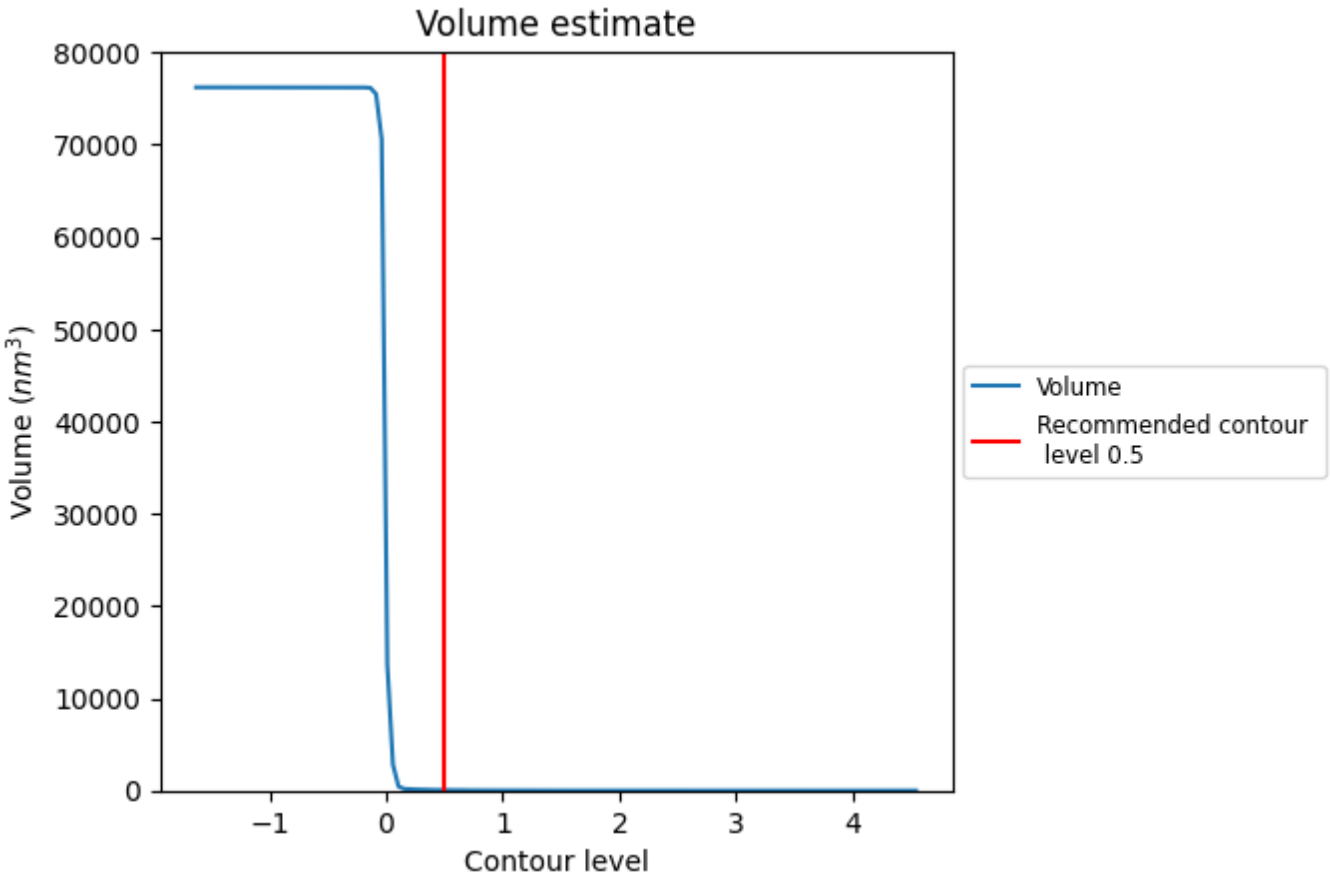
This section contains the results of statistical analysis of the map.

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.

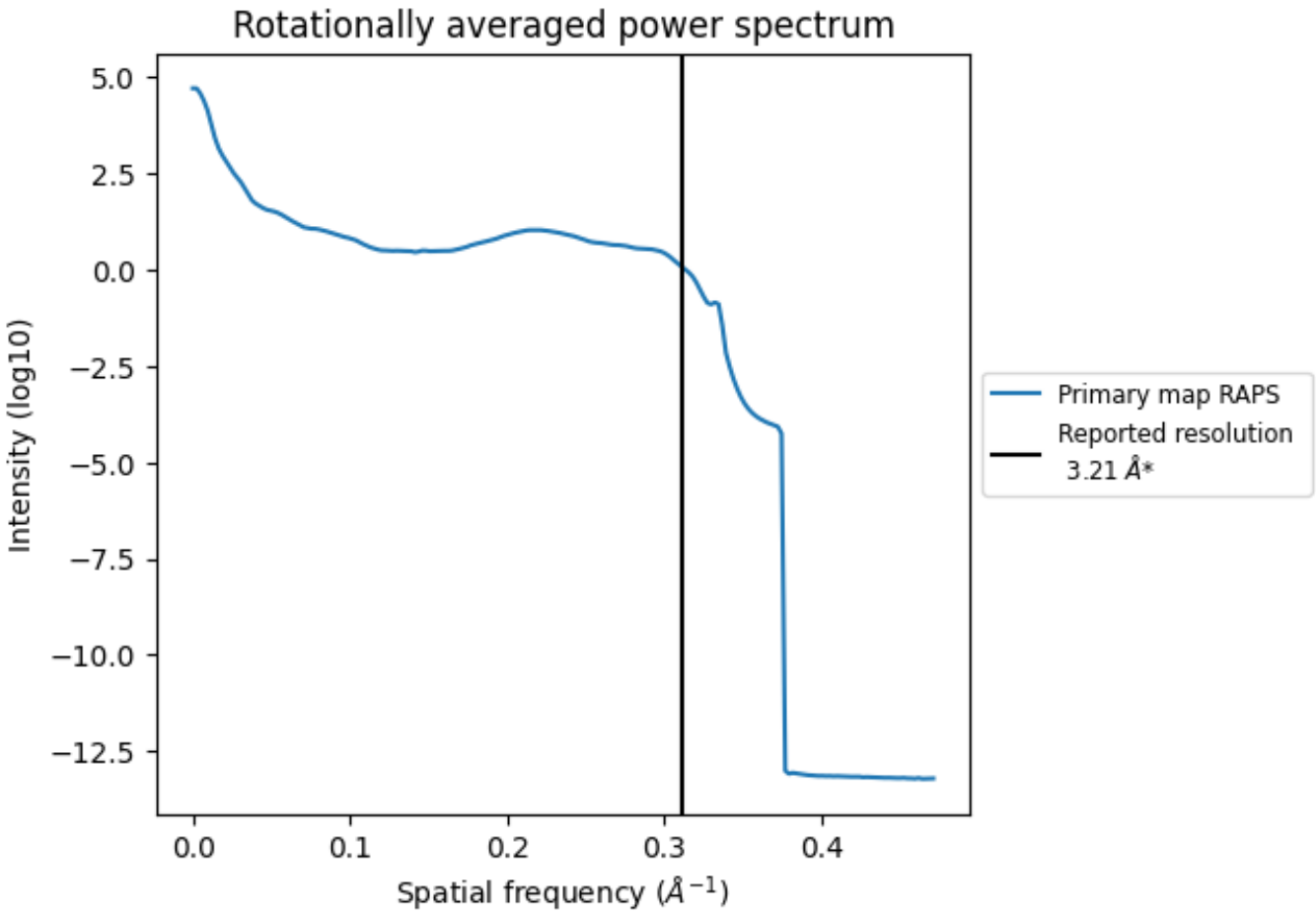
7.2 Volume estimate (i)



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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}

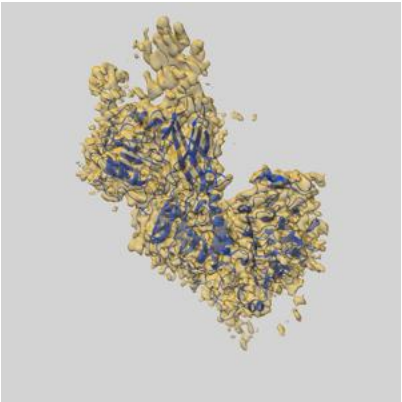
8 Fourier-Shell correlation (i)

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

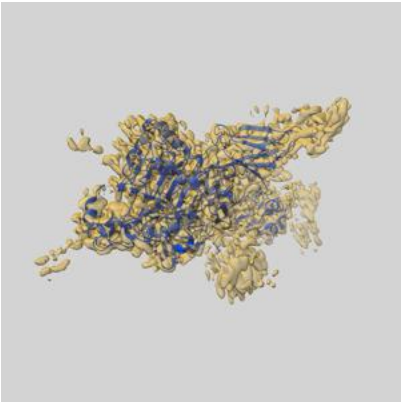
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-21415 and PDB model 6VWG. Per-residue inclusion information can be found in section 3 on page 5.

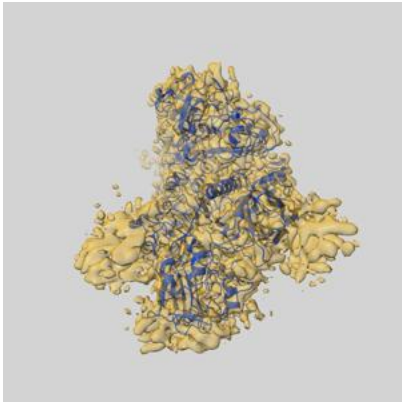
9.1 Map-model overlay (i)



X



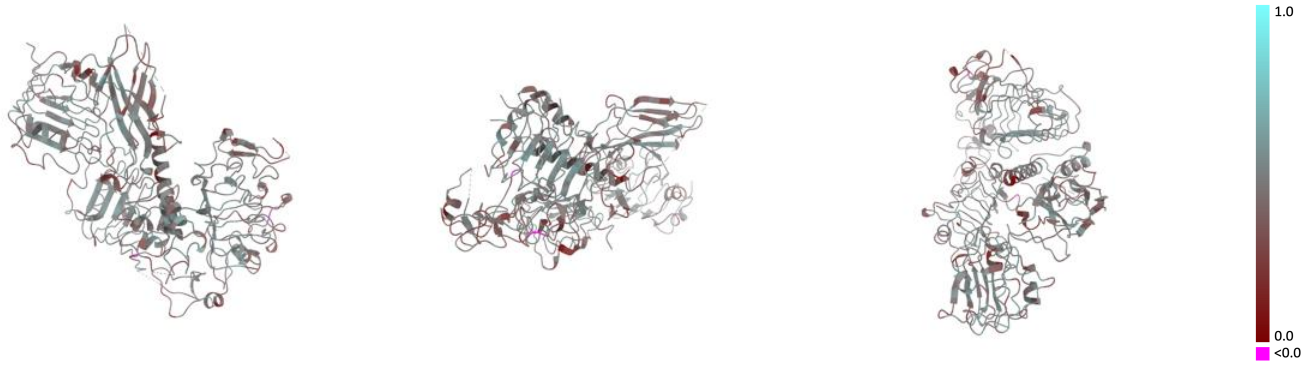
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.5 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.

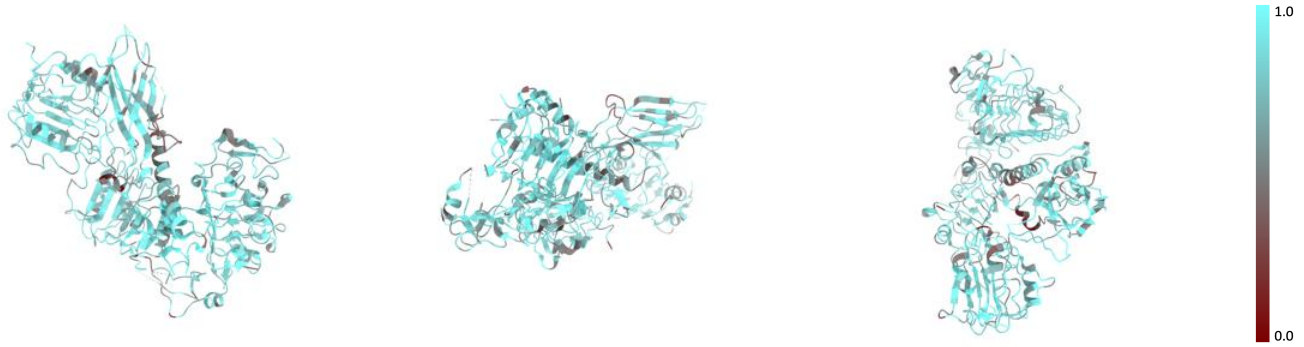
9.2 Q-score mapped to coordinate model (i)



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.

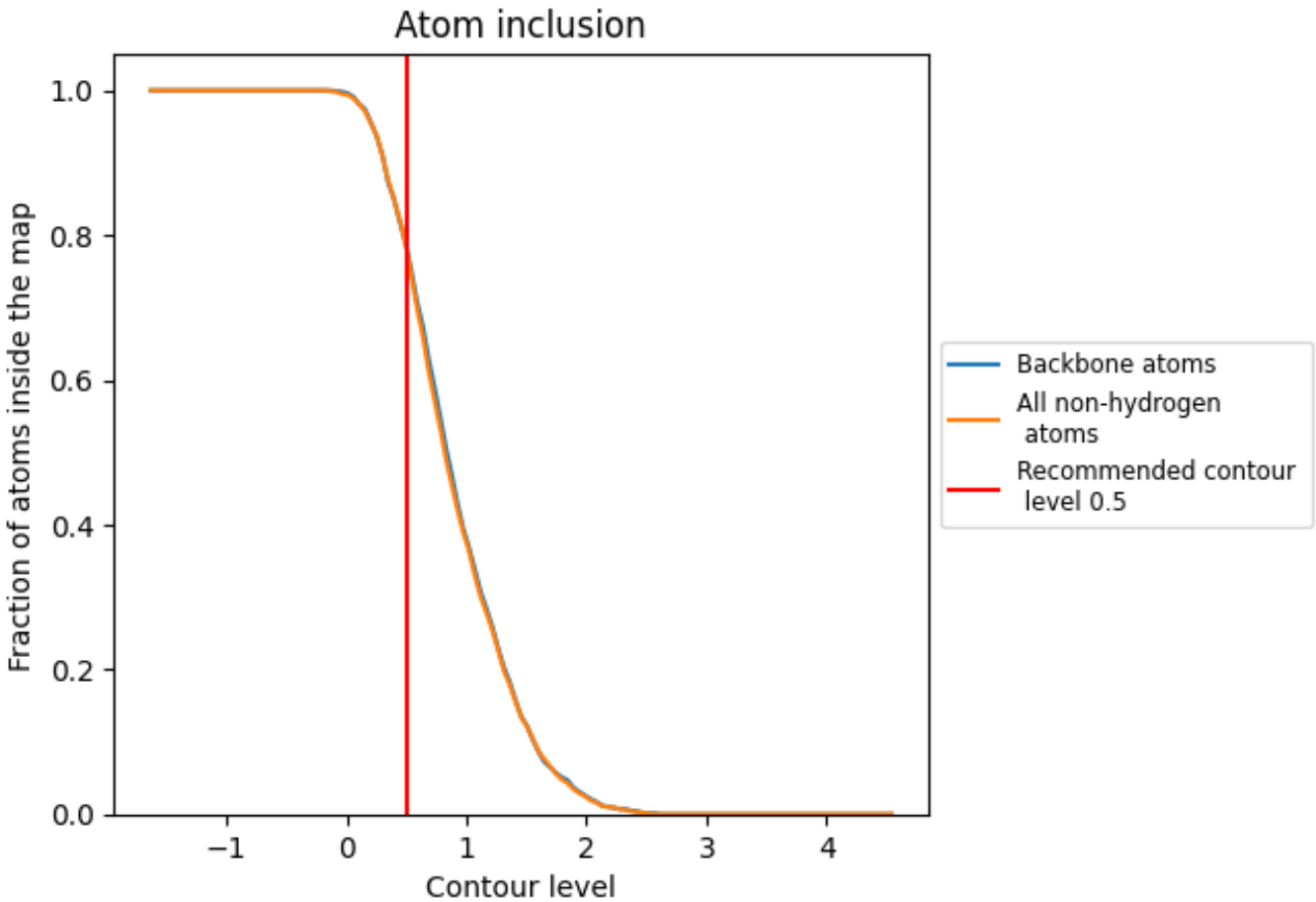
9.3 Atom inclusion mapped to coordinate model (i)



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, 78% of all backbone atoms, 78% 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	0.7830	0.4530
A	0.7800	0.4510
B	0.7630	0.4560
I	0.7980	0.4490