



Full wwPDB EM Validation Report ⓘ

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PDB ID : 9UTC / pdb_00009utc
EMDB ID : EMD-64488
Title : The VFT domains of human sweet taste receptor TAS1R2 and TAS1R3 in the sucralose-bound state
Authors : Shi, Z.J.; Xu, W.X.; Yue, X.L.; Wu, L.J.; Hua, T.; Liu, Z.J.
Deposited on : 2025-05-03
Resolution : 3.33 Å(reported)

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 ⓘ 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.dev118
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

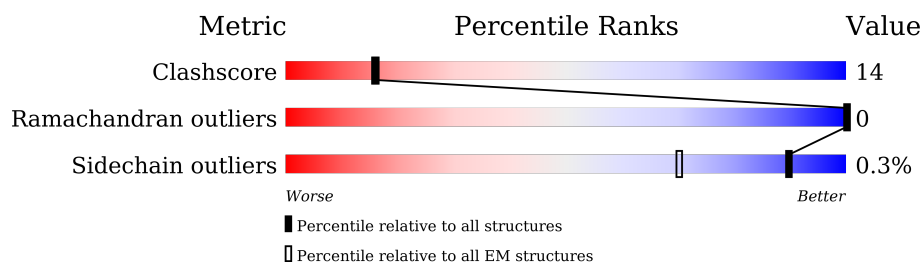
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.33 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1078	
2	B	1130	
3	C	2	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8143 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 Taste receptor type 1 member 2, Taste receptor type 1 member 2, Engineered red fluorescent protein mScarlet3.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	500	Total	C	N	O	S	0	0
			4036	2581	677	752	26		

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	initiating methionine	UNP Q8TE23
A	-2	LYS	-	expression tag	UNP Q8TE23
A	-1	THR	-	expression tag	UNP Q8TE23
A	0	ILE	-	expression tag	UNP Q8TE23
A	1	ILE	-	expression tag	UNP Q8TE23
A	2	ALA	-	expression tag	UNP Q8TE23
A	3	LEU	-	expression tag	UNP Q8TE23
A	4	SER	-	expression tag	UNP Q8TE23
A	5	TYR	-	expression tag	UNP Q8TE23
A	6	ILE	-	expression tag	UNP Q8TE23
A	7	PHE	-	expression tag	UNP Q8TE23
A	8	CYS	-	expression tag	UNP Q8TE23
A	9	LEU	-	expression tag	UNP Q8TE23
A	10	VAL	-	expression tag	UNP Q8TE23
A	11	PHE	-	expression tag	UNP Q8TE23
A	12	ALA	-	expression tag	UNP Q8TE23
A	13	GLY	-	expression tag	UNP Q8TE23
A	14	SER	-	expression tag	UNP Q8TE23
A	15	ASP	-	expression tag	UNP Q8TE23
A	16	TYR	-	expression tag	UNP Q8TE23
A	17	LYS	-	expression tag	UNP Q8TE23
A	18	ASP	-	expression tag	UNP Q8TE23
A	19	ASP	-	expression tag	UNP Q8TE23
A	20	ASP	-	expression tag	UNP Q8TE23
A	21	ASP	-	expression tag	UNP Q8TE23
A	22	LYS	-	expression tag	UNP Q8TE23
A	23	GLY	-	expression tag	UNP Q8TE23

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Chain	Residue	Modelled	Actual	Comment	Reference
A	24	SER	-	expression tag	UNP Q8TE23
A	25	ALA	-	expression tag	UNP Q8TE23

- Molecule 2 is a protein called Taste receptor type 1 member 3,mNeonGreen.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	526	Total	C	N	O	S	0	0
			4084	2577	722	752	33		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q7RTX0
B	-6	LYS	-	expression tag	UNP Q7RTX0
B	-5	THR	-	expression tag	UNP Q7RTX0
B	-4	ILE	-	expression tag	UNP Q7RTX0
B	-3	ILE	-	expression tag	UNP Q7RTX0
B	-2	ALA	-	expression tag	UNP Q7RTX0
B	-1	LEU	-	expression tag	UNP Q7RTX0
B	0	SER	-	expression tag	UNP Q7RTX0
B	1	TYR	-	expression tag	UNP Q7RTX0
B	2	ILE	-	expression tag	UNP Q7RTX0
B	3	PHE	-	expression tag	UNP Q7RTX0
B	4	CYS	-	expression tag	UNP Q7RTX0
B	5	LEU	-	expression tag	UNP Q7RTX0
B	6	VAL	-	expression tag	UNP Q7RTX0
B	7	PHE	-	expression tag	UNP Q7RTX0
B	8	ALA	-	expression tag	UNP Q7RTX0
B	9	GLY	-	expression tag	UNP Q7RTX0
B	10	SER	-	expression tag	UNP Q7RTX0
B	11	ASP	-	expression tag	UNP Q7RTX0
B	12	TYR	-	expression tag	UNP Q7RTX0
B	13	LYS	-	expression tag	UNP Q7RTX0
B	14	ASP	-	expression tag	UNP Q7RTX0
B	15	ASP	-	expression tag	UNP Q7RTX0
B	16	ASP	-	expression tag	UNP Q7RTX0
B	17	ASP	-	expression tag	UNP Q7RTX0
B	18	LYS	-	expression tag	UNP Q7RTX0
B	19	GLY	-	expression tag	UNP Q7RTX0
B	20	SER	-	expression tag	UNP Q7RTX0
B	853	GLY	-	linker	UNP Q7RTX0
B	854	SER	-	linker	UNP Q7RTX0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	855	SER	-	linker	UNP Q7RTX0
B	856	GLY	-	linker	UNP Q7RTX0
B	857	LEU	-	linker	UNP Q7RTX0
B	858	GLU	-	linker	UNP Q7RTX0
B	859	VAL	-	linker	UNP Q7RTX0
B	860	LEU	-	linker	UNP Q7RTX0
B	861	PHE	-	linker	UNP Q7RTX0
B	862	GLN	-	linker	UNP Q7RTX0
B	863	GLY	-	linker	UNP Q7RTX0
B	864	PRO	-	linker	UNP Q7RTX0
B	865	SER	-	linker	UNP Q7RTX0
B	866	GLY	-	linker	UNP Q7RTX0
B	867	GLY	-	linker	UNP Q7RTX0
B	1103	GLY	-	expression tag	UNP A0A1S4NYF2
B	1104	SER	-	expression tag	UNP A0A1S4NYF2
B	1105	GLU	-	expression tag	UNP A0A1S4NYF2
B	1106	ASN	-	expression tag	UNP A0A1S4NYF2
B	1107	LEU	-	expression tag	UNP A0A1S4NYF2
B	1108	TYR	-	expression tag	UNP A0A1S4NYF2
B	1109	PHE	-	expression tag	UNP A0A1S4NYF2
B	1110	GLN	-	expression tag	UNP A0A1S4NYF2
B	1111	SER	-	expression tag	UNP A0A1S4NYF2
B	1112	SER	-	expression tag	UNP A0A1S4NYF2
B	1113	GLY	-	expression tag	UNP A0A1S4NYF2
B	1114	HIS	-	expression tag	UNP A0A1S4NYF2
B	1115	HIS	-	expression tag	UNP A0A1S4NYF2
B	1116	HIS	-	expression tag	UNP A0A1S4NYF2
B	1117	HIS	-	expression tag	UNP A0A1S4NYF2
B	1118	HIS	-	expression tag	UNP A0A1S4NYF2
B	1119	HIS	-	expression tag	UNP A0A1S4NYF2
B	1120	HIS	-	expression tag	UNP A0A1S4NYF2
B	1121	HIS	-	expression tag	UNP A0A1S4NYF2
B	1122	HIS	-	expression tag	UNP A0A1S4NYF2

- Molecule 3 is an oligosaccharide called 4-chloro-4-deoxy-alpha-D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy-beta-D-fructofuranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	2	Total	C	Cl	O	0	0
			23	12	3	8		

- Molecule 2: Taste receptor type 1 member 3,mNeonGreen

TYR	THR	GLU	LEU	ALA	GLY	CYS	ARG	T434	F324	E203	P91	MET
ARG	LYS	VAL	LEU	THR	TRP	LEU	SER	F435	L325	N207	G92	LYS
TYR	GLY	LEU	LEU	THR	PRO	SER	ARG	H436	L325	N207	G92	THR
THR	ASP	PHE	CYS	ALA	ALA	VAL	PHE	V437	W208	V209	R94	ILE
THR	LEU	GLN	VAL	PHE	TRP	LEU	ALA	D445	W208	V209	R94	ILE
GLY	GLN	GLY	LEU	LEU	LEU	LEU	ALA	D445	L331	L212	G96	ALA
GLY	PHE	PRO	GLY	CYS	VAL	PHE	TRP	M452	L331	L212	G96	LEU
SER	SER	SER	ILE	PHE	VAL	PRO	GLY	M452	F334	D215	D98	SER
HIS	PRO	GLY	LEU	GLY	LEU	GLN	PRO	D455	F334	D215	L99	TYR
ILE	TRP	GLY	ALA	GLY	LEU	GLN	PRO	D455	L342	D216	F100	ILE
LYS	ILE	VAL	ALA	THR	ALA	PRO	ALA	L456	E217	L456	PHE	PHI
GLY	LEU	SER	PHE	PHE	MET	SER	VAL	K457	A343	Y218	CYS	CYS
GLU	VAL	LYS	HIS	LEU	LEU	PRO	LEU	L344	A343	Y218	V107	LEU
ALA	PRO	GLY	LEU	VAL	VAL	ALA	LEU	D470	A345	Q221	V108	VAL
GLN	HIS	GLU	PRO	ARG	GLU	ARG	LEU	V471	T346	G222	K111	PHI
VAL	ILE	GLU	ARG	SER	VAL	CYS	LEU	C472	D347	L223	P112	ALA
LYS	GLY	ASP	CYS	GLN	ALA	LEU	LEU	S224	S224	G222	GLY	GLY
THR	TYR	ASN	TYR	PRO	LEU	ALA	LEU	F350	F350	L225	M115	SER
GLY	GLY	MET	LEU	GLY	CYS	GLN	LEU	H487	F350	L225	M115	ASP
THR	PHE	ALA	LEU	CYS	THR	GLN	SER	H488	E356	A230	S122	TYR
GLY	PHE	ALA	LEU	CYS	THR	GLN	SER	T489	E356	A230	S122	LYS
PHI	HIS	SER	MET	TYR	TRP	PRO	LEU	S490	ARG	I235	R123	ASP
PRO	PRO	GLN	LEU	ASN	TRP	LEU	ALA	D491	GLU	I235	R123	ASP
ALA	TYR	PRO	GLN	ARG	LEU	SER	ALA	D491	GLN	I235	R123	ASP
ASP	LEU	ALA	PRO	ALA	VAL	HIS	GLY	E505	GLY	L242	A126	ASP
GLY	PRO	THR	GLY	ARG	ALA	LEU	LEU	G506	LEU	L242	A126	ASP
PRO	TYR	HIS	LEU	GLY	PHE	PRO	VAL	Q507	GLU	L245	Y131	LYS
VAL	PRO	GLU	ASN	GLY	LEU	LEU	VAL	Q507	GLU	L245	Y131	LYS
THR	ASP	LEU	THR	THR	PRO	LEU	ALA	V508	ASP	P246	Y131	GLY
MET	ASP	GLY	PRO	PHE	THR	GLY	ALA	R509	VAL	R247	Y134	SER
ASN	MET	ILE	GLU	ALA	GLY	GLY	ALA	R509	VAL	R247	Y134	SER
ASN	MET	ILE	GLU	ALA	VAL	CYS	ALA	C518	ASP	A248	L139	ALA
SER	SER	PHE	PHE	MET	VAL	LEU	GLY	Y519	V366	A248	L139	ALA
LEU	PRO	GLY	PHE	LEU	THR	SER	LEU	Y519	V366	A248	L139	ALA
THR	PHI	SER	LEU	ALA	ASP	THR	PHE	E525	R369	D250	E148	P22
ALA	GLN	ILE	GLY	TYR	TRP	LEU	VAL	E525	R369	D250	E148	P22
ALA	ALA	ASN	GLY	PHE	HIS	PHE	VAL	S528	C370	D250	E148	P22
ASP	ALA	GLY	GLY	ILE	LEU	PHI	HIS	Y529	C371	R252	L349	Y35
TRP	MET	VAL	PRO	GLY	MET	LEU	HIS	Y529	Q372	R252	L349	Y35
CYS	VAL	GLY	GLY	THR	LEU	GLN	ARG	R530	C373	L253	M151	E48
ARG	ASP	ASP	GLY	TRP	PRO	ALA	ASP	R530	C373	L253	M151	E48
SER	GLY	PHE	ASP	VAL	THR	ALA	SER	D534	T377	V256	L161	L51
LYS	SER	ASP	ALA	SER	GLU	ALA	PRO	D535	L378	L260	V165	R52
LYS	SER	MET	GLN	PHE	ALA	ILE	LEU	I536	L378	L260		

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

ASP GLU LEU TYR LYS GLY SER GLU ASN LEU TYR PHE GLN SER SER GLY HIS HIS HIS HIS HIS HIS HIS

● Molecule 3: 4-chloro-4-deoxy- α -D-galactopyranose-(1-2)-1,6-dichloro-1,6-dideoxy- β -D-fructofuranose



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	84470	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.231	Depositor
Minimum map value	-0.002	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.03	Depositor
Map size (\AA)	372.736, 372.736, 372.736	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.456, 1.456, 1.456	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: RRJ, RRY

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	0.21	0/4137	0.38	0/5637
2	B	0.20	0/4183	0.36	0/5676
All	All	0.21	0/8320	0.37	0/11313

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

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	4036	0	3903	124	0
2	B	4084	0	3969	107	0
3	C	23	0	0	1	0
All	All	8143	0	7872	228	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 14.

All (228) 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:A:439:ASP:OD1	1:A:440:PRO:CD	1.71	1.36
1:A:402:LEU:HD13	1:A:423:GLU:CG	1.73	1.18
1:A:249:MET:SD	1:A:283:HIS:HD2	1.69	1.14
2:B:509:ARG:HD2	2:B:519:TYR:CE2	1.83	1.12
2:B:509:ARG:HD2	2:B:519:TYR:CZ	1.89	1.07
1:A:402:LEU:CD1	1:A:423:GLU:HG3	1.91	0.99
1:A:439:ASP:OD1	1:A:440:PRO:HD2	0.80	0.97
2:B:509:ARG:CD	2:B:519:TYR:CZ	2.47	0.96
1:A:249:MET:SD	1:A:283:HIS:CD2	2.59	0.94
1:A:402:LEU:HD13	1:A:423:GLU:HG3	0.95	0.93
1:A:302:GLU:OE2	3:C:2:RRJ:O2	1.94	0.86
1:A:439:ASP:CG	1:A:440:PRO:HD2	1.99	0.82
2:B:509:ARG:HD3	2:B:519:TYR:CZ	2.21	0.75
2:B:507:GLN:O	2:B:530:ARG:NH1	2.19	0.75
2:B:54:ARG:NH2	2:B:58:SER:O	2.21	0.74
1:A:172:ARG:O	1:A:441:GLN:OE1	2.07	0.73
2:B:181:PRO:O	2:B:431:TYR:OH	2.04	0.73
1:A:521:LEU:O	1:A:524:THR:OG1	2.05	0.70
2:B:509:ARG:CD	2:B:519:TYR:CE2	2.70	0.70
1:A:248:ASN:OD1	1:A:248:ASN:O	2.10	0.69
1:A:274:VAL:HG11	1:A:281:LEU:HD11	1.75	0.69
2:B:331:LEU:O	2:B:331:LEU:HD23	1.94	0.68
1:A:211:SER:OG	1:A:213:ASP:OD1	2.12	0.68
1:A:321:THR:HG21	1:A:483:TRP:CE3	2.29	0.67
1:A:289:LEU:HB2	1:A:319:LEU:HD11	1.76	0.66
2:B:347:ASP:OD1	2:B:350:PHE:N	2.28	0.66
1:A:321:THR:HG21	1:A:483:TRP:CZ3	2.32	0.65
1:A:287:GLU:OE2	1:A:287:GLU:N	2.30	0.64
2:B:491:ASP:OD1	2:B:491:ASP:O	2.16	0.64
2:B:122:SER:OG	2:B:124:ASP:OD1	2.10	0.64
2:B:529:TYR:N	2:B:539:THR:O	2.31	0.63
1:A:136:VAL:HG22	1:A:420:LEU:HD12	1.80	0.62
1:A:188:ASP:OD1	1:A:189:HIS:N	2.33	0.62
1:A:402:LEU:CD1	1:A:423:GLU:CG	2.66	0.61
1:A:194:MET:O	1:A:198:MET:HG3	2.01	0.61
1:A:76:ARG:HA	1:A:76:ARG:CZ	2.31	0.61
2:B:419:ASP:OD1	2:B:419:ASP:N	2.33	0.61
2:B:317:GLN:OE1	2:B:317:GLN:N	2.34	0.60
1:A:76:ARG:HA	1:A:76:ARG:NH1	2.17	0.59
2:B:126:ALA:O	2:B:134:TYR:OH	2.20	0.59
2:B:370:CYS:SG	2:B:373:CYS:N	2.72	0.59
2:B:426:LEU:O	2:B:430:MET:N	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:THR:HA	1:A:444:VAL:HG22	1.85	0.59
2:B:457:LYS:HE2	2:B:457:LYS:HA	1.85	0.58
1:A:29:LEU:HB2	1:A:96:TYR:CE1	2.39	0.58
1:A:300:ALA:N	1:A:323:LEU:O	2.33	0.58
1:A:376:ILE:HD11	1:A:457:ARG:NH1	2.19	0.57
2:B:509:ARG:HD2	2:B:519:TYR:CD2	2.37	0.57
2:B:223:LEU:HD12	2:B:242:LEU:CD2	2.34	0.57
1:A:326:THR:O	1:A:449:GLU:N	2.33	0.57
1:A:281:LEU:HD12	1:A:285:PHE:CE2	2.40	0.57
1:A:151:ALA:HB2	1:A:180:LEU:HD13	1.86	0.56
1:A:252:GLU:OE2	1:A:252:GLU:N	2.27	0.56
1:A:363:CYS:SG	1:A:364:ASP:N	2.79	0.56
2:B:245:LEU:HD23	2:B:245:LEU:H	1.69	0.56
2:B:215:ASP:HA	2:B:242:LEU:HD13	1.88	0.55
2:B:172:GLU:HB3	2:B:225:ILE:HD11	1.87	0.55
2:B:199:GLU:O	2:B:203:GLU:HG2	2.06	0.55
1:A:81:GLU:OE2	1:A:389:TYR:OH	2.23	0.55
1:A:123:PRO:HB2	1:A:125:GLN:HE22	1.72	0.55
1:A:183:THR:HG21	1:A:391:ALA:HB2	1.88	0.54
2:B:456:LEU:N	2:B:472:GLY:O	2.39	0.54
1:A:376:ILE:HD11	1:A:457:ARG:CZ	2.37	0.54
2:B:505:GLU:OE2	2:B:530:ARG:NH2	2.41	0.54
1:A:71:LEU:HD21	1:A:384:VAL:HG23	1.88	0.54
1:A:360:ASN:O	1:A:360:ASN:ND2	2.41	0.54
1:A:384:VAL:O	1:A:387:SER:OG	2.24	0.54
2:B:148:GLU:HA	2:B:148:GLU:OE1	2.08	0.53
2:B:217:GLU:OE1	2:B:218:TYR:N	2.41	0.53
1:A:433:ASP:O	1:A:434:HIS:ND1	2.40	0.53
1:A:41:LEU:HD21	1:A:72:MET:HE1	1.91	0.53
2:B:518:CYS:SG	2:B:519:TYR:N	2.80	0.53
1:A:82:ILE:HG12	1:A:88:LEU:HD23	1.91	0.53
1:A:278:ASP:OD1	1:A:279:LEU:N	2.42	0.53
1:A:465:VAL:HG11	1:A:481:ILE:HD12	1.89	0.52
2:B:404:LEU:HA	2:B:407:THR:HG22	1.90	0.52
1:A:138:VAL:H	1:A:159:LEU:HD21	1.74	0.52
2:B:327:ARG:NH2	2:B:455:ASP:OD2	2.42	0.52
1:A:139:ILE:HD13	1:A:392:VAL:HG22	1.91	0.52
2:B:151:MET:HE1	2:B:173:LEU:HB3	1.90	0.52
2:B:534:ASP:OD1	2:B:534:ASP:N	2.43	0.52
1:A:205:TRP:O	1:A:493:SER:OG	2.28	0.52
1:A:452:GLN:OE1	1:A:453:TRP:N	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:TYR:HE2	2:B:93:LEU:HD21	1.75	0.52
2:B:161:LEU:HB3	2:B:427:LEU:HD22	1.92	0.51
1:A:316:LEU:HA	1:A:319:LEU:HD13	1.92	0.51
2:B:83:ILE:CD1	2:B:95:LEU:HD12	2.40	0.51
1:A:79:VAL:HA	1:A:82:ILE:HD12	1.93	0.51
2:B:320:THR:HG21	2:B:487:TRP:CE3	2.46	0.51
1:A:141:PRO:HB2	1:A:147:VAL:HG22	1.93	0.51
2:B:546:TRP:N	2:B:555:PHE:O	2.42	0.51
2:B:445:ASP:C	2:B:445:ASP:OD1	2.55	0.50
1:A:257:LEU:HD22	1:A:287:GLU:OE1	2.11	0.50
1:A:439:ASP:OD1	1:A:440:PRO:N	2.41	0.50
1:A:147:VAL:HG21	1:A:166:ALA:HB2	1.94	0.50
1:A:321:THR:O	1:A:321:THR:HG23	2.11	0.50
2:B:223:LEU:HD12	2:B:242:LEU:HD21	1.92	0.50
1:A:27:PHE:CD2	1:A:361:GLN:O	2.65	0.49
2:B:509:ARG:HD3	2:B:519:TYR:OH	2.12	0.49
1:A:242:THR:O	1:A:243:LEU:HD22	2.12	0.49
1:A:376:ILE:HD11	1:A:457:ARG:NH2	2.28	0.49
1:A:421:LEU:HA	1:A:424:ILE:HG22	1.93	0.49
2:B:509:ARG:CD	2:B:519:TYR:CE1	2.95	0.49
1:A:361:GLN:O	1:A:362:GLU:HG2	2.13	0.48
1:A:531:ASP:C	1:A:531:ASP:OD1	2.56	0.48
2:B:209:VAL:HG23	2:B:270:VAL:HG23	1.96	0.48
1:A:282:TYR:HE1	1:A:313:LEU:HD13	1.79	0.48
2:B:287:SER:CB	2:B:318:MET:HE1	2.44	0.48
2:B:124:ASP:OD1	2:B:124:ASP:N	2.37	0.48
2:B:172:GLU:OE1	2:B:172:GLU:HA	2.13	0.48
1:A:119:ASP:N	1:A:119:ASP:OD1	2.40	0.48
1:A:162:ILE:HD13	1:A:395:VAL:CG2	2.44	0.48
2:B:139:LEU:HD13	2:B:426:LEU:HD11	1.96	0.48
2:B:488:HIS:CD2	2:B:489:THR:HG23	2.49	0.48
2:B:344:LEU:HD11	2:B:350:PHE:CD1	2.49	0.47
1:A:172:ARG:HG2	1:A:443:ASP:OD2	2.13	0.47
1:A:361:GLN:O	1:A:361:GLN:HG3	2.14	0.47
1:A:527:ASN:ND2	1:A:530:GLU:OE1	2.48	0.47
2:B:150:ALA:HB1	2:B:183:PHE:CZ	2.49	0.47
1:A:159:LEU:C	1:A:159:LEU:HD23	2.39	0.47
2:B:505:GLU:O	2:B:530:ARG:NH2	2.44	0.47
2:B:212:LEU:HB3	2:B:273:LEU:HD12	1.96	0.47
2:B:256:VAL:O	2:B:260:LEU:HD22	2.13	0.47
2:B:196:ALA:HB1	2:B:324:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:THR:O	2:B:305:THR:OG1	2.26	0.47
1:A:294:THR:OG1	1:A:295:GLY:N	2.48	0.46
2:B:249:ASP:O	2:B:252:ARG:N	2.44	0.46
1:A:27:PHE:CE1	1:A:72:MET:SD	3.09	0.46
1:A:70:ASN:ND2	1:A:377:LEU:HD22	2.32	0.45
1:A:124:ILE:HB	2:B:115:MET:HE3	1.98	0.45
2:B:435:PHE:HD2	2:B:437:VAL:HG23	1.82	0.45
1:A:215:TYR:O	1:A:219:ASN:ND2	2.49	0.45
1:A:255:GLN:OE1	1:A:255:GLN:C	2.59	0.45
1:A:333:PRO:HD3	1:A:432:LEU:HD11	1.98	0.45
2:B:115:MET:HE2	2:B:115:MET:HA	1.97	0.45
2:B:167:TYR:O	2:B:187:VAL:HG21	2.17	0.45
2:B:194:LEU:HD21	2:B:274:PHE:CD1	2.52	0.45
1:A:172:ARG:NH1	1:A:443:ASP:OD2	2.49	0.45
1:A:257:LEU:O	1:A:261:VAL:HG22	2.17	0.45
2:B:434:THR:HG23	2:B:434:THR:O	2.16	0.45
2:B:111:LYS:N	2:B:112:PRO:HD2	2.32	0.45
1:A:204:ASN:OD1	1:A:204:ASN:C	2.60	0.45
1:A:221:GLN:HE22	2:B:242:LEU:HD12	1.80	0.45
1:A:464:SER:O	1:A:479:GLN:NE2	2.50	0.45
1:A:450:ILE:HB	1:A:466:ALA:HB3	1.99	0.45
2:B:230:ALA:HB1	2:B:235:ILE:O	2.17	0.45
2:B:166:SER:OG	2:B:167:TYR:N	2.49	0.44
2:B:76:MET:HE2	2:B:99:LEU:HD22	1.99	0.44
1:A:293:PHE:CZ	1:A:296:ALA:HB2	2.53	0.44
2:B:79:ALA:O	2:B:83:ILE:HG12	2.17	0.44
2:B:171:MET:HE3	2:B:221:GLN:HG3	1.98	0.44
1:A:261:VAL:HG12	1:A:288:VAL:HG22	1.98	0.44
1:A:531:ASP:OD1	1:A:531:ASP:O	2.36	0.44
1:A:109:GLN:C	1:A:109:GLN:CD	2.86	0.44
1:A:96:TYR:HD2	1:A:98:ILE:HG12	1.82	0.44
1:A:174:LYS:HD2	1:A:174:LYS:N	2.32	0.44
1:A:281:LEU:O	1:A:282:TYR:C	2.61	0.44
1:A:524:THR:HA	1:A:537:ALA:HA	2.00	0.44
2:B:535:ASP:OD1	2:B:535:ASP:N	2.51	0.44
1:A:76:ARG:CZ	1:A:96:TYR:CE1	3.01	0.44
2:B:97:TYR:CD1	2:B:97:TYR:N	2.84	0.44
1:A:88:LEU:O	1:A:400:HIS:CD2	2.71	0.43
1:A:169:ASP:OD1	1:A:172:ARG:HD3	2.19	0.43
2:B:342:LEU:O	2:B:346:THR:HG23	2.18	0.43
1:A:520:CYS:SG	1:A:524:THR:OG1	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:HD2	1:A:361:GLN:O	2.02	0.43
1:A:477:ASN:OD1	1:A:477:ASN:O	2.36	0.43
1:A:91:GLY:O	1:A:92:VAL:C	2.61	0.43
1:A:281:LEU:HD12	1:A:285:PHE:CD2	2.54	0.43
2:B:223:LEU:HD12	2:B:242:LEU:HD23	2.00	0.43
2:B:470:ASP:OD1	2:B:470:ASP:C	2.62	0.43
2:B:165:VAL:HG23	2:B:184:PHE:O	2.18	0.43
2:B:400:VAL:HG22	2:B:430:MET:HE1	2.00	0.43
2:B:545:GLU:HA	2:B:556:ARG:HA	2.00	0.43
2:B:299:ALA:HB3	2:B:304:LEU:HD13	2.01	0.43
1:A:28:TYR:CD1	1:A:29:LEU:N	2.87	0.43
2:B:80:VAL:O	2:B:83:ILE:HG13	2.19	0.43
2:B:151:MET:HE2	2:B:171:MET:HE2	2.00	0.42
2:B:326:GLN:NE2	2:B:452:MET:SD	2.87	0.42
2:B:528:SER:HA	2:B:540:PHE:HA	2.01	0.42
2:B:70:LEU:O	2:B:74:LEU:HG	2.19	0.42
2:B:307:ASP:O	2:B:307:ASP:OD1	2.37	0.42
2:B:59:SER:HG	2:B:107:VAL:C	2.27	0.42
1:A:127:ASP:OD1	1:A:127:ASP:C	2.63	0.42
1:A:159:LEU:HA	1:A:417:PRO:HB2	2.01	0.42
2:B:76:MET:HE2	2:B:99:LEU:CD2	2.49	0.42
2:B:274:PHE:HA	2:B:300:SER:OG	2.19	0.42
1:A:498:ARG:NH1	1:A:499:CYS:O	2.53	0.42
2:B:65:PHE:CZ	2:B:67:SER:HA	2.55	0.42
2:B:249:ASP:HA	2:B:252:ARG:HB2	2.02	0.42
2:B:83:ILE:HD12	2:B:95:LEU:HD12	2.01	0.42
2:B:131:TYR:CD1	2:B:131:TYR:C	2.97	0.42
1:A:147:VAL:HG13	1:A:180:LEU:HD11	2.02	0.42
1:A:109:GLN:N	1:A:110:PRO:CD	2.83	0.41
1:A:173:ASP:OD1	1:A:175:VAL:HG12	2.20	0.41
2:B:549:GLU:O	2:B:550:ARG:HG2	2.20	0.41
1:A:138:VAL:HG21	1:A:154:LEU:HD11	2.03	0.41
1:A:194:MET:HE2	1:A:325:ILE:CD1	2.50	0.41
1:A:510:ILE:HD13	2:B:265:GLN:NE2	2.35	0.41
1:A:463:GLN:OE1	1:A:464:SER:N	2.53	0.41
1:A:276:SER:HB2	1:A:281:LEU:CD2	2.50	0.41
1:A:402:LEU:HD21	1:A:419:GLN:HB3	2.03	0.41
2:B:91:PRO:HG3	2:B:411:ASN:O	2.21	0.41
2:B:331:LEU:HD23	2:B:334:PHE:HB2	2.02	0.41
2:B:207:ASN:OD1	2:B:207:ASN:N	2.53	0.41
1:A:33:TYR:O	1:A:94:LEU:HA	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:N	1:A:364:ASP:OD1	2.45	0.41
1:A:504:LYS:N	1:A:518:ILE:O	2.52	0.41
2:B:93:LEU:HD12	2:B:93:LEU:HA	1.99	0.41
2:B:108:VAL:HG22	2:B:108:VAL:O	2.21	0.41
2:B:377:THR:OG1	2:B:378:LEU:N	2.53	0.41
1:A:82:ILE:HG13	1:A:393:TYR:CE1	2.56	0.40
2:B:487:TRP:O	2:B:488:HIS:ND1	2.54	0.40
2:B:140:ALA:HB3	2:B:400:VAL:HG11	2.02	0.40
2:B:304:LEU:HD21	2:B:457:LYS:HB2	2.02	0.40
2:B:387:HIS:O	2:B:390:THR:HG22	2.21	0.40
2:B:426:LEU:O	2:B:427:LEU:C	2.64	0.40
1:A:166:ALA:HB1	1:A:171:LEU:CD1	2.51	0.40
1:A:302:GLU:HA	1:A:325:ILE:O	2.21	0.40
1:A:308:PRO:HB3	1:A:376:ILE:HG21	2.02	0.40
1:A:58:MET:SD	1:A:58:MET:N	2.94	0.40
1:A:283:HIS:O	1:A:287:GLU:OE2	2.39	0.40
2:B:26:SER:HB3	2:B:369:ARG:HA	2.03	0.40
1:A:167:ILE:HD13	1:A:167:ILE:HA	1.93	0.40
1:A:182:ARG:HB3	1:A:443:ASP:OD1	2.21	0.40
1:A:192:GLU:CD	1:A:473:ARG:HE	2.29	0.40
1:A:225:GLU:CD	1:A:225:GLU:C	2.89	0.40
2:B:98:ASP:O	2:B:100:PHE:HD1	2.04	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	494/1078 (46%)	451 (91%)	43 (9%)	0	100	100
2	B	522/1130 (46%)	470 (90%)	52 (10%)	0	100	100
All	All	1016/2208 (46%)	921 (91%)	95 (9%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	455/955 (48%)	453 (100%)	2 (0%)	89	93
2	B	442/941 (47%)	441 (100%)	1 (0%)	92	95
All	All	897/1896 (47%)	894 (100%)	3 (0%)	90	94

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	303	SER
1	A	393	TYR
2	B	97	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	120	ASN
1	A	125	GLN
1	A	248	ASN
1	A	283	HIS
1	A	441	GLN
1	A	541	ASN
2	B	341	HIS
2	B	462	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

2 monosaccharides 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	RRY	C	1	3	10,12,12	0.72	0	8,18,18	0.64	0
3	RRJ	C	2	3	10,11,12	1.20	1 (10%)	11,15,17	1.14	1 (9%)

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	RRY	C	1	3	-	0/5/24/24	0/1/1/1
3	RRJ	C	2	3	-	0/2/19/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2	RRJ	C4-C5	2.59	1.55	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	RRJ	C1-O5-C5	2.17	115.13	112.19

There are no chirality outliers.

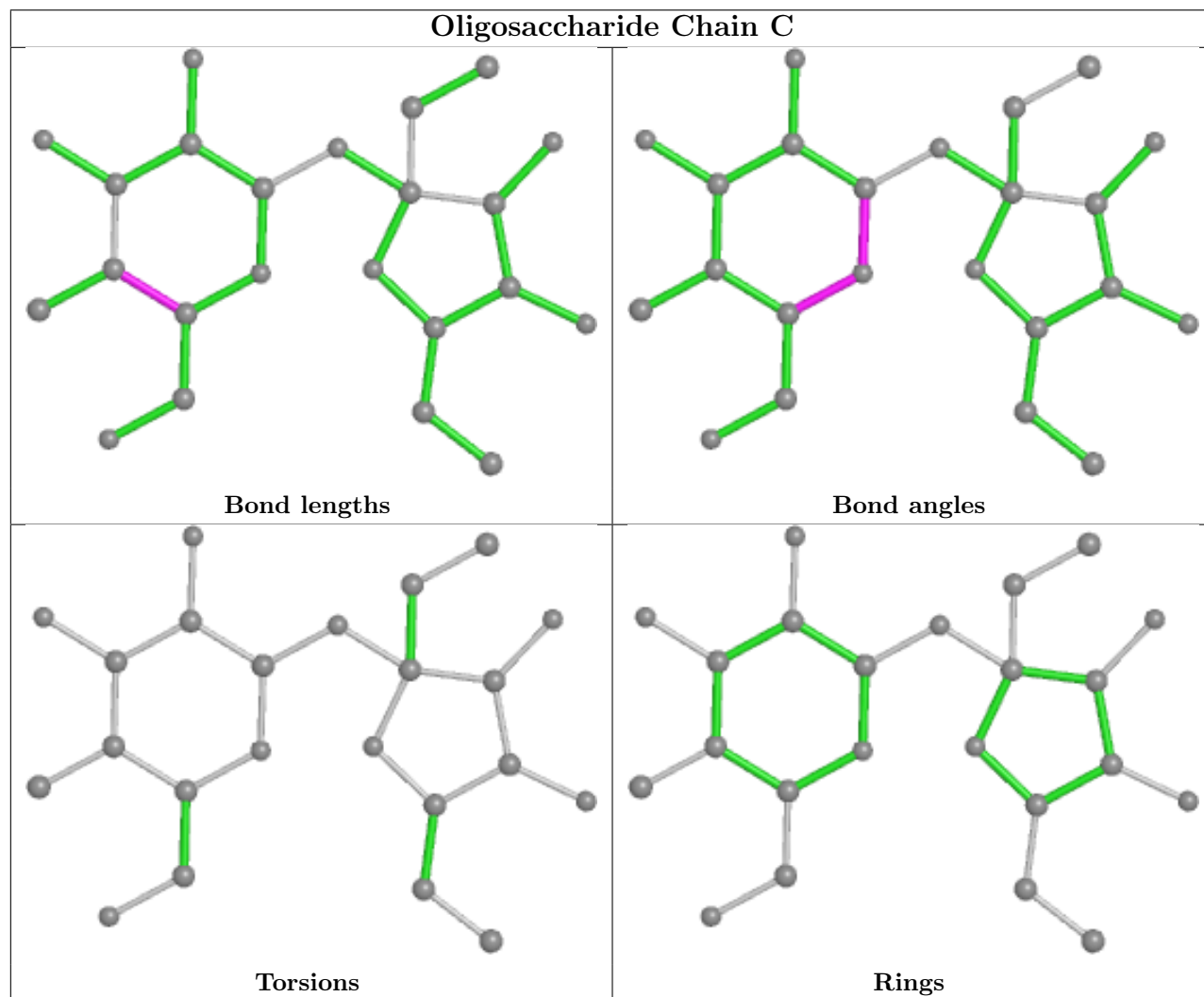
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2	RRJ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

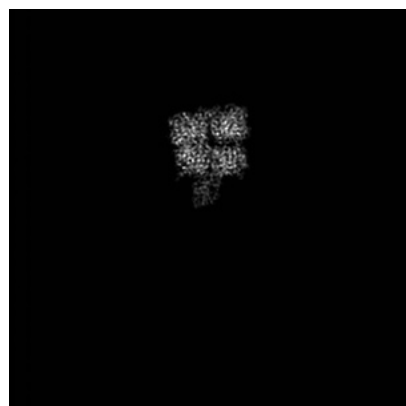
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64488. These allow visual inspection of the internal detail of the map and identification of artifacts.

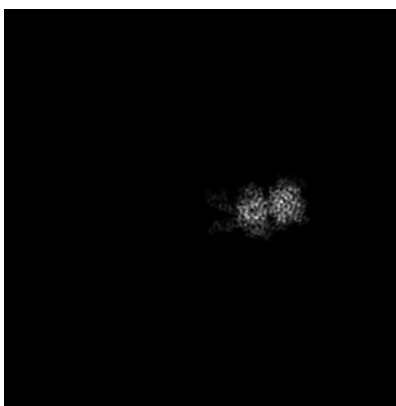
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

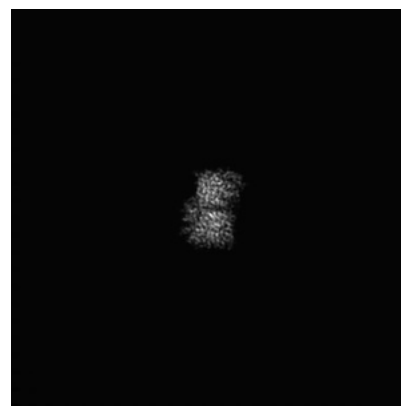
6.1.1 Primary map



X

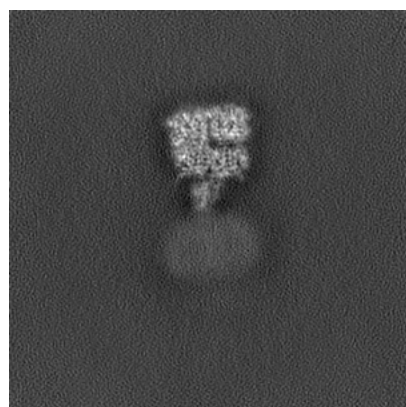


Y

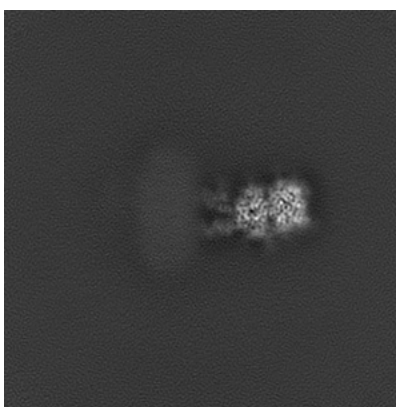


Z

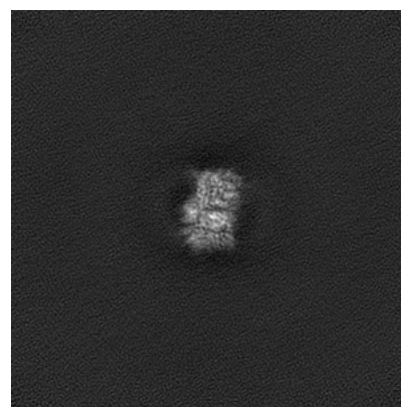
6.1.2 Raw map



X



Y

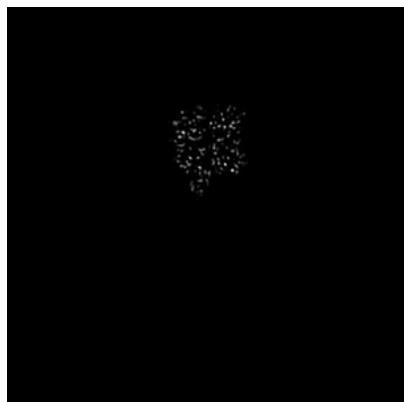


Z

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

6.2 Central slices [i](#)

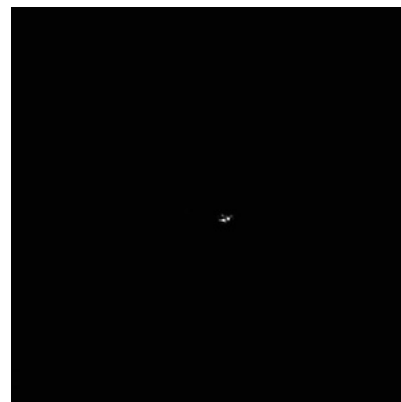
6.2.1 Primary map



X Index: 128

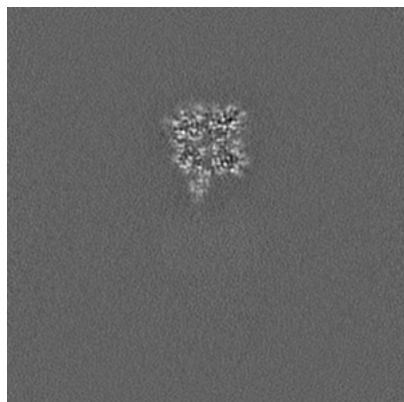


Y Index: 128

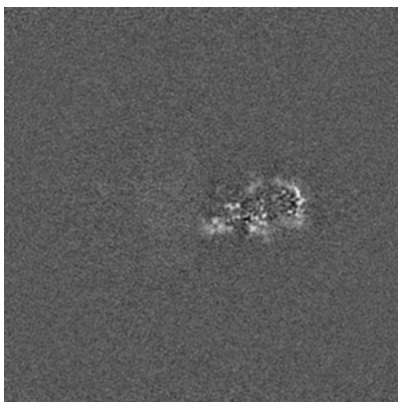


Z Index: 128

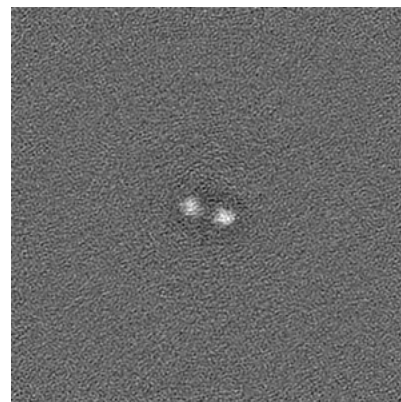
6.2.2 Raw map



X Index: 128



Y Index: 128

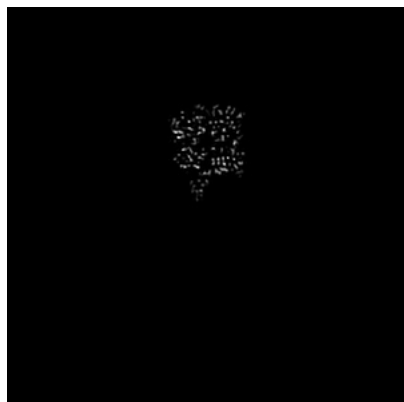


Z Index: 128

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

6.3 Largest variance slices [i](#)

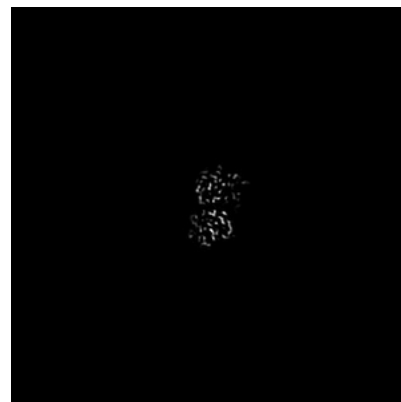
6.3.1 Primary map



X Index: 129

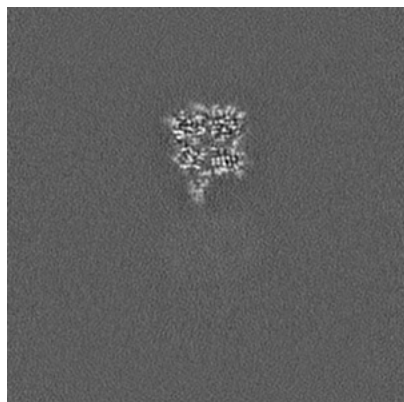


Y Index: 117

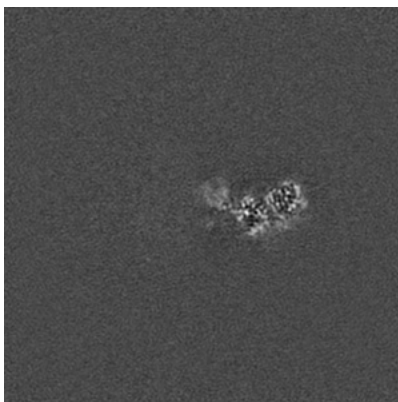


Z Index: 175

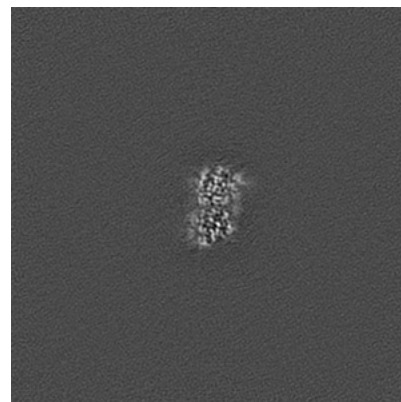
6.3.2 Raw map



X Index: 129



Y Index: 122



Z Index: 176

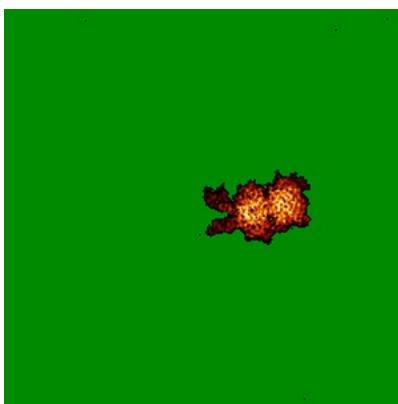
The images above show the largest variance slices of the map in three orthogonal directions.

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

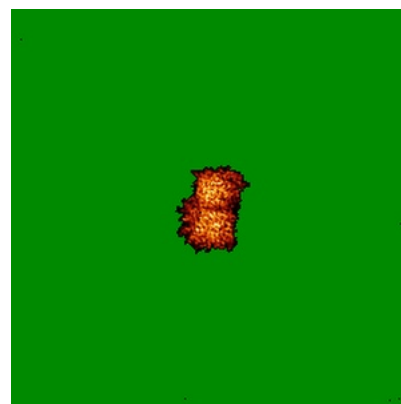
6.4.1 Primary map



X

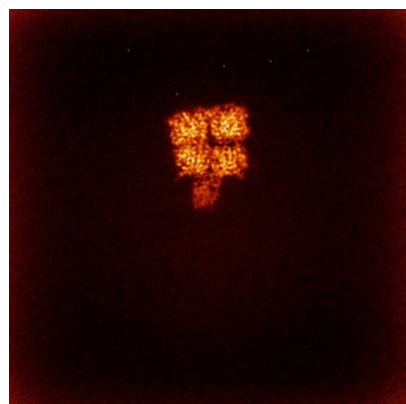


Y

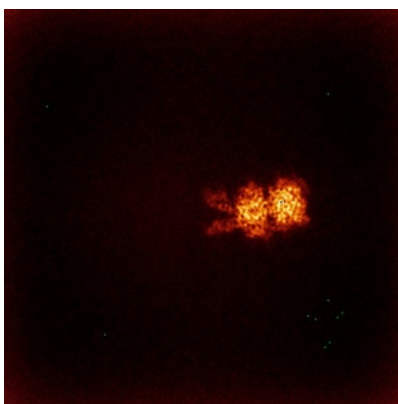


Z

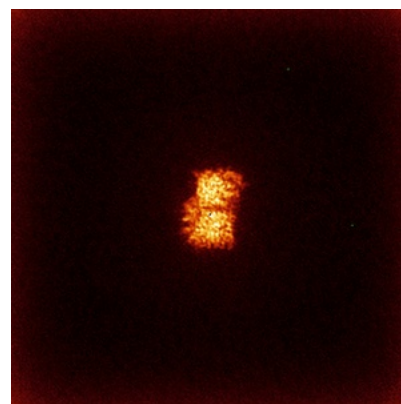
6.4.2 Raw map



X



Y

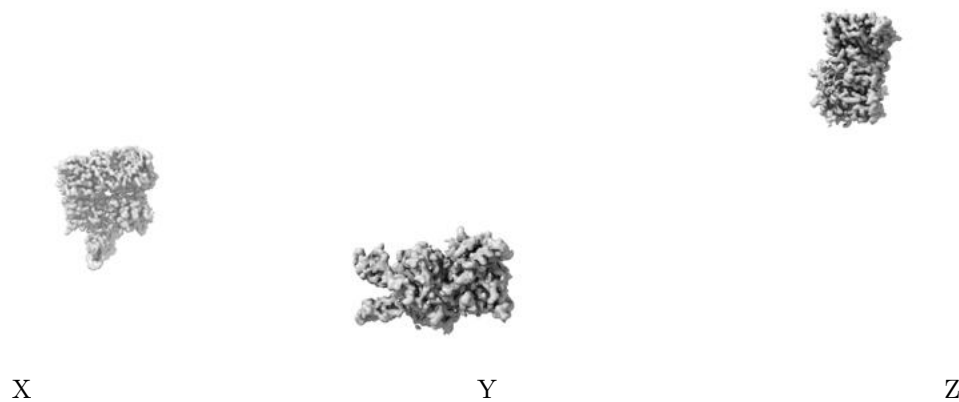


Z

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.

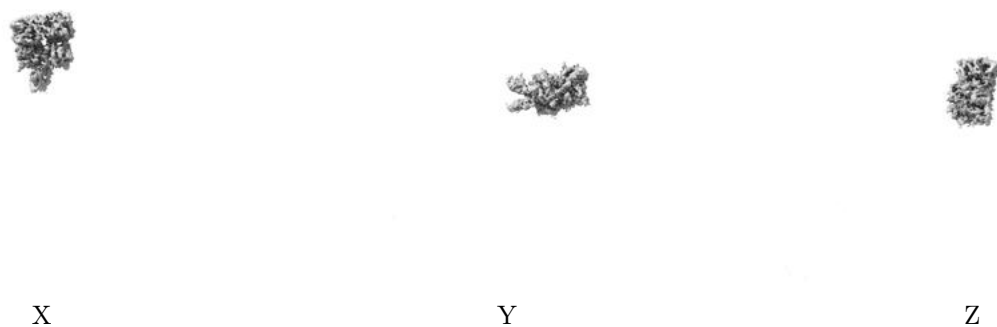
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

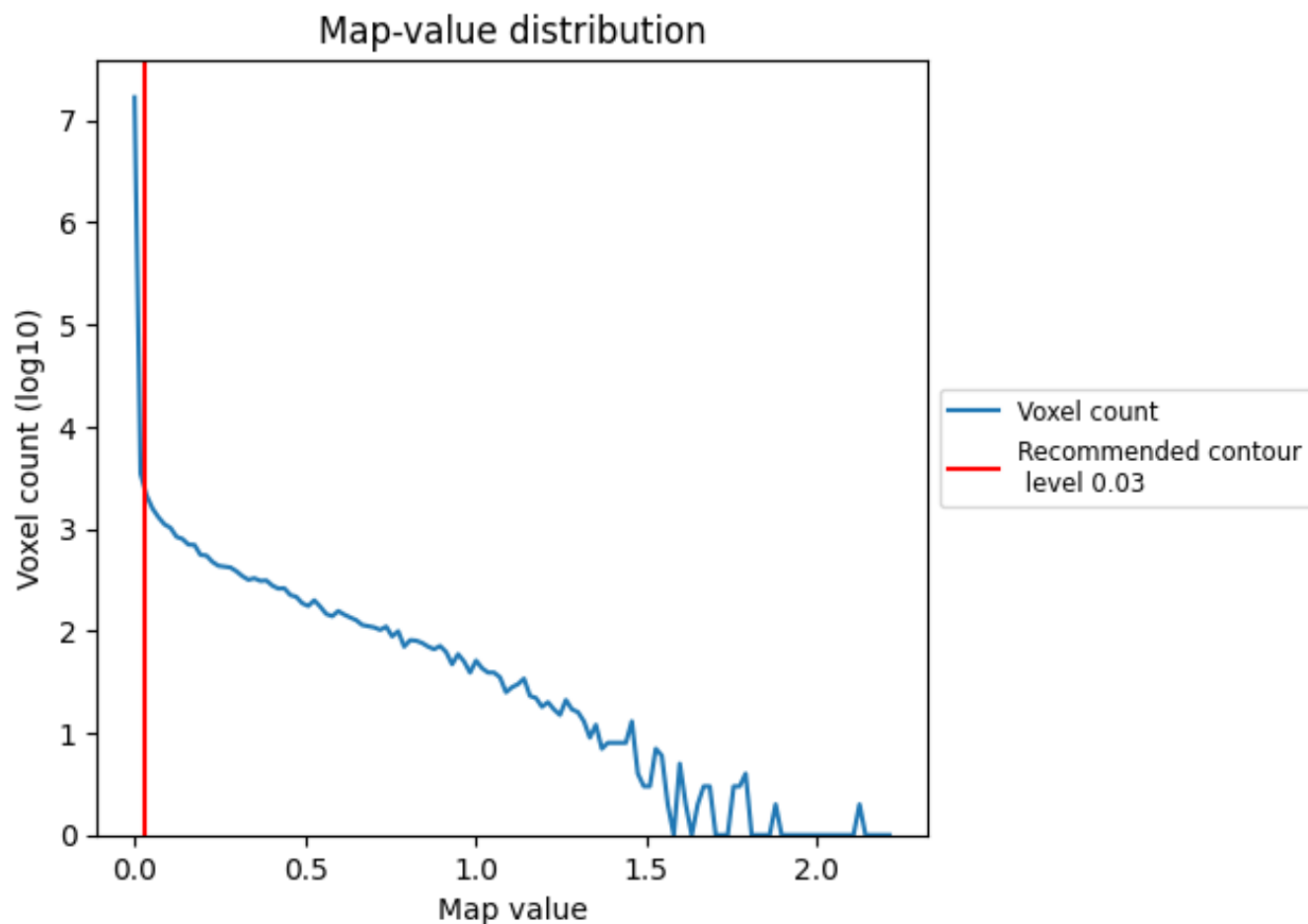
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

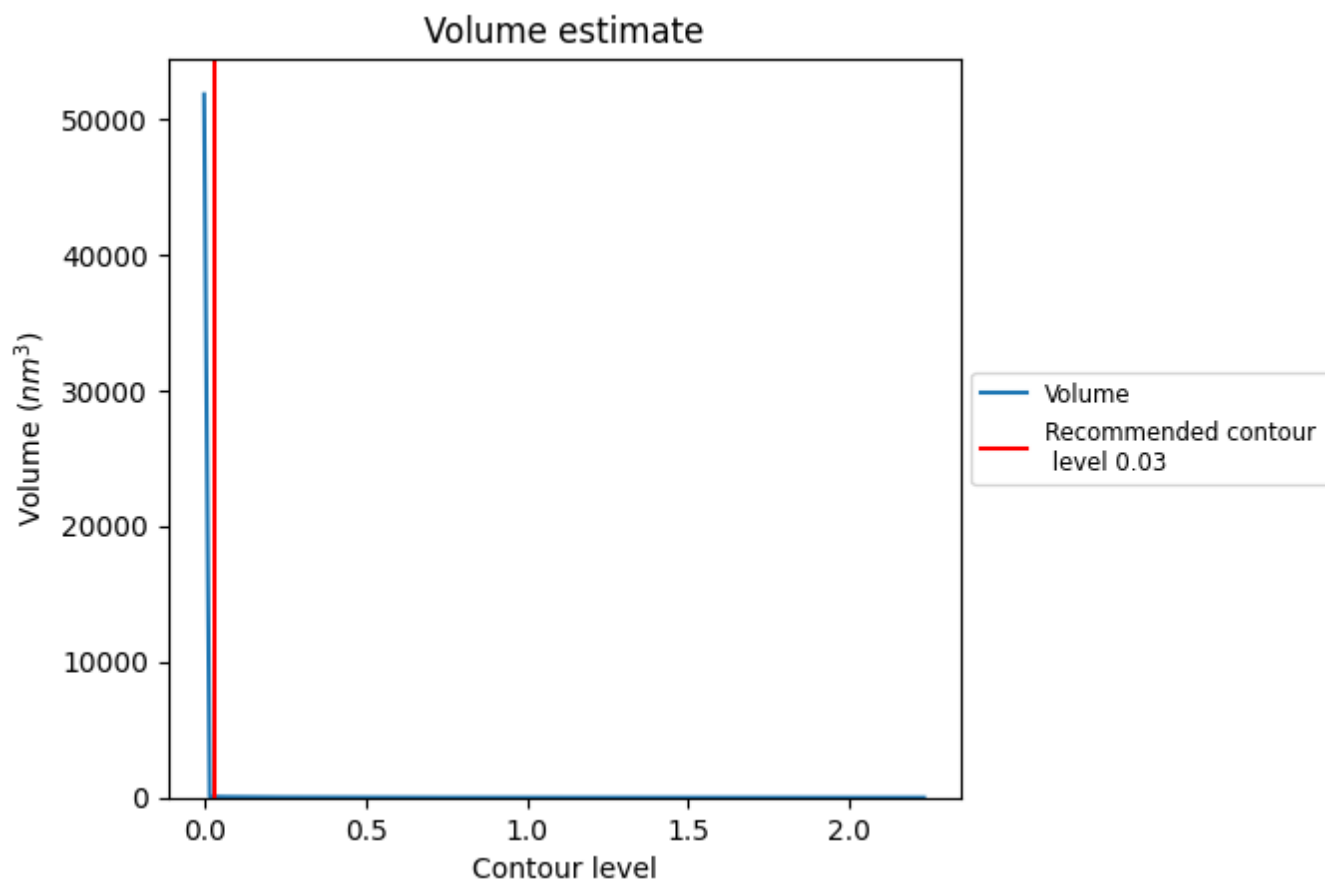
This section contains the results of statistical analysis of the map.

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.

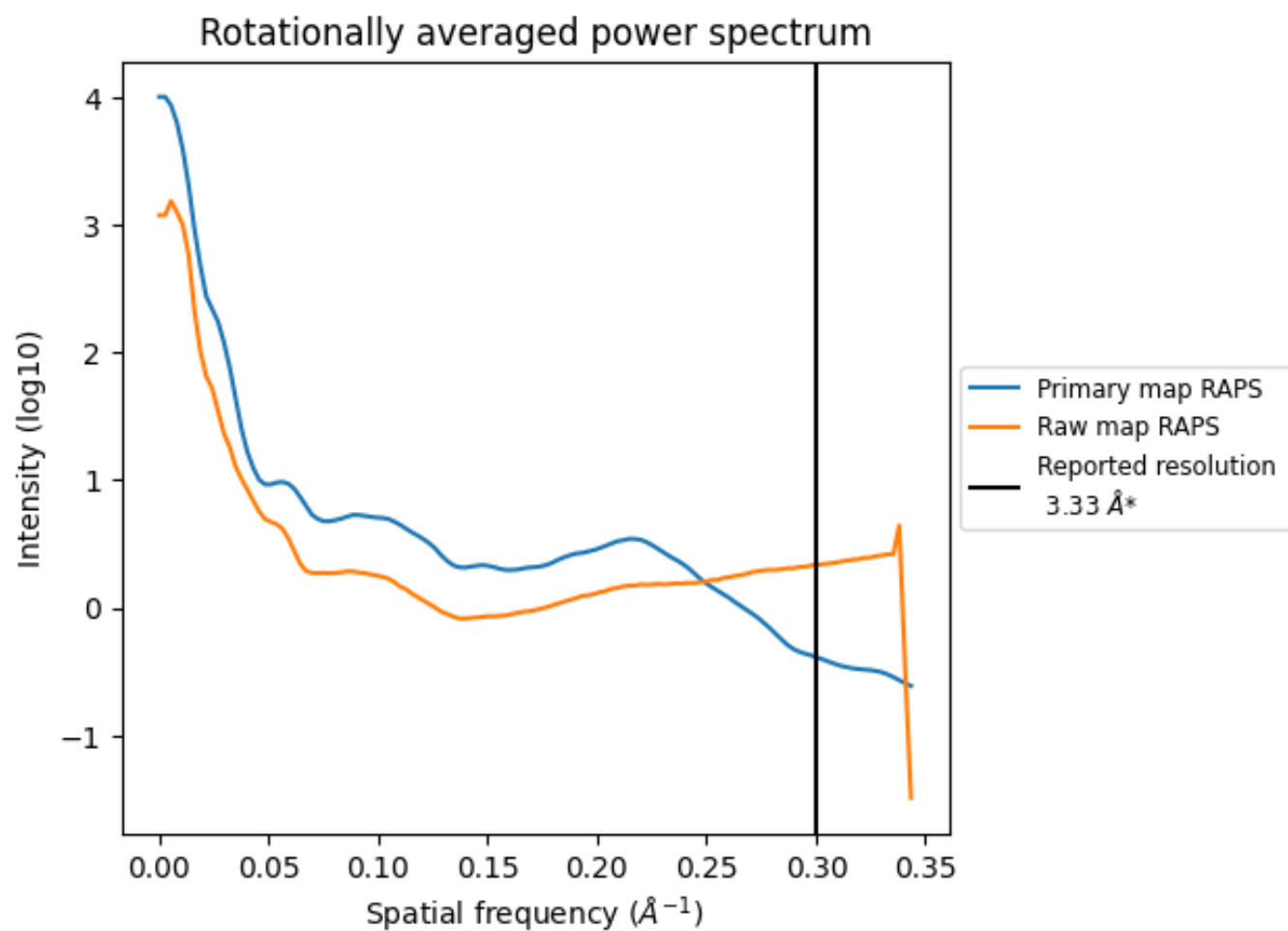
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 64 nm^3 ; this corresponds to an approximate mass of 57 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 ⓘ

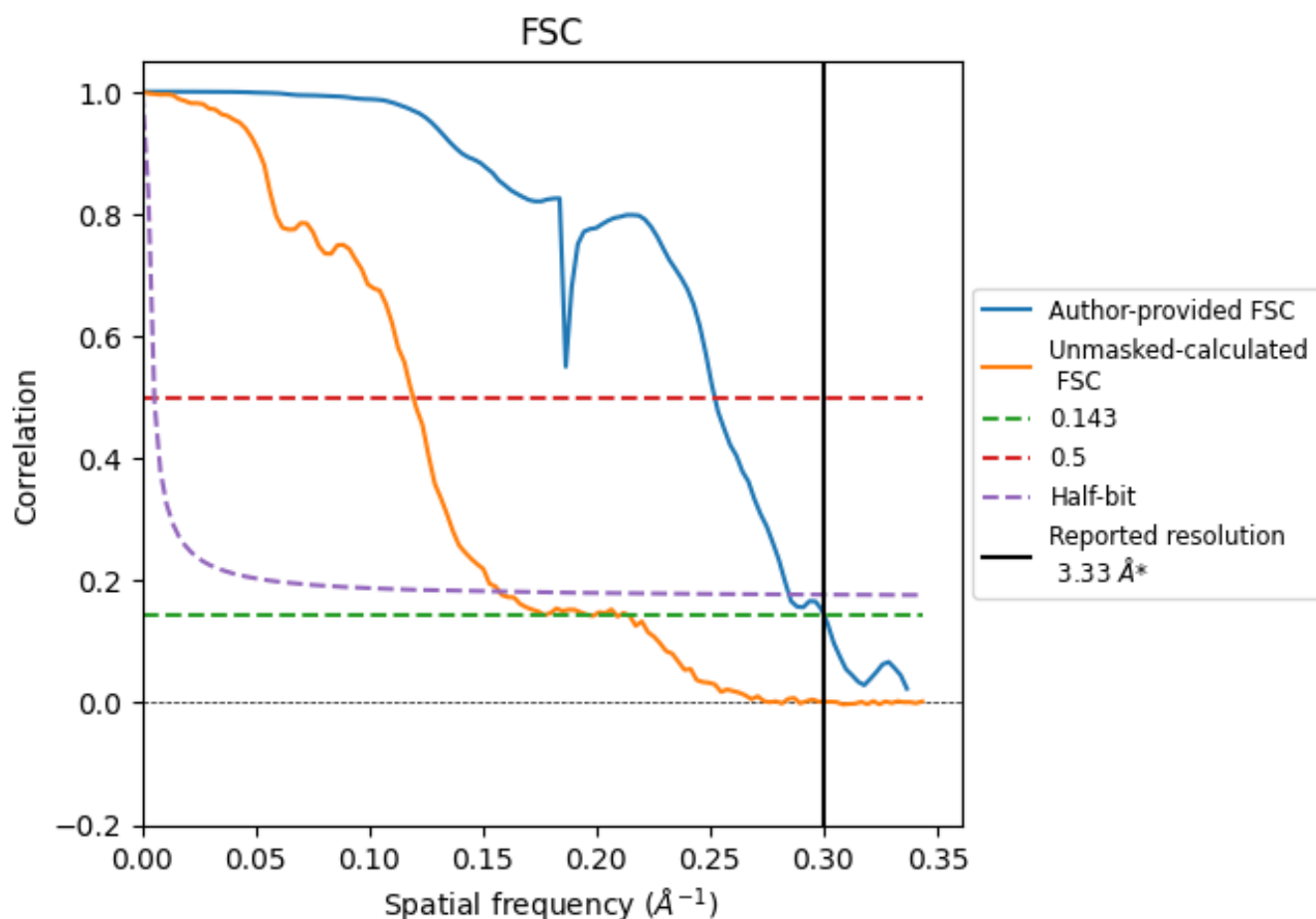


*Reported resolution corresponds to spatial frequency of 0.300 \AA^{-1}

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.300 \AA^{-1}

8.2 Resolution estimates [i](#)

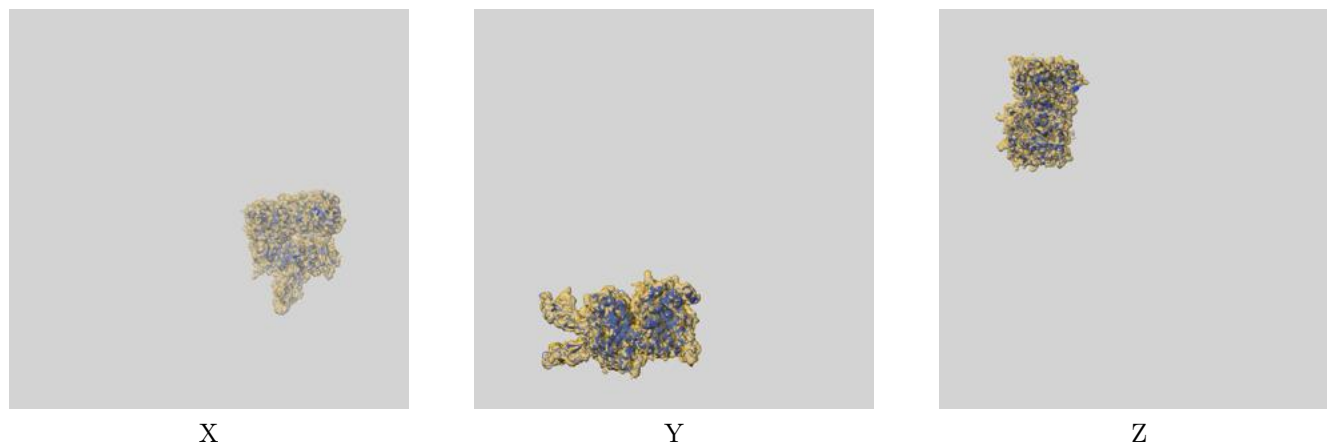
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.33	-	-
Author-provided FSC curve	3.33	3.97	3.51
Unmasked-calculated*	5.07	8.38	6.36

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.07 differs from the reported value 3.33 by more than 10 %

9 Map-model fit [i](#)

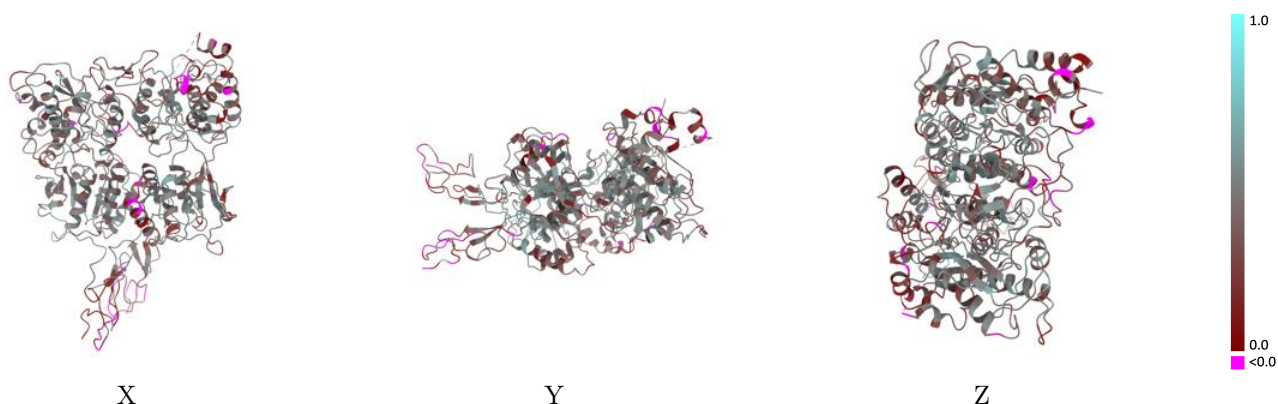
This section contains information regarding the fit between EMDB map EMD-64488 and PDB model 9UTC. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



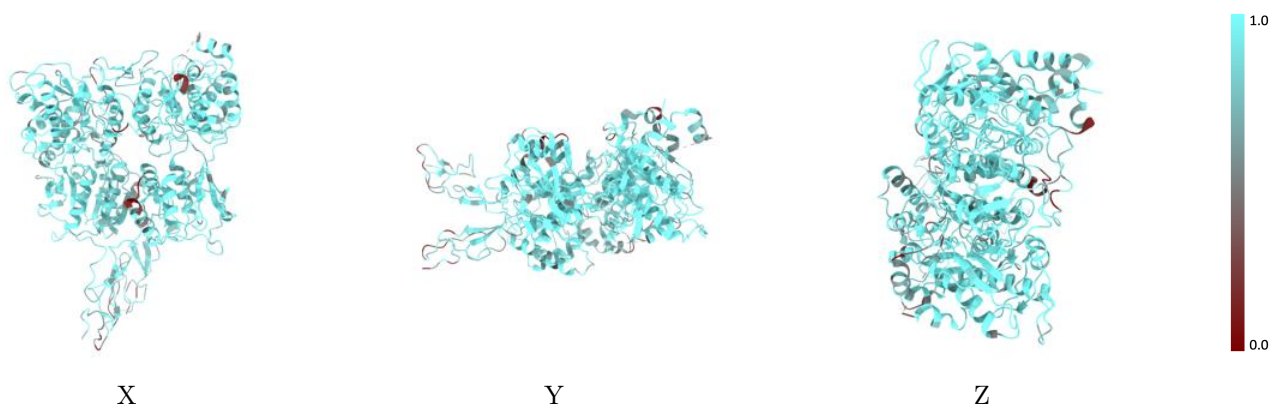
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



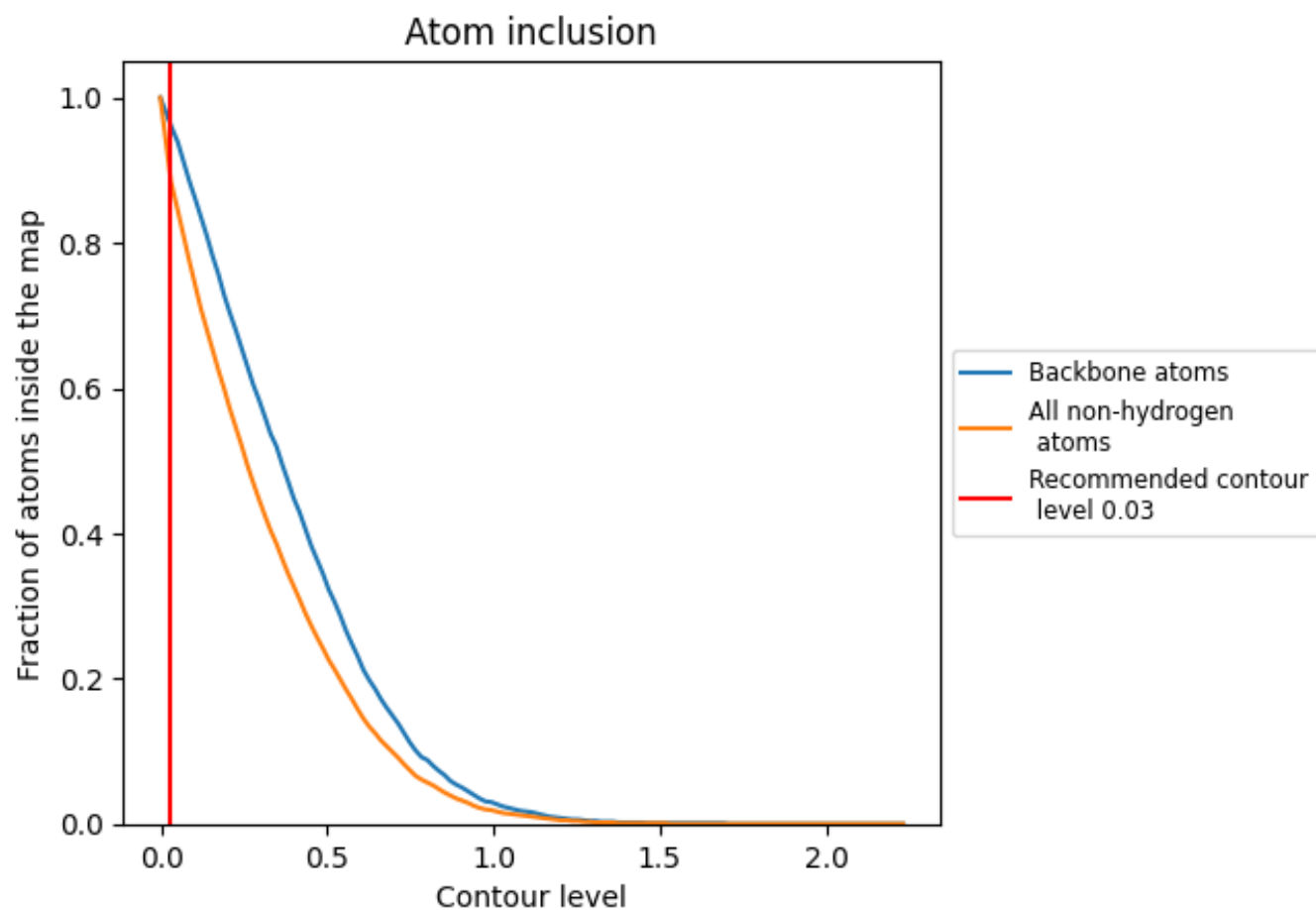
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 88% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8850	<div></div> 0.3930
A	<div></div> 0.8920	<div></div> 0.3980
B	<div></div> 0.8810	<div></div> 0.3900
C	<div></div> 0.4350	<div></div> 0.2610

