Full wwPDB EM Validation Report ⓘ

Aug 1, 2022 – 05:24 pm BST

PDB ID	:	7QVM
EMDB ID	:	EMD-14180
Title	:	Human Oxytocin receptor (OTR) oxytocin Gq chimera (mGoqi) complex
Authors	:	Waltenspuhl, Y.; Ehrenmann, J.; Vacca, S.; Thom, C.; Medalia, O.; Pluckthun, A.
Deposited on	:	2022-01-21
Resolution	:	3.25 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:

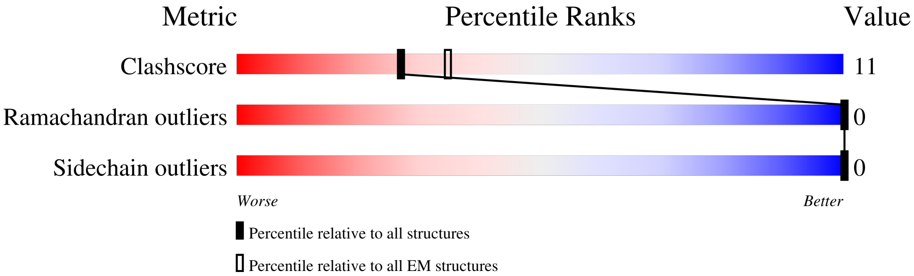
EMDB validation analysis	:	0.0.1.dev8
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 3.25 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	228	• 73% 19% 8%
2	B	354	• 71% 25% 5%
3	G	71	• 56% 23% 21%
4	L	10	10% 60% 40%
5	R	359	13% 56% 13% 30%
6	S	251	• 68% 24% 8%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8528 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 Guanine nucleotide-binding protein G(o) subunit alpha,cDNA FLJ31446 fis, clone NT2NE2000909, highly similar to Guanine nucleotide-binding protein G(o) subunit alpha 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	210	1662	1058	277	316	11	0	0

There are 25 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	ASP	GLU	engineered mutation	UNP A0A1W2PS82
A	10	LYS	ARG	engineered mutation	UNP A0A1W2PS82
A	13	VAL	LEU	engineered mutation	UNP A0A1W2PS82
A	18	MET	ALA	engineered mutation	UNP A0A1W2PS82
A	42	ASP	GLY	conflict	UNP A0A1W2PS82
A	43	ASN	GLU	conflict	UNP A0A1W2PS82
A	174	GLY	-	linker	UNP A0A1W2PS82
A	175	GLY	-	linker	UNP A0A1W2PS82
A	176	SER	-	linker	UNP A0A1W2PS82
A	177	GLY	-	linker	UNP A0A1W2PS82
A	178	GLY	-	linker	UNP A0A1W2PS82
A	179	SER	-	linker	UNP A0A1W2PS82
A	180	GLY	-	linker	UNP A0A1W2PS82
A	181	GLY	-	linker	UNP A0A1W2PS82
A	227	ASP	ALA	conflict	UNP B3KP89
A	230	ASP	GLY	conflict	UNP B3KP89
A	332	ALA	ILE	conflict	UNP P09471
A	335	ILE	VAL	conflict	UNP P09471
A	344	LEU	ILE	engineered mutation	UNP P09471
A	345	GLN	ALA	engineered mutation	UNP P09471
A	346	MET	ASN	conflict	UNP P09471
A	350	GLU	GLY	engineered mutation	UNP P09471
A	351	TYR	CYS	engineered mutation	UNP P09471
A	352	ASN	GLY	engineered mutation	UNP P09471
A	354	VAL	-	expression tag	UNP P09471

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	338	Total 2600	C 1604	N 467	O 508	S 21	0	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	initiating methionine	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	HIS	-	expression tag	UNP P62873
B	-9	HIS	-	expression tag	UNP P62873
B	-8	HIS	-	expression tag	UNP P62873
B	-7	HIS	-	expression tag	UNP P62873
B	-6	HIS	-	expression tag	UNP P62873
B	-5	HIS	-	expression tag	UNP P62873
B	-4	HIS	-	expression tag	UNP P62873
B	-3	HIS	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	56	Total 433	C 271	N 76	O 83	S 3	0	0

- Molecule 4 is a protein called Oxytocin.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	10	Total 69	C 43	N 12	O 12	S 2	0	1

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	10	NH2	-	amidation	UNP P01178

- Molecule 5 is a protein called Oxytocin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	250	Total 1994	C 1349	N 312	O 315	S 18	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	153	TYR	ASP	conflict	UNP P30559
R	218	THR	ALA	variant	UNP P30559
R	359	LYS	GLU	conflict	UNP P30559

- Molecule 6 is a protein called Antibody fragment scFv16.

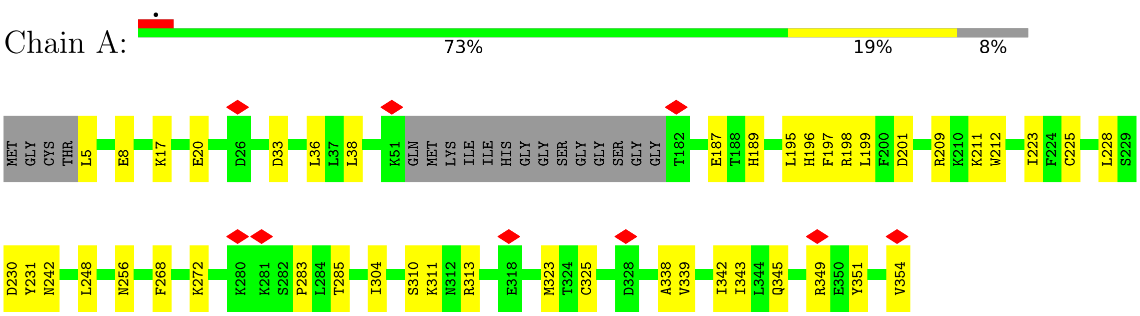
Mol	Chain	Residues	Atoms					AltConf	Trace
6	S	231	Total 1770	C 1125	N 294	O 341	S 10	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

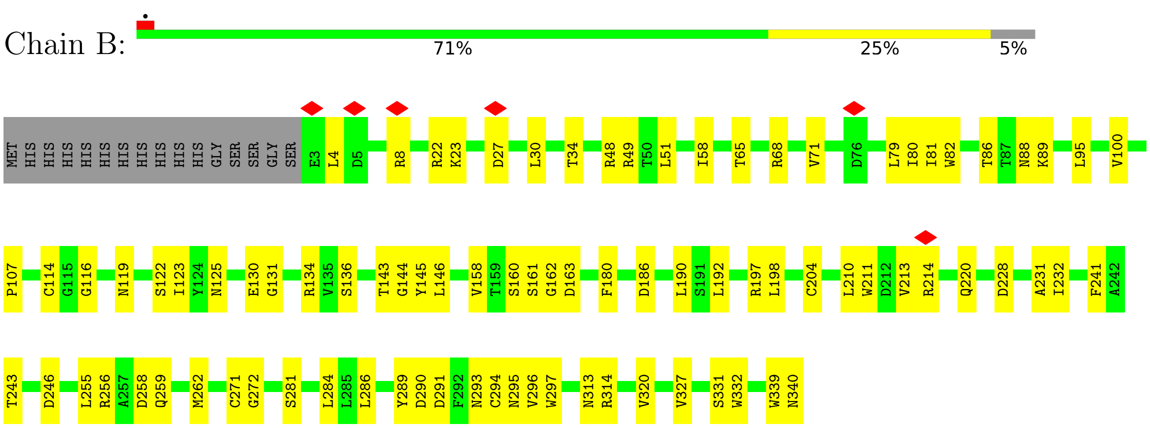
• Molecule 1: Guanine nucleotide-binding protein G(o) subunit alpha,cDNA FLJ31446 fis, clone NT2NE2000909, highly similar to Guanine nucleotide-binding protein G(o) subunit alpha 1

Chain A:



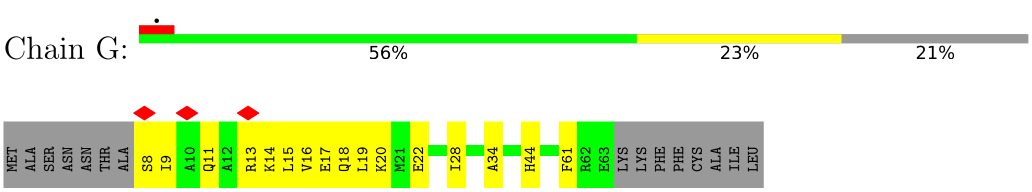
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



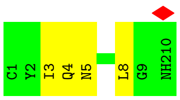
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:



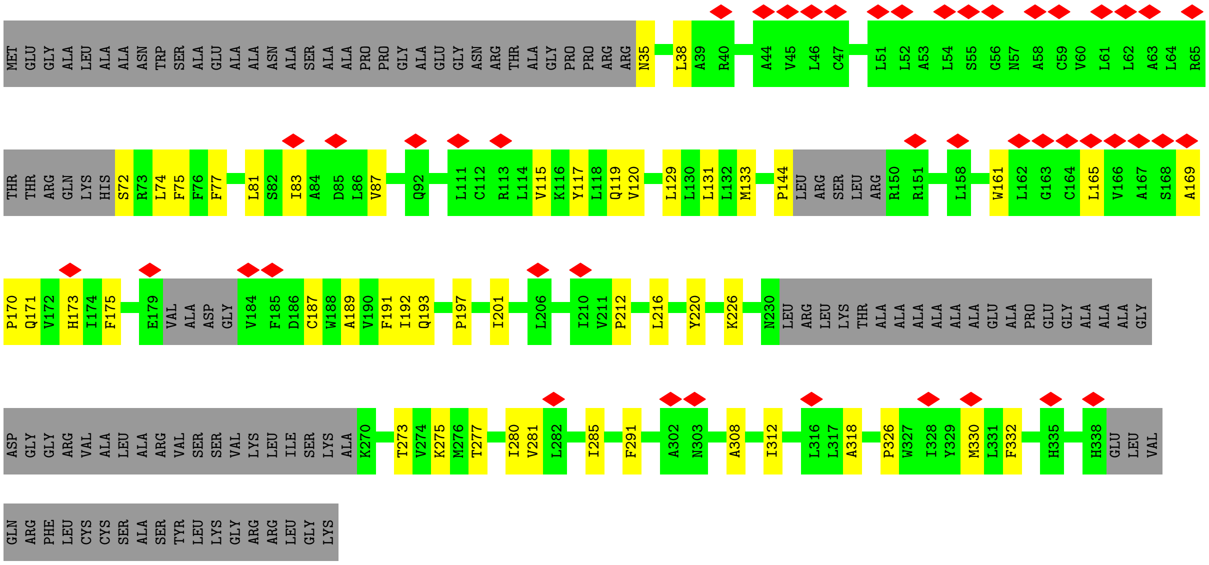
• Molecule 4: Oxytocin

Chain L:



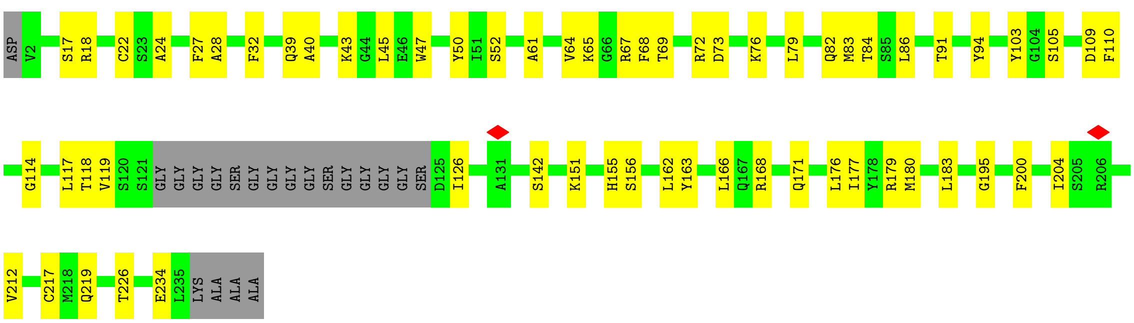
• Molecule 5: Oxytocin receptor

Chain R:

• Molecule 6: Antibody fragment scFv16

Chain S:

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	392369	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	63.78	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.388	Depositor
Minimum map value	-0.655	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.169	Depositor
Map size (Å)	268.212, 268.212, 268.212	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.651, 0.651, 0.651	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: NH2

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	0.26	0/1689	0.48	0/2272
2	B	0.26	0/2647	0.55	0/3589
3	G	0.29	0/439	0.52	0/592
4	L	0.57	0/69	0.55	0/93
5	R	0.27	0/2050	0.45	0/2801
6	S	0.28	0/1814	0.52	0/2460
All	All	0.27	0/8708	0.51	0/11807

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	1662	0	1650	36	0
2	B	2600	0	2505	67	0
3	G	433	0	442	16	0
4	L	69	0	65	4	0
5	R	1994	0	2051	32	0
6	S	1770	0	1700	43	0
All	All	8528	0	8413	184	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 11.

All (184) 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)
3:G:9:ILE:HG22	3:G:13:ARG:HH12	1.53	0.74
2:B:160:SER:HB3	2:B:190:LEU:HD23	1.70	0.74
2:B:213:VAL:HG23	2:B:214:ARG:HG3	1.70	0.74
6:S:39:GLN:HB2	6:S:45:LEU:HD23	1.71	0.72
2:B:246:ASP:HA	2:B:272:GLY:HA3	1.72	0.70
3:G:17:GLU:HA	3:G:20:LYS:HG2	1.74	0.70
6:S:40:ALA:HB3	6:S:43:LYS:HB2	1.75	0.69
2:B:286:LEU:HG	2:B:296:VAL:HG22	1.75	0.68
2:B:271:CYS:SG	2:B:272:GLY:N	2.66	0.68
6:S:52:SER:O	6:S:72:ARG:NH1	2.27	0.68
6:S:94:TYR:O	6:S:114:GLY:HA2	1.94	0.67
2:B:22:ARG:O	2:B:259:GLN:NE2	2.28	0.67
6:S:105:SER:O	6:S:179:ARG:NH2	2.27	0.67
1:A:310:SER:OG	1:A:311:LYS:NZ	2.28	0.66
2:B:210:LEU:HD22	2:B:255:LEU:HD12	1.78	0.66
2:B:125:ASN:HB2	2:B:136:SER:HB2	1.79	0.64
3:G:13:ARG:HA	3:G:16:VAL:HG22	1.79	0.64
1:A:38:LEU:HD23	1:A:201:ASP:HB2	1.81	0.62
2:B:65:THR:OG1	2:B:107:PRO:O	2.16	0.62
1:A:231:TYR:O	1:A:242:ASN:N	2.32	0.62
4:L:8:LEU:HD12	5:R:312:ILE:HD11	1.81	0.62
5:R:192:ILE:HG13	5:R:193:GLN:HG2	1.83	0.61
6:S:69:THR:HG22	6:S:82:GLN:HB3	1.83	0.61
2:B:232:ILE:HG13	2:B:243:THR:HB	1.82	0.61
1:A:33:ASP:OD2	1:A:198:ARG:NH1	2.32	0.61
1:A:38:LEU:HD22	1:A:199:LEU:HD23	1.82	0.60
2:B:313:ASN:HB3	2:B:332:TRP:HB2	1.83	0.60
6:S:64:VAL:HG13	6:S:68:PHE:HD2	1.67	0.60
2:B:290:ASP:HA	2:B:314:ARG:HE	1.66	0.60
3:G:9:ILE:HG22	3:G:13:ARG:NH1	2.16	0.59
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.84	0.59
5:R:77:PHE:HB3	5:R:133:MET:HG3	1.84	0.59
1:A:311:LYS:O	1:A:313:ARG:NH1	2.36	0.58
6:S:162:LEU:HB3	6:S:180:MET:HB2	1.85	0.58
4:L:3:ILE:HA	5:R:171:GLN:HE22	1.68	0.58
3:G:17:GLU:HA	3:G:20:LYS:HZ2	1.69	0.58
5:R:326:PRO:O	5:R:330:MET:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:22:CYS:HB3	6:S:79:LEU:HB3	1.85	0.58
5:R:175:PHE:HA	5:R:189:ALA:HA	1.84	0.58
5:R:35:ASN:HB2	5:R:38:LEU:HB3	1.86	0.57
6:S:166:LEU:HB2	6:S:176:LEU:HD11	1.87	0.57
1:A:248:LEU:HD21	1:A:311:LYS:HE2	1.85	0.57
6:S:212:VAL:HG23	6:S:234:GLU:HA	1.87	0.57
2:B:197:ARG:HA	2:B:197:ARG:NH1	2.20	0.57
2:B:86:THR:OG1	2:B:88:ASN:OD1	2.23	0.56
1:A:228:LEU:HD11	1:A:304:ILE:HD13	1.85	0.56
2:B:198:LEU:HD13	2:B:210:LEU:HD21	1.86	0.56
2:B:49:ARG:HE	3:G:61:PHE:HD1	1.55	0.55
2:B:186:ASP:O	2:B:204:CYS:N	2.37	0.55
1:A:283:PRO:HB2	1:A:285:THR:HG22	1.87	0.55
2:B:51:LEU:HB3	2:B:82:TRP:CZ3	2.41	0.55
5:R:281:VAL:O	5:R:285:ILE:HG12	2.07	0.55
2:B:281:SER:OG	3:G:44:HIS:O	2.25	0.55
2:B:289:TYR:OH	2:B:297:TRP:NE1	2.39	0.55
6:S:32:PHE:O	6:S:72:ARG:NH2	2.29	0.54
2:B:198:LEU:HB3	2:B:210:LEU:HD11	1.88	0.54
2:B:82:TRP:HA	2:B:89:LYS:HA	1.89	0.54
1:A:351:TYR:HD2	5:R:74:LEU:HD13	1.72	0.54
1:A:338:ALA:O	1:A:342:ILE:HG12	2.08	0.54
2:B:119:ASN:ND2	2:B:143:THR:O	2.37	0.53
2:B:145:TYR:O	2:B:162:GLY:N	2.42	0.53
6:S:69:THR:CG2	6:S:82:GLN:HB3	2.38	0.53
2:B:186:ASP:HB3	2:B:204:CYS:SG	2.49	0.53
1:A:256:ASN:OD1	1:A:313:ARG:NH2	2.41	0.53
4:L:8:LEU:HB2	5:R:312:ILE:HD13	1.90	0.53
6:S:61:ALA:O	6:S:65:LYS:N	2.40	0.53
6:S:91:THR:OG1	6:S:119:VAL:N	2.39	0.52
5:R:273:THR:O	5:R:277:THR:HG23	2.10	0.52
1:A:8:GLU:OE2	6:S:163:TYR:OH	2.25	0.51
6:S:142:SER:HA	6:S:204:ILE:O	2.10	0.51
5:R:275:LYS:HE2	5:R:332:PHE:CE1	2.46	0.51
2:B:95:LEU:HD13	2:B:100:VAL:HG11	1.92	0.51
1:A:33:ASP:OD1	1:A:196:HIS:ND1	2.37	0.51
2:B:256:ARG:HB3	3:G:28:ILE:HG12	1.93	0.51
6:S:109:ASP:OD1	6:S:110:PHE:N	2.44	0.51
2:B:4:LEU:O	2:B:8:ARG:HG2	2.11	0.50
6:S:168:ARG:NE	6:S:171:GLN:OE1	2.44	0.50
1:A:228:LEU:HD11	1:A:304:ILE:HG21	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:LEU:HD23	2:B:262:MET:HE3	1.94	0.50
2:B:289:TYR:HH	2:B:297:TRP:HE1	1.53	0.50
2:B:158:VAL:HG21	2:B:192:LEU:HD21	1.94	0.49
2:B:123:ILE:O	2:B:136:SER:N	2.45	0.49
2:B:144:GLY:H	2:B:163:ASP:HB2	1.77	0.49
1:A:339:VAL:O	1:A:343:ILE:HG13	2.12	0.49
2:B:162:GLY:HA2	2:B:186:ASP:OD1	2.13	0.49
5:R:291:PHE:CD1	5:R:318:ALA:HB2	2.48	0.49
2:B:80:ILE:HB	2:B:82:TRP:HE1	1.77	0.49
2:B:231:ALA:O	2:B:243:THR:OG1	2.24	0.49
2:B:23:LYS:HA	2:B:23:LYS:HE2	1.95	0.49
1:A:20:GLU:OE2	2:B:89:LYS:NZ	2.45	0.49
1:A:209:ARG:HG3	1:A:209:ARG:HH11	1.78	0.49
2:B:22:ARG:HG2	2:B:258:ASP:HB2	1.95	0.48
6:S:83:MET:HG3	6:S:86:LEU:HD21	1.95	0.48
2:B:131:GLY:HA3	6:S:28:ALA:HB3	1.94	0.48
5:R:220:TYR:HB3	5:R:277:THR:HG22	1.96	0.48
5:R:170:PRO:HA	5:R:173:HIS:HB3	1.95	0.48
2:B:204:CYS:HA	2:B:228:ASP:OD1	2.14	0.48
5:R:275:LYS:HE2	5:R:332:PHE:HE1	1.77	0.48
6:S:162:LEU:HD22	6:S:200:PHE:CD1	2.49	0.48
2:B:30:LEU:O	2:B:34:THR:N	2.44	0.48
2:B:293:ASN:OD1	2:B:294:CYS:N	2.47	0.48
6:S:219:GLN:HE21	6:S:226:THR:H	1.62	0.47
2:B:30:LEU:HD13	3:G:34:ALA:HB1	1.96	0.47
2:B:58:ILE:HB	2:B:331:SER:O	2.14	0.47
6:S:94:TYR:O	6:S:114:GLY:CA	2.62	0.47
6:S:195:GLY:HA3	6:S:200:PHE:CD1	2.50	0.47
1:A:345:GLN:HB3	1:A:349:ARG:HH12	1.79	0.47
6:S:64:VAL:HG13	6:S:68:PHE:CD2	2.49	0.47
2:B:232:ILE:HD11	2:B:241:PHE:CE2	2.49	0.47
2:B:48:ARG:HG3	2:B:340:ASN:HB2	1.96	0.47
2:B:100:VAL:HA	2:B:116:GLY:HA3	1.97	0.47
6:S:162:LEU:HD11	6:S:217:CYS:SG	2.54	0.47
1:A:36:LEU:HD13	1:A:223:ILE:HD11	1.97	0.47
6:S:180:MET:SD	6:S:195:GLY:N	2.88	0.47
6:S:24:ALA:HB1	6:S:27:PHE:CE1	2.50	0.47
2:B:114:CYS:SG	2:B:122:SER:HB2	2.55	0.46
2:B:197:ARG:HA	2:B:197:ARG:CZ	2.46	0.46
2:B:158:VAL:HG12	2:B:190:LEU:HD22	1.96	0.46
4:L:4:GLN:HG2	4:L:5:ASN:H	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:LYS:HD3	1:A:323:MET:HG3	1.97	0.46
2:B:27:ASP:N	2:B:27:ASP:OD1	2.49	0.46
6:S:91:THR:HA	6:S:117:LEU:O	2.16	0.45
6:S:67:ARG:O	6:S:84:THR:OG1	2.33	0.45
5:R:175:PHE:HD2	5:R:187:CYS:HB3	1.82	0.45
3:G:18:GLN:O	3:G:22:GLU:HG3	2.17	0.45
5:R:115:VAL:O	5:R:119:GLN:HG3	2.16	0.45
5:R:117:TYR:HE2	5:R:169:ALA:HA	1.81	0.45
1:A:354:VAL:OXT	1:A:354:VAL:HG22	2.17	0.44
1:A:5:LEU:N	6:S:155:HIS:HE1	2.16	0.44
2:B:289:TYR:CE1	2:B:295:ASN:HB2	2.53	0.44
2:B:220:GLN:NE2	2:B:255:LEU:O	2.36	0.44
3:G:8:SER:O	3:G:11:GLN:NE2	2.51	0.44
3:G:13:ARG:O	3:G:14:LYS:C	2.55	0.44
5:R:120:VAL:HG21	5:R:171:GLN:HG2	1.99	0.44
1:A:211:LYS:HA	1:A:211:LYS:HD3	1.80	0.44
1:A:311:LYS:HD3	1:A:311:LYS:HA	1.71	0.43
2:B:146:LEU:HA	2:B:161:SER:HA	1.99	0.43
5:R:191:PHE:HB3	5:R:197:PRO:HD3	2.00	0.43
2:B:286:LEU:HD22	2:B:327:VAL:HG11	2.00	0.43
1:A:187:GLU:OE2	1:A:198:ARG:NE	2.39	0.43
5:R:308:ALA:O	5:R:312:ILE:HG13	2.18	0.43
6:S:91:THR:HG23	6:S:118:THR:HA	2.00	0.43
2:B:79:LEU:HB2	2:B:95:LEU:HD21	1.99	0.43
3:G:8:SER:OG	3:G:9:ILE:N	2.51	0.43
6:S:73:ASP:OD2	6:S:76:LYS:NZ	2.51	0.43
1:A:189:HIS:HB2	1:A:196:HIS:NE2	2.32	0.43
5:R:216:LEU:HD21	5:R:280:ILE:HG22	2.00	0.43
6:S:47:TRP:HZ2	6:S:50:TYR:HB3	1.83	0.43
6:S:155:HIS:CG	6:S:156:SER:H	2.37	0.43
2:B:130:GLU:HG2	2:B:134:ARG:HH21	1.84	0.43
5:R:161:TRP:O	5:R:165:LEU:HD23	2.19	0.43
1:A:343:ILE:HG22	5:R:144:PRO:HB2	2.00	0.42
1:A:230:ASP:OD1	1:A:242:ASN:ND2	2.52	0.42
1:A:272:LYS:HE2	1:A:325:CYS:HA	2.01	0.42
2:B:68:ARG:HD3	6:S:103:TYR:CZ	2.54	0.42
5:R:117:TYR:HE1	5:R:165:LEU:HD13	1.85	0.42
6:S:76:LYS:NZ	6:S:76:LYS:HB2	2.33	0.42
5:R:226:LYS:HA	5:R:226:LYS:HD3	1.66	0.42
1:A:17:LYS:HA	1:A:17:LYS:HD3	1.83	0.42
2:B:180:PHE:HB3	2:B:211:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:162:LEU:HD22	6:S:200:PHE:CG	2.55	0.42
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.89	0.42
3:G:15:LEU:O	3:G:19:LEU:HD23	2.20	0.42
6:S:126:ILE:HD11	6:S:151:LYS:NZ	2.35	0.42
6:S:177:ILE:HD13	6:S:183:LEU:HA	2.01	0.42
3:G:11:GLN:O	3:G:15:LEU:HD23	2.20	0.41
5:R:83:ILE:O	5:R:87:VAL:HG23	2.20	0.41
3:G:14:LYS:HA	3:G:14:LYS:HD2	1.72	0.41
5:R:72:SER:HB2	5:R:75:PHE:HD1	1.86	0.41
5:R:81:LEU:HA	5:R:129:LEU:HD23	2.01	0.41
6:S:18:ARG:O	6:S:83:MET:CB	2.68	0.41
1:A:197:PHE:CZ	1:A:339:VAL:HG11	2.56	0.41
1:A:225:CYS:HA	1:A:268:PHE:HB2	2.02	0.41
1:A:209:ARG:HA	1:A:212:TRP:NE1	2.36	0.41
2:B:284:LEU:HD12	2:B:296:VAL:CG1	2.51	0.41
2:B:290:ASP:OD1	2:B:291:ASP:N	2.54	0.41
2:B:339:TRP:CD1	2:B:339:TRP:N	2.89	0.41
5:R:131:LEU:HD12	5:R:212:PRO:HA	2.02	0.41
2:B:130:GLU:HA	2:B:130:GLU:OE2	2.21	0.41
2:B:197:ARG:HH12	2:B:213:VAL:HG21	1.86	0.41
6:S:17:SER:HA	6:S:83:MET:O	2.21	0.41
5:R:197:PRO:O	5:R:201:ILE:HG12	2.21	0.40
2:B:71:VAL:HG23	2:B:81:ILE:HG12	2.03	0.40
1:A:228:LEU:HD12	1:A:228:LEU:HA	1.97	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	204/228 (90%)	196 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	336/354 (95%)	323 (96%)	13 (4%)	0	100	100
3	G	54/71 (76%)	52 (96%)	2 (4%)	0	100	100
4	L	8/10 (80%)	6 (75%)	2 (25%)	0	100	100
5	R	240/359 (67%)	234 (98%)	6 (2%)	0	100	100
6	S	227/251 (90%)	220 (97%)	7 (3%)	0	100	100
All	All	1069/1273 (84%)	1031 (96%)	38 (4%)	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	184/199 (92%)	184 (100%)	0	100	100
2	B	281/295 (95%)	281 (100%)	0	100	100
3	G	46/58 (79%)	46 (100%)	0	100	100
4	L	8/8 (100%)	8 (100%)	0	100	100
5	R	215/291 (74%)	215 (100%)	0	100	100
6	S	193/201 (96%)	193 (100%)	0	100	100
All	All	927/1052 (88%)	927 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
5	R	230	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 monosaccharides in this entry.

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 (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	231:TYR	C	242:ASN	N	3.45

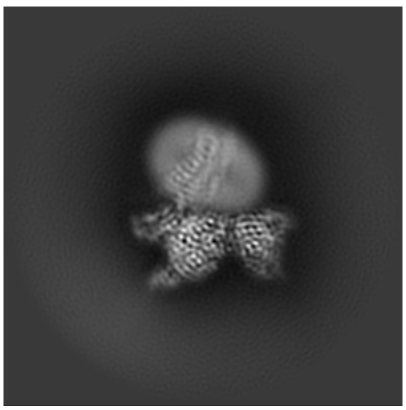
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-14180. These allow visual inspection of the internal detail of the map and identification of artifacts.

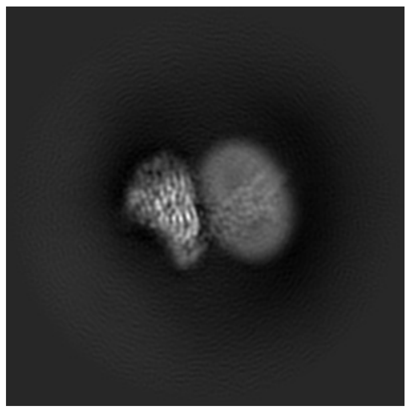
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

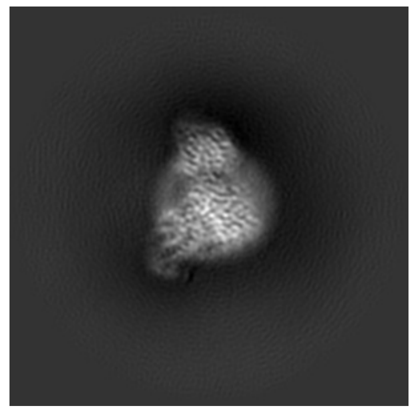
6.1.1 Primary map



X



Y

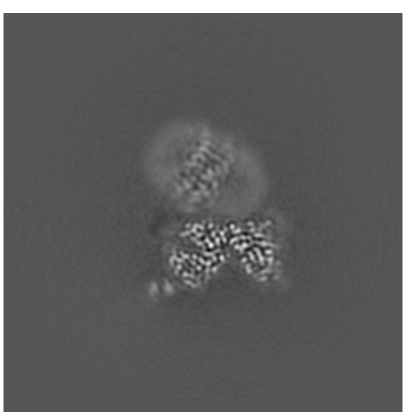


Z

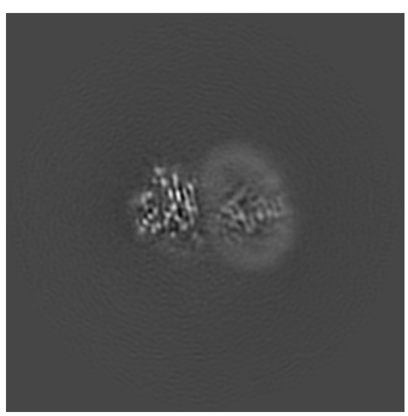
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

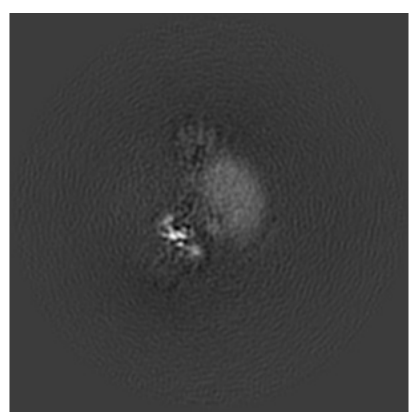
6.2.1 Primary map



X Index: 206



Y Index: 206

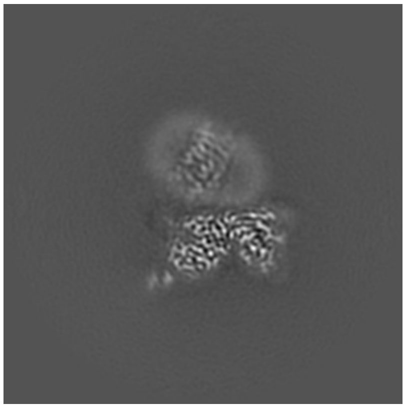


Z Index: 206

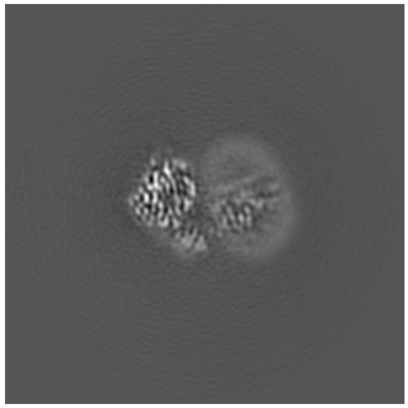
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

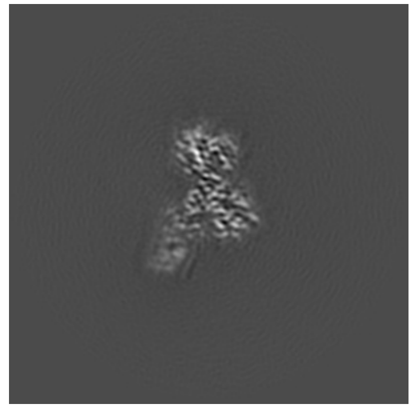
6.3.1 Primary map



X Index: 203



Y Index: 196



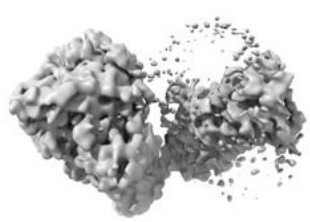
Z Index: 174

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

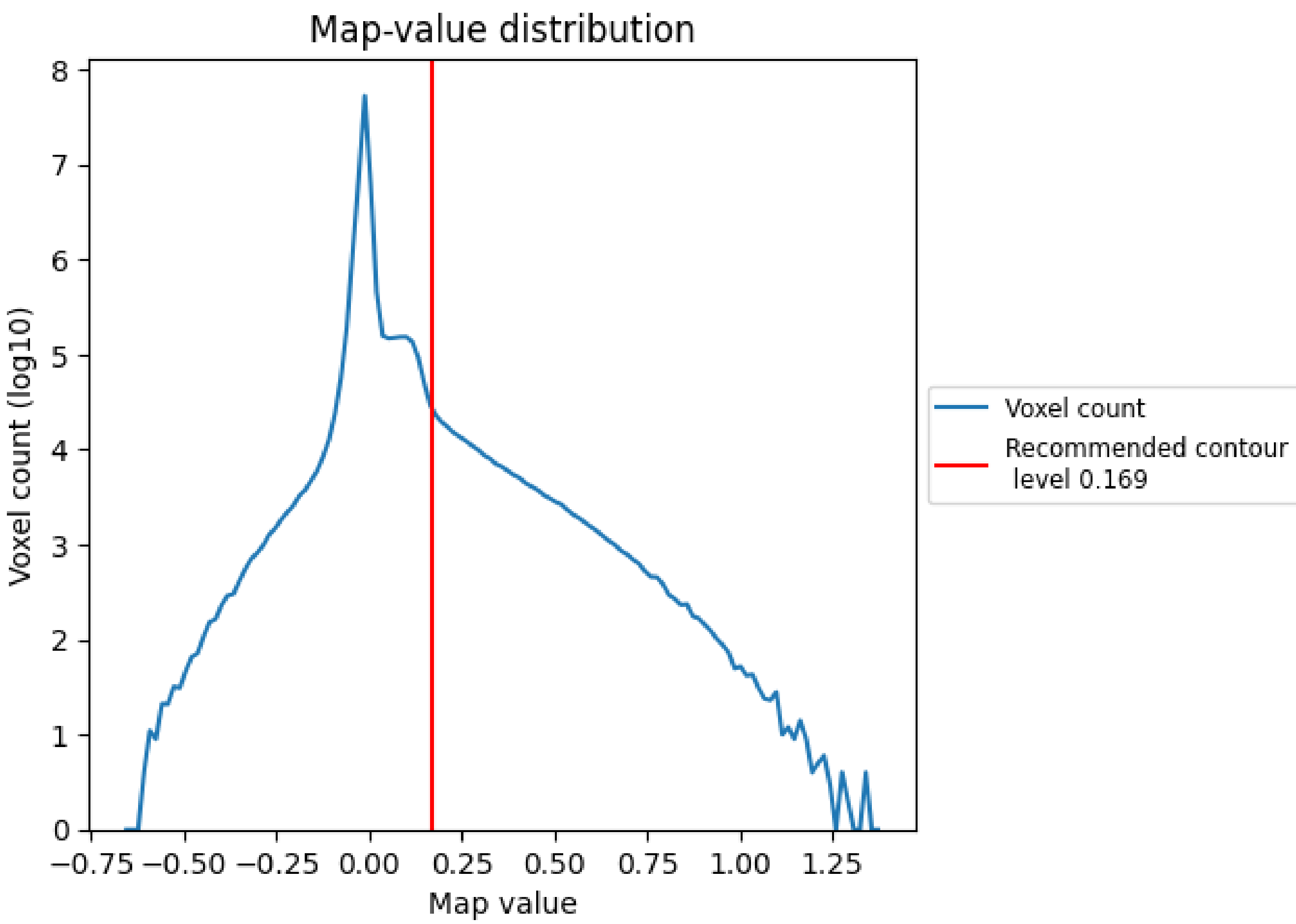
6.5 Mask visualisation (i)

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

7 Map analysis ⓘ

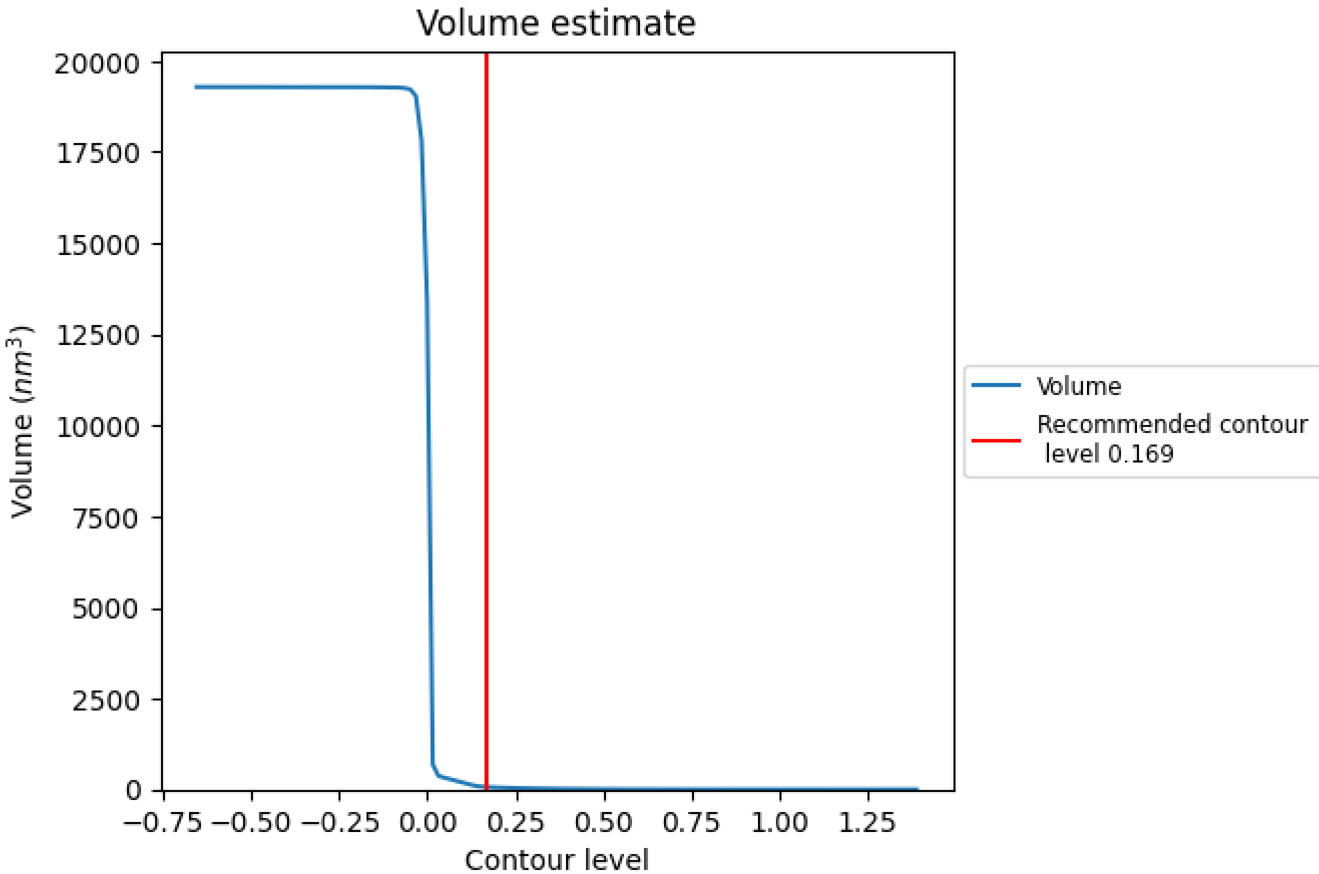
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



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.

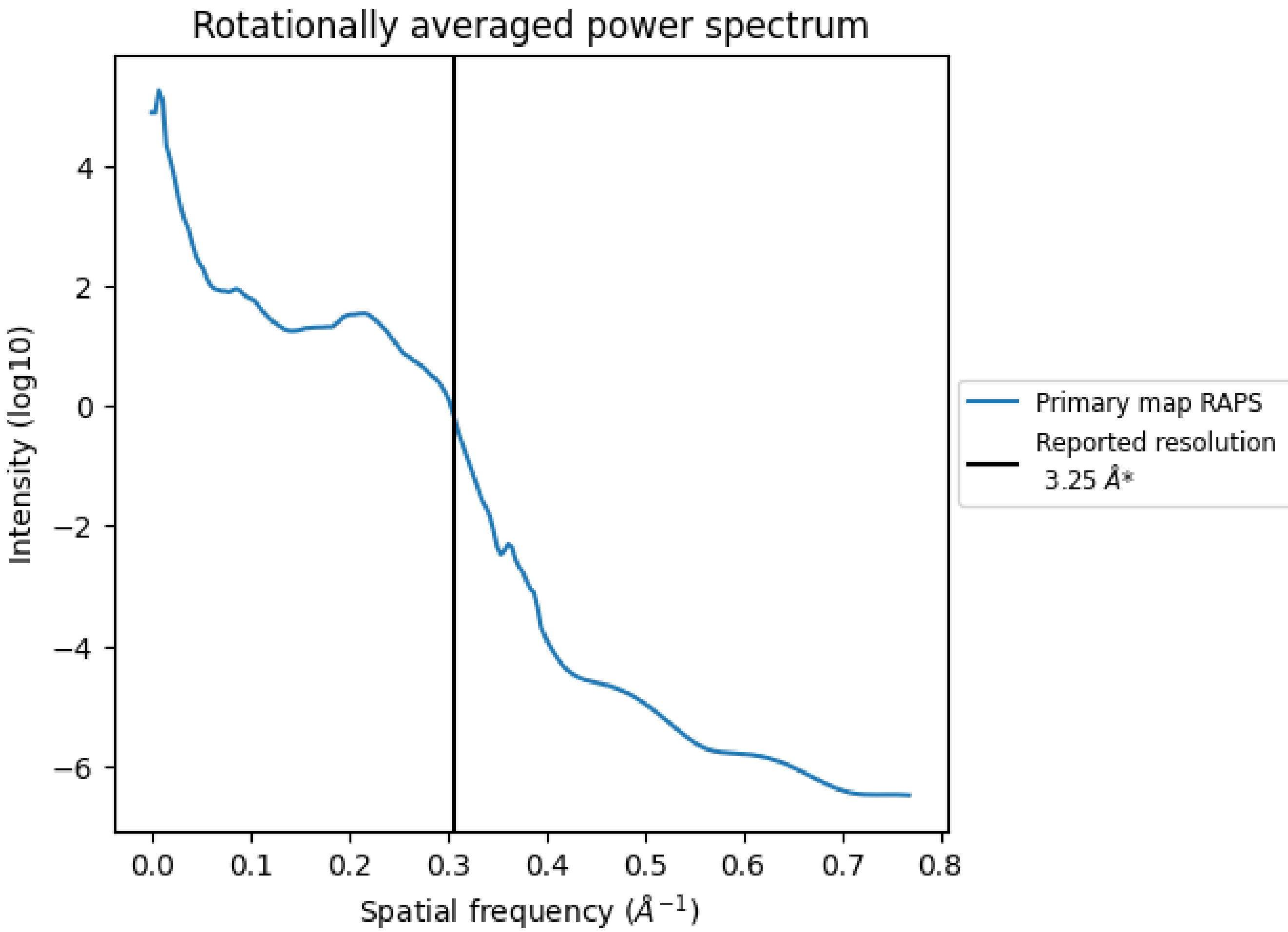
7.2 Volume estimate (i)



The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 59 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 0.308 $Å^{-1}$

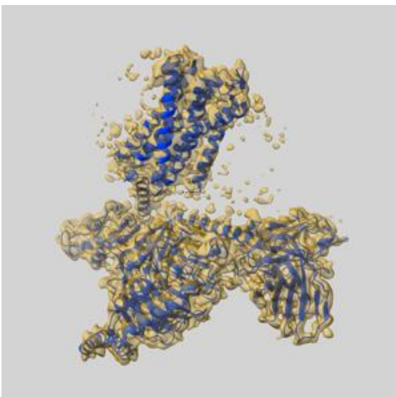
8 Fourier-Shell correlation

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

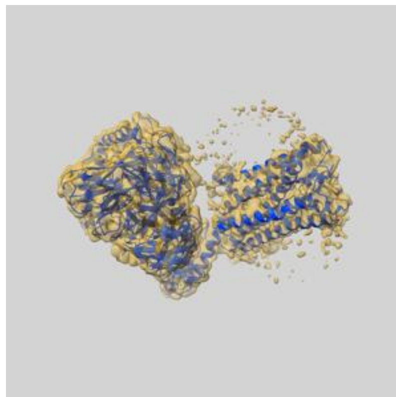
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-14180 and PDB model 7QVM. Per-residue inclusion information can be found in section 3 on page 6.

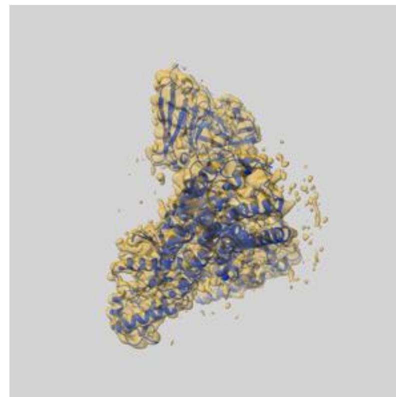
9.1 Map-model overlay (i)



X



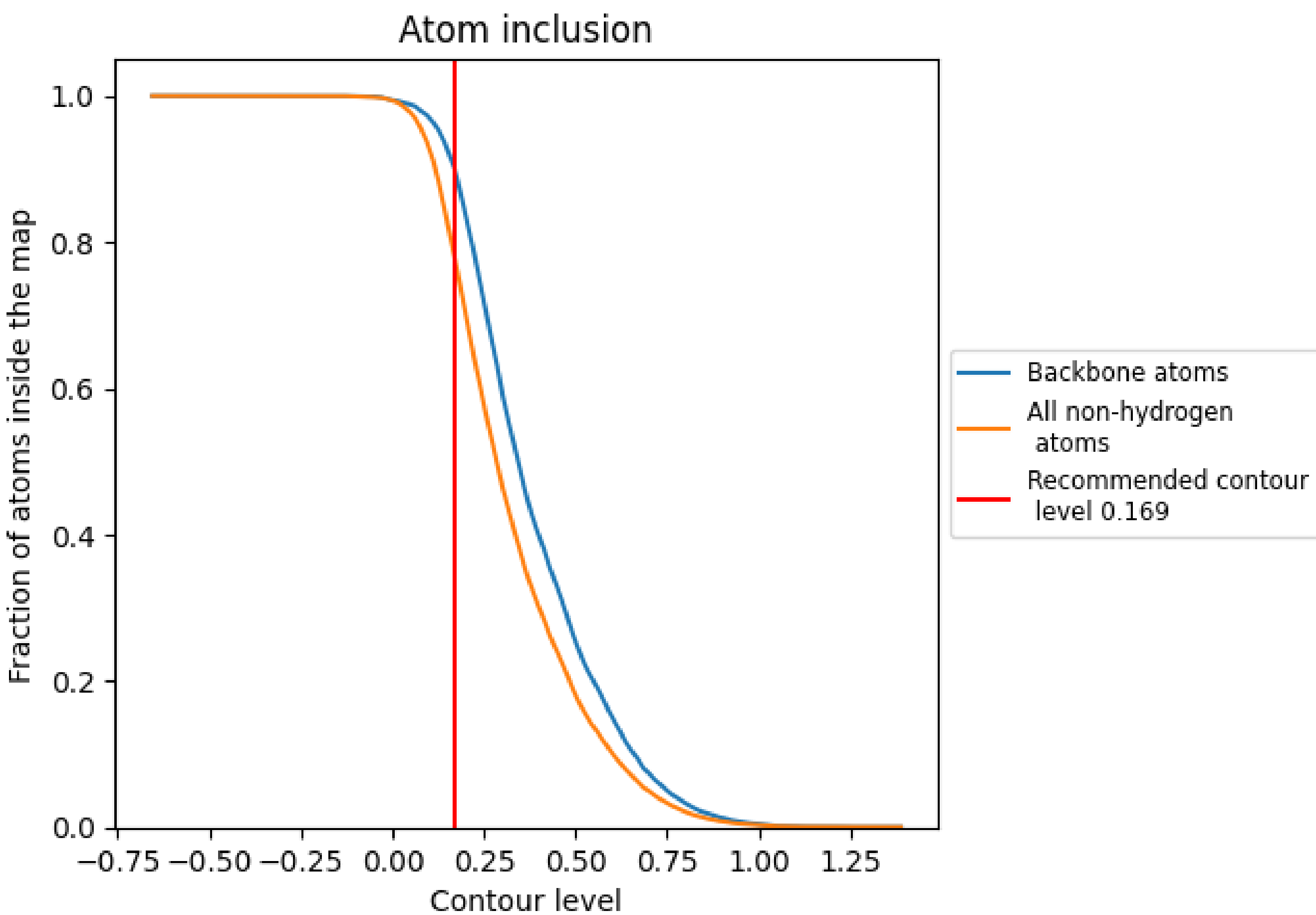
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.169 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 Atom inclusion (i)



At the recommended contour level, 90% of all backbone atoms, 78% of all non-hydrogen atoms, are inside the map.