



## Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 04:36 PM JST

PDB ID : 7WU5  
EMDB ID : EMD-32820  
Title : Cryo-EM structure of the adhesion GPCR ADGRF1(H565A/T567A) in complex with miniGi  
Authors : Qu, X.; Qiu, N.; Wang, M.; Zhao, Q.; Wu, B.  
Deposited on : 2022-02-05  
Resolution : 3.00 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
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

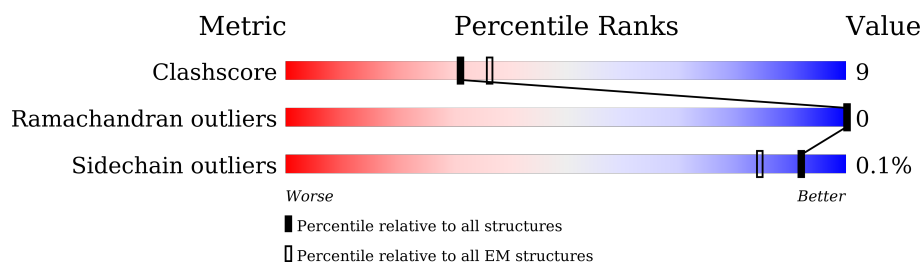
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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  $\geq 3$ , 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	241	<div> <div>8%</div> <div>68%</div> <div>18%</div> <div>14%</div> </div>
2	B	351	<div> <div>5%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
3	C	71	<div> <div>13%</div> <div>65%</div> <div>13%</div> <div>.</div> <div>21%</div> </div>
4	R	674	<div> <div>11%</div> <div>35%</div> <div>8%</div> <div>58%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6948 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(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	207	Total	C	N	O	S	0	0
			1677	1066	282	317	12		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP A0A3B3IUA8
A	-10	GLY	-	expression tag	UNP A0A3B3IUA8
A	-9	HIS	-	expression tag	UNP A0A3B3IUA8
A	-8	HIS	-	expression tag	UNP A0A3B3IUA8
A	-7	HIS	-	expression tag	UNP A0A3B3IUA8
A	-6	HIS	-	expression tag	UNP A0A3B3IUA8
A	-5	HIS	-	expression tag	UNP A0A3B3IUA8
A	-4	HIS	-	expression tag	UNP A0A3B3IUA8
A	-3	GLU	-	expression tag	UNP A0A3B3IUA8
A	-2	ASN	-	expression tag	UNP A0A3B3IUA8
A	-1	LEU	-	expression tag	UNP A0A3B3IUA8
A	0	TYR	-	expression tag	UNP A0A3B3IUA8
A	1	PHE	-	expression tag	UNP A0A3B3IUA8
A	2	GLN	-	expression tag	UNP A0A3B3IUA8
A	3	GLY	-	expression tag	UNP A0A3B3IUA8
A	42	ASP	GLY	conflict	UNP A0A3B3IUA8
A	43	ASN	GLU	conflict	UNP A0A3B3IUA8
A	173	GLY	-	linker	UNP A0A3B3IUA8
A	174	GLY	-	linker	UNP A0A3B3IUA8
A	175	GLY	-	linker	UNP A0A3B3IUA8
A	176	GLY	-	linker	UNP A0A3B3IUA8
A	177	GLY	-	linker	UNP A0A3B3IUA8
A	178	GLY	-	linker	UNP A0A3B3IUA8
A	179	GLY	-	linker	UNP A0A3B3IUA8
A	180	GLY	-	linker	UNP A0A3B3IUA8
A	217	ASP	GLY	conflict	UNP P63096
A	219	ALA	THR	conflict	UNP P63096

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Chain	Residue	Modelled	Actual	Comment	Reference
A	226	ASP	ALA	conflict	UNP P63096
A	?	-	ASP	deletion	UNP P63096
A	?	-	LEU	deletion	UNP P63096
A	?	-	VAL	deletion	UNP P63096
A	?	-	LEU	deletion	UNP P63096
A	?	-	ALA	deletion	UNP P63096
A	?	-	GLU	deletion	UNP P63096
A	?	-	ASP	deletion	UNP P63096
A	?	-	GLU	deletion	UNP P63096
A	?	-	GLU	deletion	UNP P63096
A	?	-	MET	deletion	UNP P63096
A	288	GLN	PRO	conflict	UNP P63096
A	332	ALA	VAL	conflict	UNP P63096
A	335	ILE	VAL	conflict	UNP P63096

- 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	339	Total	C	N	O	S	0	0
			2586	1597	464	504	21		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	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	GLY	-	expression tag	UNP P62873
B	-2	SER	-	expression tag	UNP P62873
B	-1	LEU	-	expression tag	UNP P62873
B	0	LEU	-	expression tag	UNP P62873
B	1	GLN	-	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	C	56	Total	C	N	O	S	0	0
			420	263	73	81	3		

- Molecule 4 is a protein called Adhesion G-protein coupled receptor F1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	286	Total	C	N	O	S	0	0
			2204	1488	352	350	14		

There are 66 discrepancies between the modelled and reference sequences:

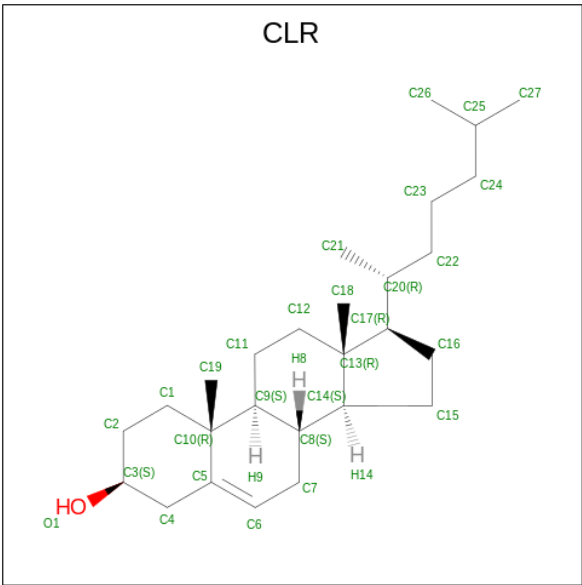
Chain	Residue	Modelled	Actual	Comment	Reference
R	225	MET	-	initiating methionine	UNP Q5T601
R	226	LYS	-	expression tag	UNP Q5T601
R	227	THR	-	expression tag	UNP Q5T601
R	228	ILE	-	expression tag	UNP Q5T601
R	229	ILE	-	expression tag	UNP Q5T601
R	230	ALA	-	expression tag	UNP Q5T601
R	231	LEU	-	expression tag	UNP Q5T601
R	232	SER	-	expression tag	UNP Q5T601
R	233	TYR	-	expression tag	UNP Q5T601
R	234	ILE	-	expression tag	UNP Q5T601
R	235	PHE	-	expression tag	UNP Q5T601
R	236	CYS	-	expression tag	UNP Q5T601
R	237	LEU	-	expression tag	UNP Q5T601
R	238	VAL	-	expression tag	UNP Q5T601
R	239	PHE	-	expression tag	UNP Q5T601
R	240	ALA	-	expression tag	UNP Q5T601
R	241	ASP	-	expression tag	UNP Q5T601
R	242	TYR	-	expression tag	UNP Q5T601
R	243	LYS	-	expression tag	UNP Q5T601
R	244	ASP	-	expression tag	UNP Q5T601
R	245	ASP	-	expression tag	UNP Q5T601
R	246	ASP	-	expression tag	UNP Q5T601
R	247	ASP	-	expression tag	UNP Q5T601
R	248	GLY	-	expression tag	UNP Q5T601
R	249	ALA	-	expression tag	UNP Q5T601
R	250	PRO	-	expression tag	UNP Q5T601
R	565	ALA	HIS	engineered mutation	UNP Q5T601
R	567	ALA	THR	engineered mutation	UNP Q5T601
R	861	GLU	-	expression tag	UNP Q5T601
R	862	PHE	-	expression tag	UNP Q5T601
R	863	LEU	-	expression tag	UNP Q5T601

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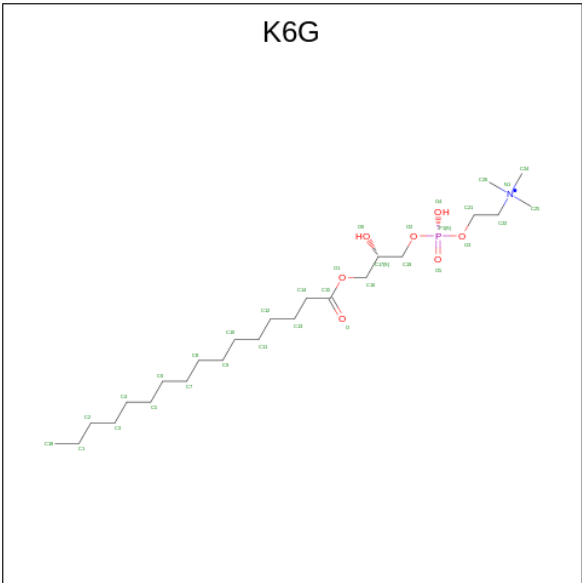
Chain	Residue	Modelled	Actual	Comment	Reference
R	864	GLU	-	expression tag	UNP Q5T601
R	865	VAL	-	expression tag	UNP Q5T601
R	866	LEU	-	expression tag	UNP Q5T601
R	867	PHE	-	expression tag	UNP Q5T601
R	868	GLN	-	expression tag	UNP Q5T601
R	869	GLY	-	expression tag	UNP Q5T601
R	870	PRO	-	expression tag	UNP Q5T601
R	871	TRP	-	expression tag	UNP Q5T601
R	872	SER	-	expression tag	UNP Q5T601
R	873	HIS	-	expression tag	UNP Q5T601
R	874	PRO	-	expression tag	UNP Q5T601
R	875	GLN	-	expression tag	UNP Q5T601
R	876	PHE	-	expression tag	UNP Q5T601
R	877	GLU	-	expression tag	UNP Q5T601
R	878	LYS	-	expression tag	UNP Q5T601
R	879	GLY	-	expression tag	UNP Q5T601
R	880	GLY	-	expression tag	UNP Q5T601
R	881	GLY	-	expression tag	UNP Q5T601
R	882	SER	-	expression tag	UNP Q5T601
R	883	GLY	-	expression tag	UNP Q5T601
R	884	GLY	-	expression tag	UNP Q5T601
R	885	GLY	-	expression tag	UNP Q5T601
R	886	SER	-	expression tag	UNP Q5T601
R	887	GLY	-	expression tag	UNP Q5T601
R	888	GLY	-	expression tag	UNP Q5T601
R	889	SER	-	expression tag	UNP Q5T601
R	890	ALA	-	expression tag	UNP Q5T601
R	891	TRP	-	expression tag	UNP Q5T601
R	892	SER	-	expression tag	UNP Q5T601
R	893	HIS	-	expression tag	UNP Q5T601
R	894	PRO	-	expression tag	UNP Q5T601
R	895	GLN	-	expression tag	UNP Q5T601
R	896	PHE	-	expression tag	UNP Q5T601
R	897	GLU	-	expression tag	UNP Q5T601
R	898	LYS	-	expression tag	UNP Q5T601

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: C<sub>27</sub>H<sub>46</sub>O).



Mol	Chain	Residues	Atoms			AltConf
5	R	1	Total	C	O	0
			28	27	1	

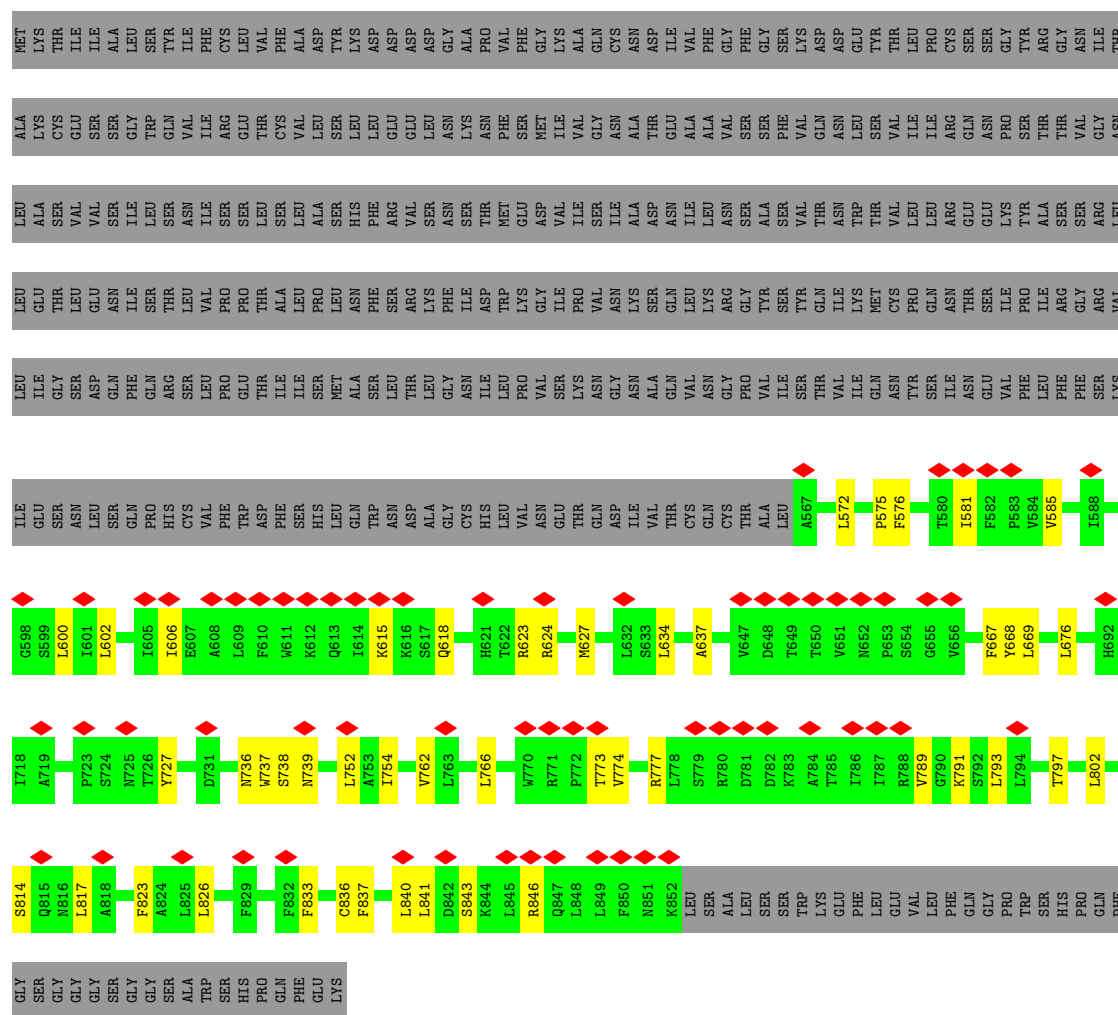
- Molecule 6 is [(2 {R})-2-oxidanyl-3-[oxidanyl-[2-(trimethyl- $\text{N}^{\text{+}}$ {4}-azanyl)ethoxy]phosphoryl]oxy-propyl] hexadecanoate (three-letter code: K6G) (formula:  $\text{C}_{24}\text{H}_{51}\text{NO}_7\text{P}$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	N	O	P	0
			33	24	1	7	1	







## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	799431	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 ( $e^-/\text{\AA}^2$ )	70	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.114	Depositor
Minimum map value	-0.070	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0115	Depositor
Map size (Å)	274.176, 274.176, 274.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.071, 1.071, 1.071	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: CLR, K6G

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	0/1706	0.45	0/2287
2	B	0.27	0/2633	0.53	0/3571
3	C	0.24	0/426	0.41	0/576
4	R	0.24	0/2264	0.45	0/3095
All	All	0.26	0/7029	0.48	0/9529

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	1677	0	1655	28	0
2	B	2586	0	2483	55	0
3	C	420	0	421	9	0
4	R	2204	0	2293	37	0
5	R	28	0	46	0	0
6	R	33	0	0	0	0
All	All	6948	0	6898	119	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 9.

All (119) 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:320:TYR:HA	4:R:777:ARG:HD3	1.69	0.73
1:A:208:ARG:HH22	1:A:253:ILE:HG22	1.53	0.73
2:B:294:CYS:HB2	2:B:308:LEU:HB2	1.70	0.72
4:R:615:LYS:HE2	4:R:624:ARG:HG3	1.72	0.71
1:A:251:ASP:OD1	1:A:255:ASN:ND2	2.26	0.68
4:R:774:VAL:H	4:R:777:ARG:HH21	1.44	0.64
1:A:207:GLU:OE2	1:A:209:LYS:NZ	2.31	0.64
2:B:30:LEU:HD13	3:C:34:ALA:HB1	1.80	0.64
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.80	0.62
2:B:274:THR:HG21	2:B:316:SER:HA	1.81	0.61
4:R:843:SER:HB2	4:R:846:ARG:HH21	1.66	0.61
4:R:766:LEU:HD21	4:R:793:LEU:HD21	1.84	0.60
1:A:325:CYS:SG	1:A:326:ALA:N	2.75	0.60
4:R:623:ARG:HH11	4:R:624:ARG:HH22	1.49	0.60
1:A:251:ASP:O	1:A:255:ASN:ND2	2.35	0.60
1:A:348:LEU:HB3	1:A:354:PHE:HB2	1.83	0.59
4:R:676:LEU:HB2	4:R:754:ILE:HD12	1.83	0.59
4:R:774:VAL:H	4:R:777:ARG:NH2	2.01	0.59
1:A:39:LEU:HD13	1:A:253:ILE:HG21	1.85	0.58
3:C:24:ASN:ND2	3:C:24:ASN:O	2.36	0.58
4:R:797:THR:HG23	4:R:802:LEU:HB2	1.85	0.58
4:R:623:ARG:NH1	4:R:624:ARG:HH22	2.02	0.57
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.86	0.56
1:A:311:ASN:HD21	1:A:317:LYS:HB2	1.71	0.56
4:R:576:PHE:O	4:R:814:SER:OG	2.23	0.56
2:B:128:THR:HG22	2:B:130:GLU:H	1.70	0.55
2:B:146:LEU:HD11	2:B:159:THR:HB	1.88	0.55
1:A:50:VAL:HG13	1:A:51:LYS:HG2	1.88	0.55
2:B:231:ALA:HB1	2:B:276:VAL:HG22	1.90	0.53
2:B:260:GLU:OE2	2:B:263:THR:OG1	2.27	0.53
4:R:736:ASN:OD1	4:R:737:TRP:N	2.42	0.53
1:A:315:ASP:OD1	1:A:316:THR:N	2.42	0.53
2:B:286:LEU:HD22	2:B:327:VAL:HG21	1.89	0.53
2:B:4:LEU:HD11	3:C:9:ILE:HA	1.90	0.53
2:B:200:VAL:HG12	2:B:234:PHE:CE1	2.44	0.52
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.91	0.52
4:R:581:ILE:HD13	4:R:817:LEU:HD12	1.91	0.52
4:R:600:LEU:HD21	4:R:634:LEU:HD23	1.91	0.52
2:B:160:SER:HB2	2:B:190:LEU:HD23	1.90	0.51
2:B:210:LEU:HD22	2:B:255:LEU:HD22	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:ILE:HD13	2:B:91:HIS:HB2	1.93	0.51
1:A:184:ILE:HD11	2:B:99:TRP:CD1	2.46	0.51
1:A:209:LYS:NZ	2:B:228:ASP:OD2	2.40	0.50
4:R:762:VAL:HG21	4:R:802:LEU:HD11	1.92	0.50
4:R:806:PHE:HB2	4:R:823:PHE:HD1	1.76	0.50
2:B:18:ILE:HD11	3:C:23:ALA:HA	1.93	0.50
4:R:791:LYS:HG3	4:R:841:LEU:HD21	1.94	0.50
2:B:266:HIS:HB3	2:B:269:ILE:HG12	1.93	0.49
1:A:271:LYS:HD2	1:A:323:PHE:HB3	1.95	0.49
2:B:64:GLY:HA2	2:B:105:TYR:CD2	2.47	0.49
2:B:331:SER:OG	2:B:333:ASP:OD1	2.29	0.49
4:R:738:SER:OG	4:R:739:ASN:N	2.46	0.49
3:C:55:PRO:HG2	3:C:58:GLU:HG2	1.95	0.48
2:B:230:ASN:ND2	2:B:246:ASP:OD1	2.46	0.48
4:R:581:ILE:HG13	4:R:585:VAL:HB	1.96	0.48
4:R:637:ALA:HB2	4:R:667:PHE:HB3	1.96	0.48
1:A:186:GLU:HG2	1:A:199:PHE:CD1	2.49	0.47
2:B:79:LEU:HD23	2:B:93:ILE:HD13	1.97	0.47
2:B:79:LEU:HD21	2:B:112:VAL:HG11	1.97	0.47
1:A:282:PRO:HG2	1:A:285:ILE:HD12	1.97	0.47
2:B:85:TYR:CE1	3:C:60:PRO:HB2	2.50	0.47
2:B:311:HIS:CG	2:B:331:SER:HG	2.31	0.47
4:R:717:THR:HG22	4:R:727:TYR:HE1	1.80	0.46
1:A:188:HIS:HB3	1:A:195:HIS:CE1	2.51	0.46
1:A:250:PHE:HE1	1:A:264:ILE:HG21	1.81	0.46
4:R:575:PRO:HB3	4:R:737:TRP:CD2	2.51	0.46
4:R:797:THR:HA	4:R:802:LEU:HD12	1.98	0.45
2:B:192:LEU:HD13	2:B:199:PHE:HB3	1.98	0.45
4:R:752:LEU:HD11	4:R:808:ILE:HB	1.99	0.45
2:B:123:ILE:HD13	2:B:171:ILE:HD12	1.99	0.45
2:B:254:ASP:HB3	2:B:257:ALA:HB3	2.00	0.44
2:B:296:VAL:HG12	2:B:305:ALA:HB3	1.98	0.44
4:R:773:THR:HA	4:R:777:ARG:NH2	2.32	0.44
2:B:51:LEU:HD23	2:B:87:THR:HG23	1.99	0.44
2:B:124:TYR:CE2	2:B:135:VAL:HG22	2.52	0.44
2:B:68:ARG:HE	2:B:85:TYR:HD2	1.65	0.44
2:B:67:SER:O	2:B:67:SER:OG	2.31	0.44
1:A:208:ARG:HA	1:A:211:TRP:CE2	2.53	0.43
1:A:227:LEU:HD21	1:A:303:ILE:HG21	2.00	0.43
4:R:833:PHE:O	4:R:837:PHE:HB2	2.18	0.43
2:B:225:HIS:NE2	2:B:243:THR:OG1	2.41	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:289:TYR:HE2	2:B:295:ASN:HB2	1.84	0.43
2:B:42:ARG:NH1	2:B:44:GLN:HB3	2.34	0.43
1:A:185:VAL:HG22	1:A:200:ASP:HB3	2.02	0.42
1:A:348:LEU:HG	1:A:353:LEU:HD22	2.01	0.42
4:R:618:GLN:HE21	4:R:695:GLN:HB2	1.84	0.42
2:B:198:LEU:HD12	2:B:210:LEU:HD21	2.00	0.42
2:B:256:ARG:HB3	3:C:28:ILE:HG12	2.01	0.42
2:B:289:TYR:CE2	2:B:295:ASN:HB2	2.54	0.42
2:B:58:ILE:HG13	2:B:334:SER:HA	2.02	0.42
2:B:254:ASP:OD2	3:C:33:ALA:HB1	2.19	0.42
4:R:602:LEU:O	4:R:606:ILE:HG12	2.20	0.42
4:R:615:LYS:HG3	4:R:624:ARG:HG3	2.00	0.42
4:R:709:CYS:HB3	4:R:710:PRO:HD3	2.01	0.42
1:A:10:LYS:HA	1:A:10:LYS:HD2	1.90	0.41
2:B:180:PHE:CE1	2:B:216:GLY:HA2	2.54	0.41
4:R:806:PHE:HE2	4:R:826:LEU:HD12	1.85	0.41
2:B:10:GLU:O	2:B:13:GLN:HG3	2.20	0.41
4:R:623:ARG:O	4:R:627:MET:HG2	2.20	0.41
2:B:275:SER:O	2:B:288:GLY:N	2.36	0.41
2:B:115:GLY:HA3	2:B:146:LEU:HD23	2.02	0.41
2:B:280:LYS:HD2	3:C:47:GLU:O	2.21	0.41
2:B:18:ILE:HD13	2:B:18:ILE:HA	1.93	0.41
2:B:34:THR:OG1	2:B:300:LEU:O	2.28	0.41
2:B:71:VAL:HG21	2:B:112:VAL:HG11	2.03	0.41
2:B:170:ASP:HB3	2:B:173:THR:HG22	2.03	0.41
1:A:33:GLU:OE1	1:A:195:HIS:HB3	2.20	0.41
1:A:36:LEU:N	1:A:197:LYS:O	2.53	0.41
2:B:30:LEU:HB3	2:B:262:MET:HE3	2.02	0.41
1:A:295:THR:OG1	1:A:297:GLU:OE1	2.36	0.40
4:R:669:LEU:HB3	4:R:710:PRO:HB3	2.02	0.40
4:R:836:CYS:O	4:R:840:LEU:HB3	2.21	0.40
1:A:38:LEU:HD21	1:A:46:LYS:HG2	2.03	0.40
2:B:7:LEU:HD23	2:B:7:LEU:HA	1.89	0.40
4:R:572:LEU:HD21	4:R:668:TYR:CE2	2.56	0.40
1:A:194:LEU:HD12	1:A:194:LEU:HA	1.97	0.40
4:R:789:VAL:O	4:R:793:LEU:HD23	2.22	0.40
2:B:259:GLN:HG2	2:B:260:GLU:N	2.37	0.40
4:R:668:TYR:HD1	4:R:668:TYR:HA	1.77	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	203/241 (84%)	197 (97%)	6 (3%)	0	100	100
2	B	337/351 (96%)	330 (98%)	7 (2%)	0	100	100
3	C	54/71 (76%)	53 (98%)	1 (2%)	0	100	100
4	R	284/674 (42%)	277 (98%)	7 (2%)	0	100	100
All	All	878/1337 (66%)	857 (98%)	21 (2%)	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	183/208 (88%)	183 (100%)	0	100	100
2	B	277/293 (94%)	277 (100%)	0	100	100
3	C	43/58 (74%)	42 (98%)	1 (2%)	45	75
4	R	236/591 (40%)	236 (100%)	0	100	100
All	All	739/1150 (64%)	738 (100%)	1 (0%)	92	98

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	24	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

### 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 ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	CLR	R	901	-	31,31,31	0.29	0	48,48,48	0.40	0
6	K6G	R	902	-	32,32,32	1.00	2 (6%)	37,39,39	0.68	1 (2%)

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
5	CLR	R	901	-	-	0/10/68/68	0/4/4/4
6	K6G	R	902	-	-	25/34/34/34	-

All (2) bond length outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	902	K6G	O1-C15	2.35	1.40	1.33
6	R	902	K6G	O1-C16	-2.14	1.40	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	902	K6G	O1-C15-C14	2.53	119.86	111.91

There are no chirality outliers.

All (25) torsion outliers are listed below:

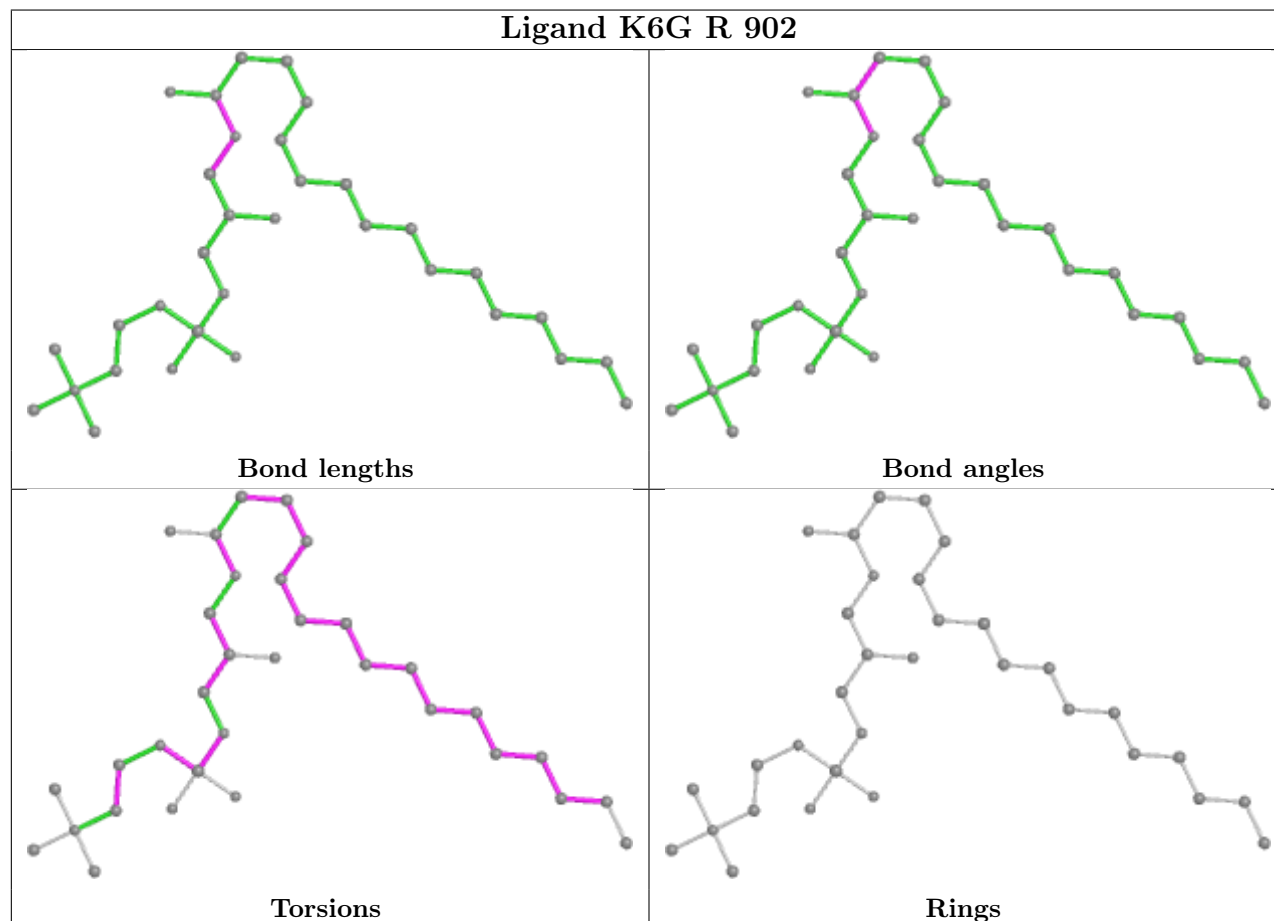
Mol	Chain	Res	Type	Atoms
6	R	902	K6G	C19-O2-P1-O4
6	R	902	K6G	C19-O2-P1-O5
6	R	902	K6G	C21-O3-P1-O2
6	R	902	K6G	C21-O3-P1-O4
6	R	902	K6G	C21-O3-P1-O5
6	R	902	K6G	O-C15-O1-C16
6	R	902	K6G	C14-C15-O1-C16
6	R	902	K6G	C7-C8-C9-C10
6	R	902	K6G	C5-C6-C7-C8
6	R	902	K6G	C3-C4-C5-C6
6	R	902	K6G	C9-C10-C11-C12
6	R	902	K6G	C19-O2-P1-O3
6	R	902	K6G	C1-C2-C3-C4
6	R	902	K6G	C10-C11-C12-C13
6	R	902	K6G	O1-C16-C17-O6
6	R	902	K6G	C12-C13-C14-C15
6	R	902	K6G	C11-C10-C9-C8
6	R	902	K6G	C2-C3-C4-C5
6	R	902	K6G	C18-C1-C2-C3
6	R	902	K6G	O3-C21-C22-N1
6	R	902	K6G	C6-C7-C8-C9
6	R	902	K6G	O6-C17-C19-O2
6	R	902	K6G	C4-C5-C6-C7
6	R	902	K6G	C11-C12-C13-C14
6	R	902	K6G	O1-C16-C17-C19

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

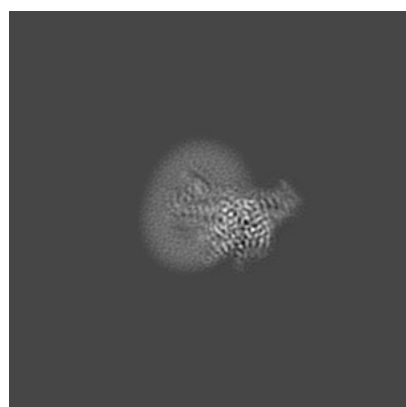
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32820. These allow visual inspection of the internal detail of the map and identification of artifacts.

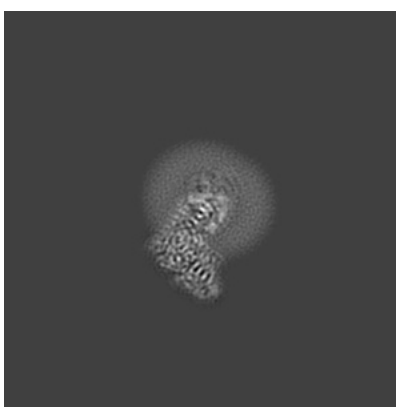
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

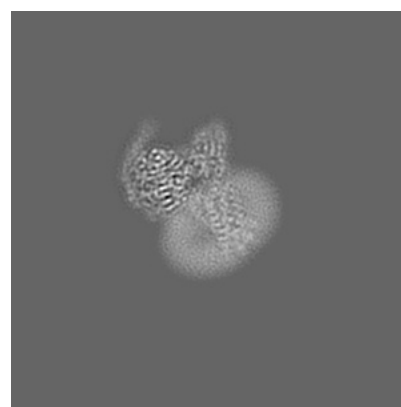
#### 6.1.1 Primary map



X



Y

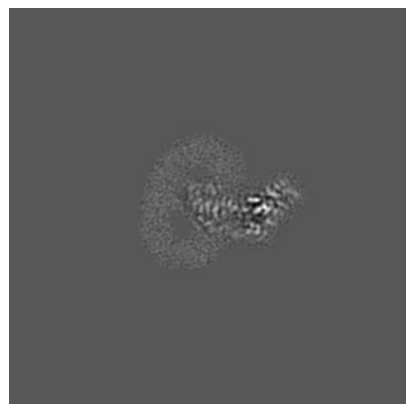


Z

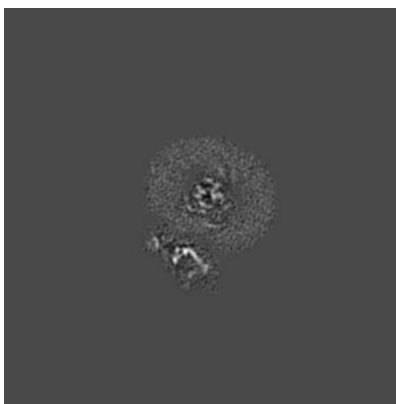
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



X Index: 128



Y Index: 128

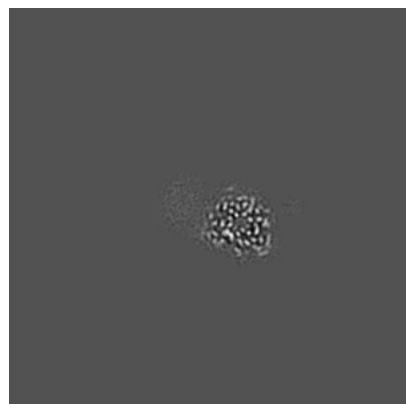


Z Index: 128

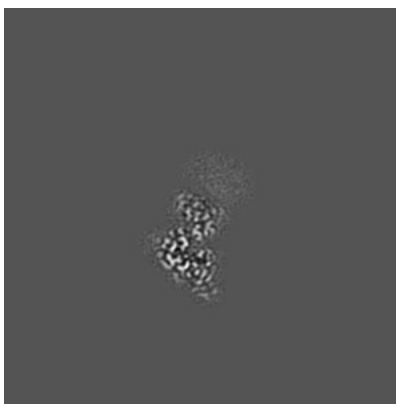
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

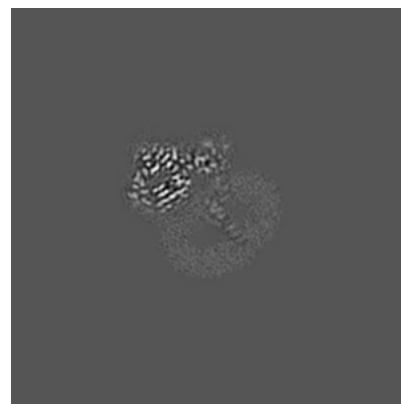
### 6.3.1 Primary map



X Index: 96



Y Index: 152

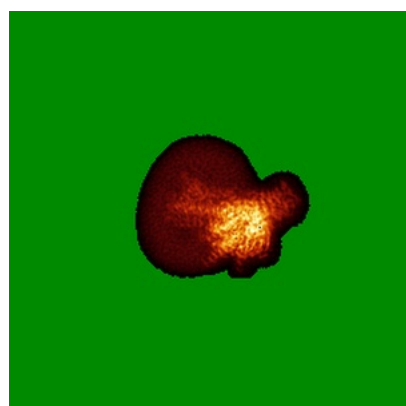


Z Index: 117

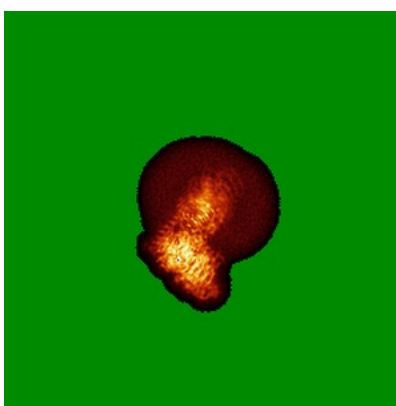
The images above show the largest variance slices of the map in three orthogonal directions.

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

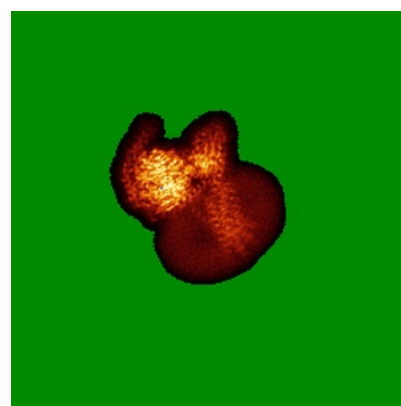
### 6.4.1 Primary map



X



Y

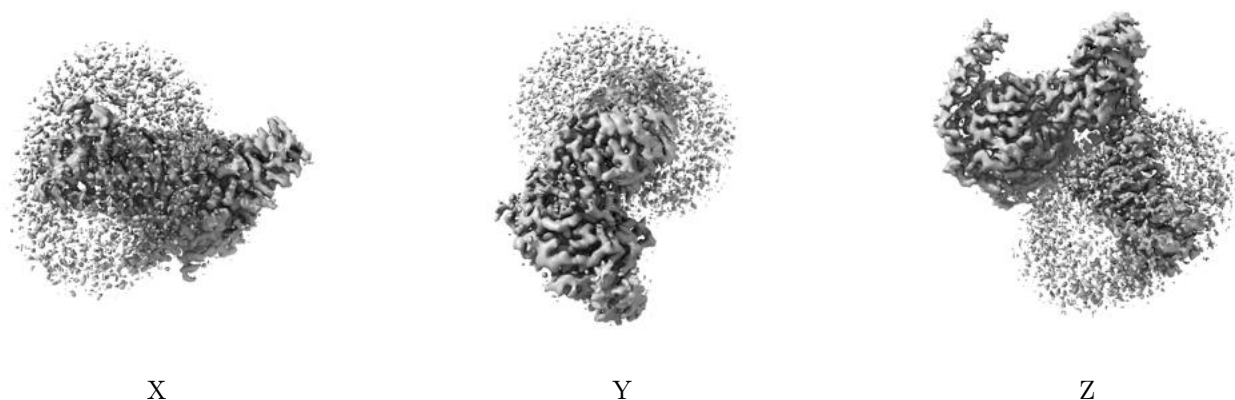


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.0115. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

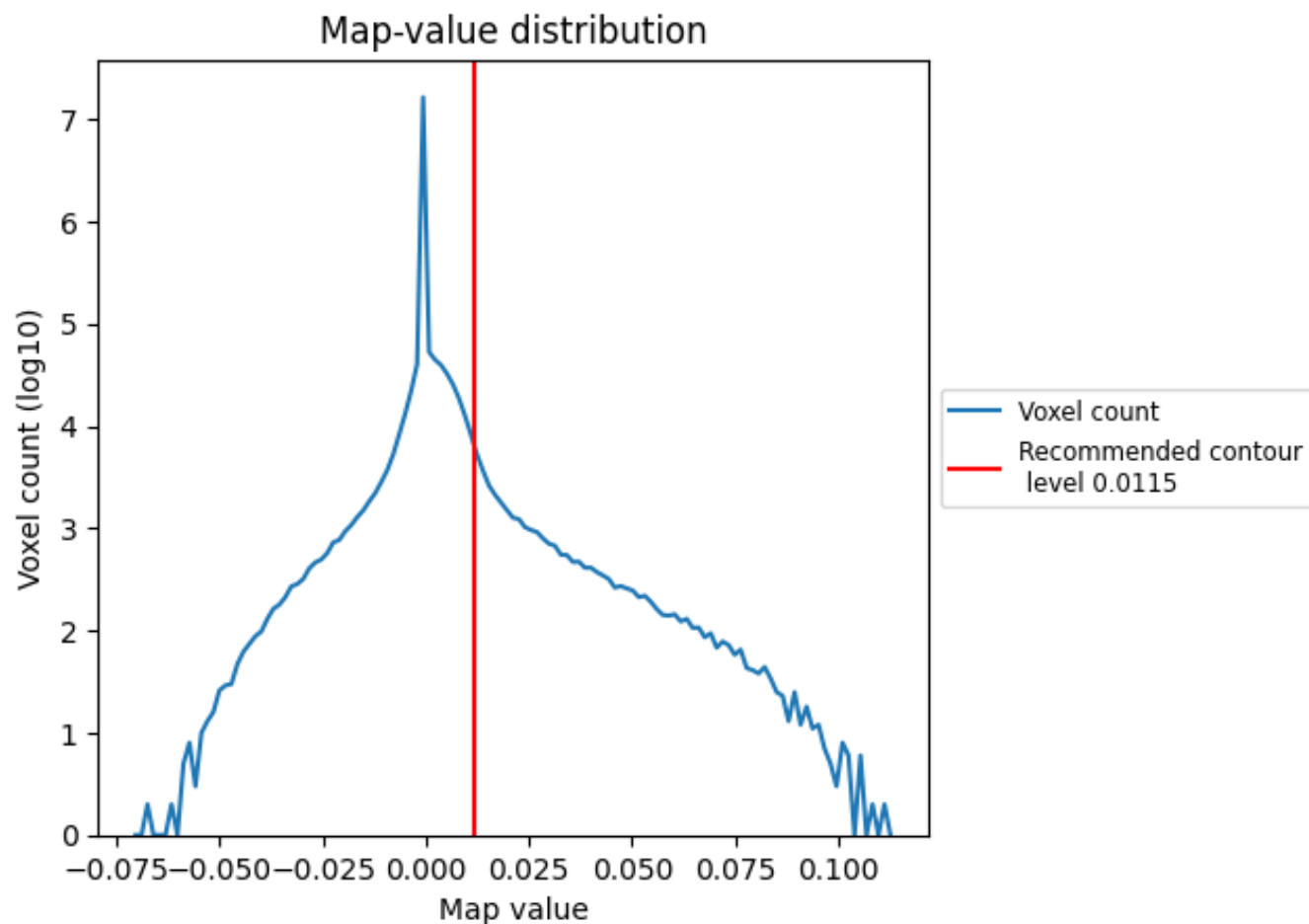
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

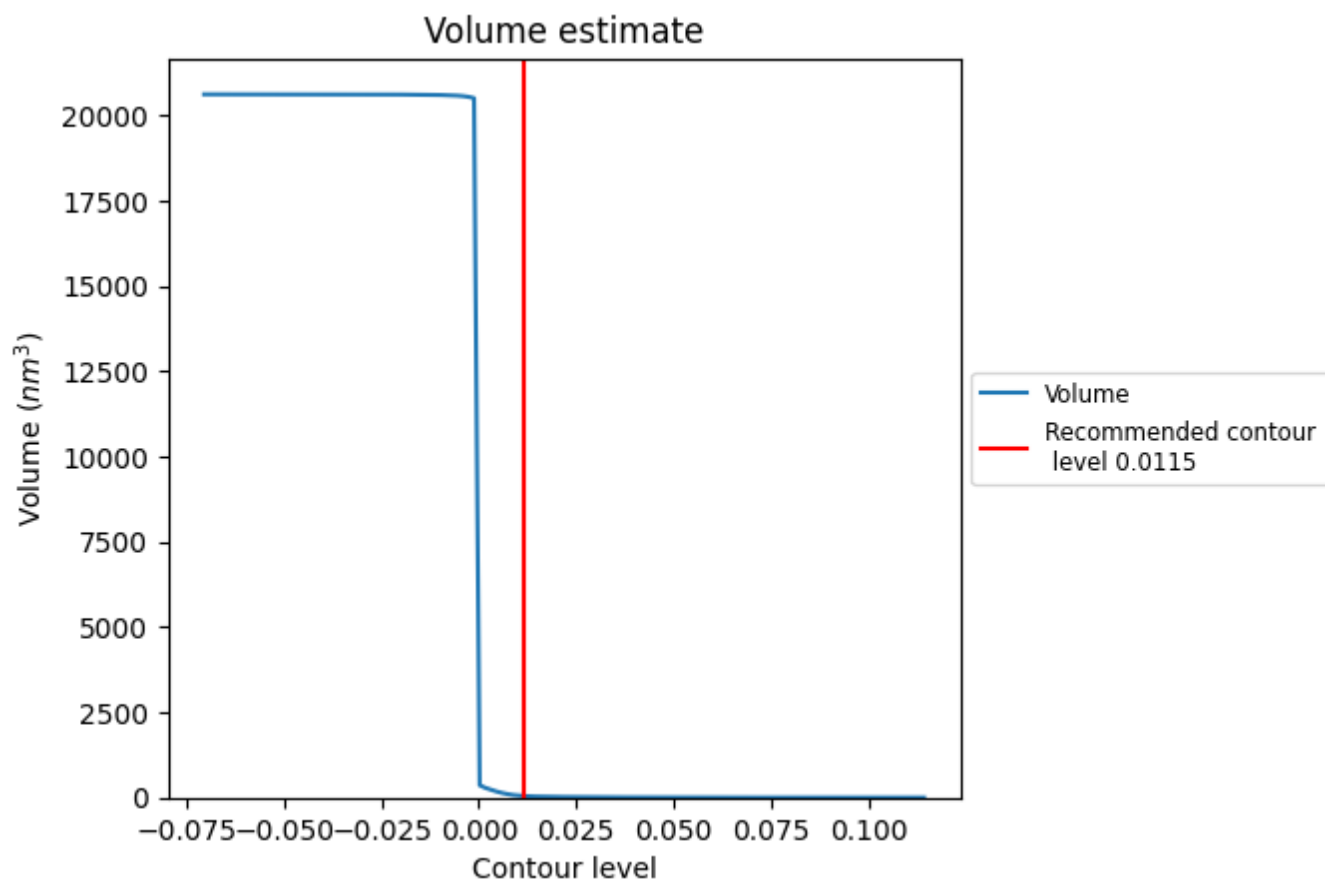
This section contains the results of statistical analysis of the map.

### 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.

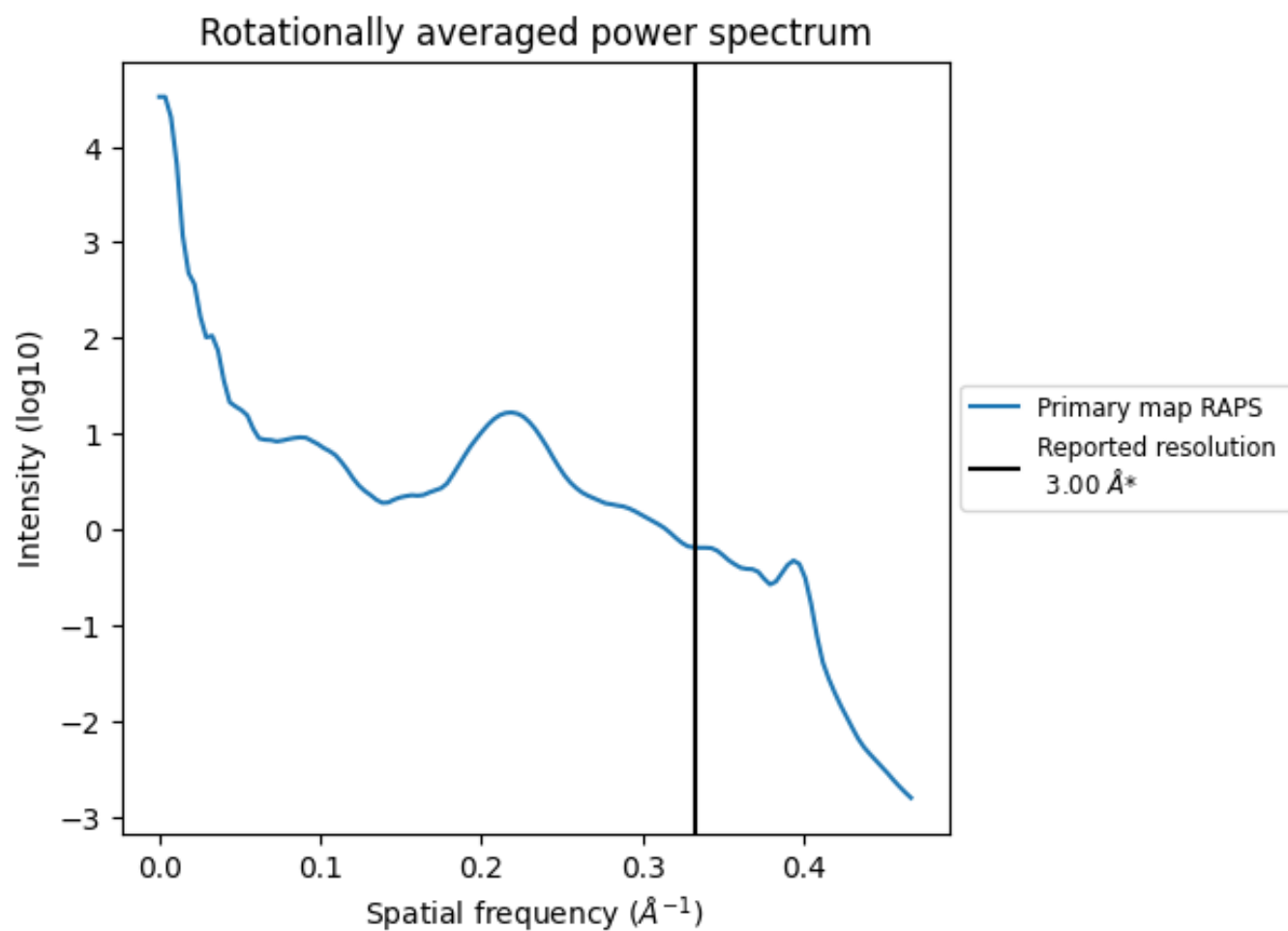
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 46  $\text{nm}^3$ ; this corresponds to an approximate mass of 41 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 0.333 Å<sup>-1</sup>



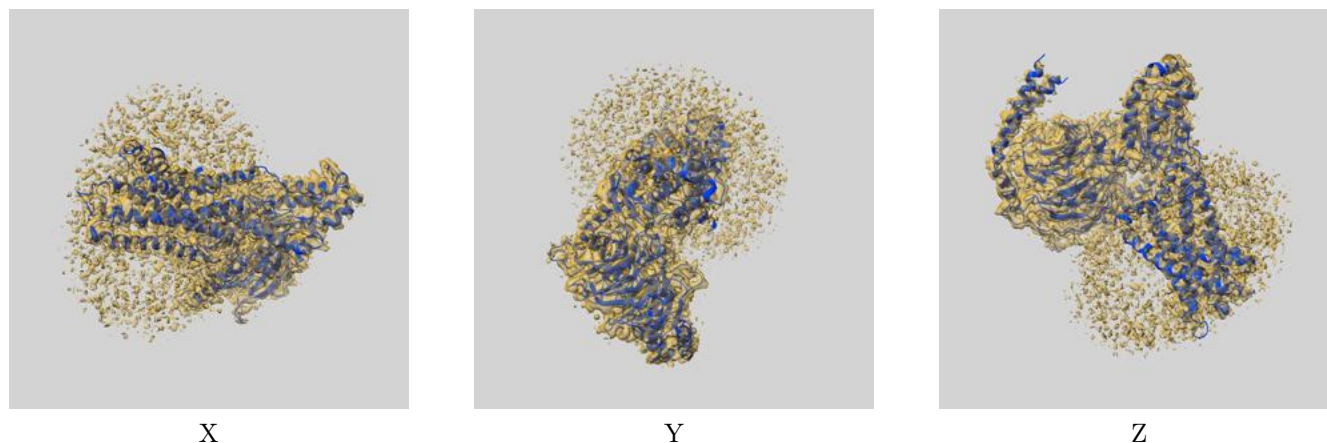
## 8 Fourier-Shell correlation

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

## 9 Map-model fit [i](#)

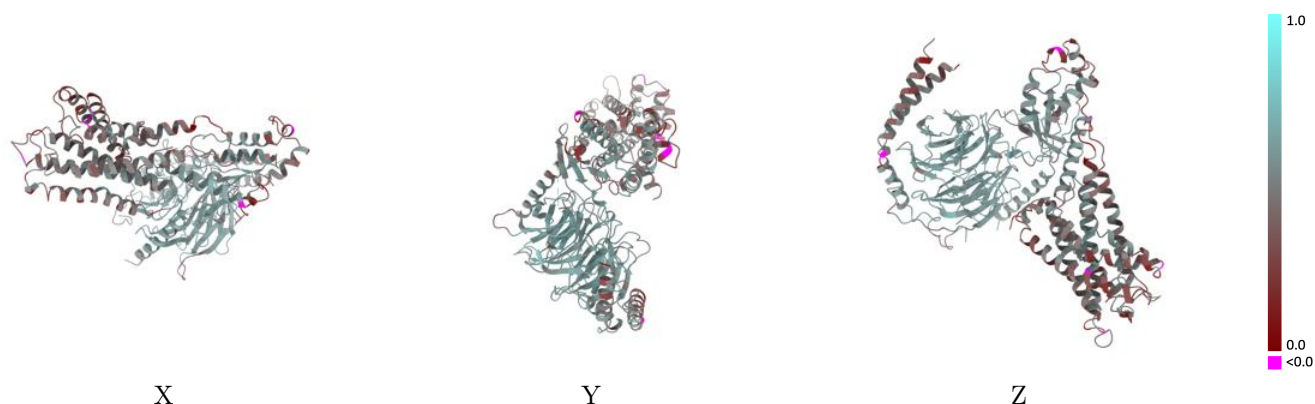
This section contains information regarding the fit between EMDB map EMD-32820 and PDB model 7WU5. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

### 9.1 Map-model overlay [i](#)



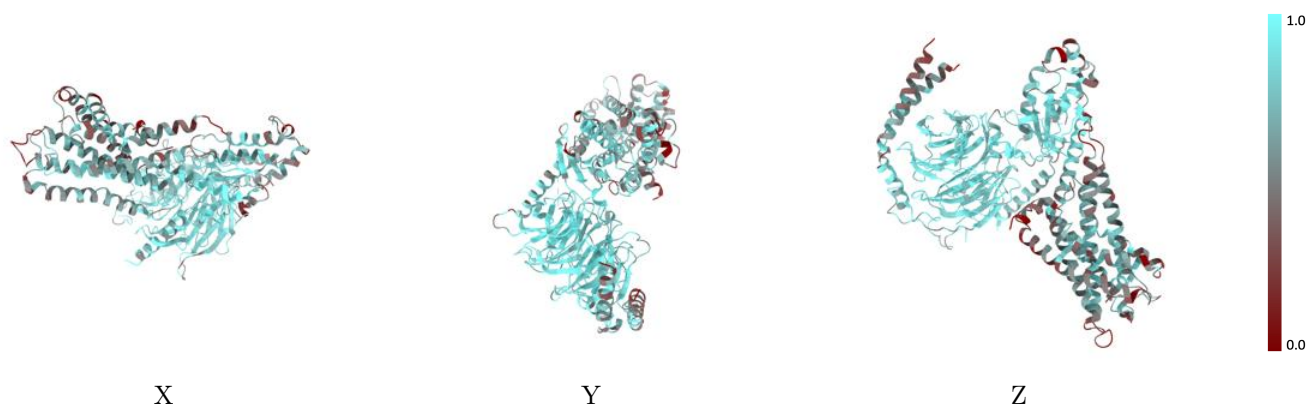
The images above show the 3D surface view of the map at the recommended contour level 0.0115 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



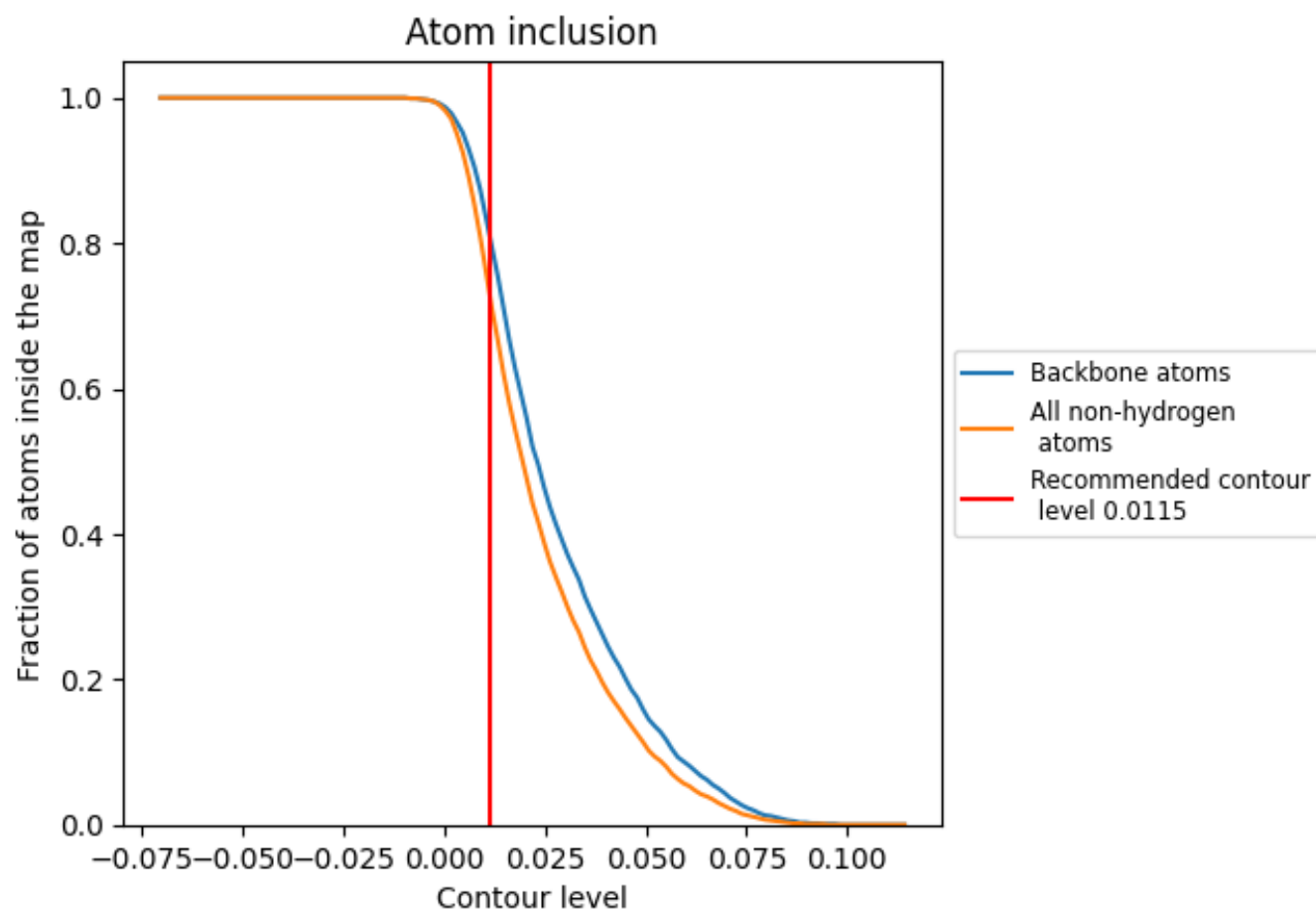
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0115).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 72% 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 (0.0115) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7220	<div></div> 0.4920
A	<div></div> 0.7490	<div></div> 0.4980
B	<div></div> 0.8500	<div></div> 0.5630
C	<div></div> 0.6940	<div></div> 0.4900
R	<div></div> 0.5630	<div></div> 0.4060

