



# wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 06:09 AM EDT

PDB ID : 7MTA  
EMDB ID : EMD-23979  
Title : Rhodopsin kinase (GRK1)-S5E/S488E/T489E in complex with rhodopsin and Fab1  
Authors : Chen, Q.; Chen, C.-L.; Tesmer, J.J.G.  
Deposited on : 2021-05-13  
Resolution : 4.10 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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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 : 2022.3.0, CSD as543be (2022)  
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

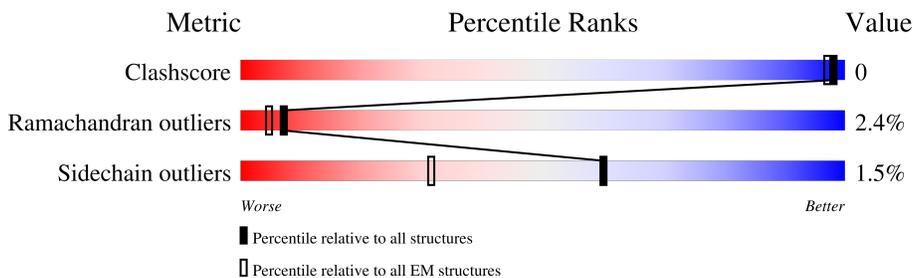
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.10 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  $\leq 5\%$ .

Mol	Chain	Length	Quality of chain
1	1-G	543	60% (Green), 36% (Grey), 2% (Yellow), 2% (Orange), 0% (Red)
1	2-G	543	60% (Green), 36% (Grey), 2% (Yellow), 2% (Orange), 0% (Red)
1	3-G	543	60% (Green), 36% (Grey), 2% (Yellow), 2% (Orange), 0% (Red)
1	4-G	543	61% (Green), 36% (Grey), 2% (Yellow), 1% (Orange), 0% (Red)
1	5-G	543	61% (Green), 36% (Grey), 2% (Yellow), 1% (Orange), 0% (Red)
1	6-G	543	61% (Green), 36% (Grey), 2% (Yellow), 1% (Orange), 0% (Red)
2	1-H	234	92% (Green), 5% (Grey), 2% (Yellow), 1% (Orange), 0% (Red)
2	2-H	234	91% (Green), 5% (Grey), 2% (Yellow), 1% (Orange), 0% (Red)
2	3-H	234	91% (Green), 5% (Grey), 2% (Yellow), 1% (Orange), 0% (Red)

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Mol	Chain	Length	Quality of chain
2	4-H	234	 92% • 5%
2	5-H	234	 91% • 5%
2	6-H	234	 92% • 5%
3	1-L	217	 92% 6% ••
3	2-L	217	 92% 6% ••
3	3-L	217	 92% 6% ••
3	4-L	217	 91% 7% ••
3	5-L	217	 93% 6% ••
3	6-L	217	 92% 6% •
4	1-R	348	 89% • 7%
4	2-R	348	 91% • 7%
4	3-R	348	 90% • 7%
4	4-R	348	 89% • 7%
4	5-R	348	 88% 5% 7%
4	6-R	348	 89% • 7%

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 52194 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 Rhodopsin kinase GRK1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1-G	346	2746	1756	470	507	13	0	0
1	2-G	346	2746	1756	470	507	13	0	0
1	3-G	346	2746	1756	470	507	13	0	0
1	4-G	346	2746	1756	470	507	13	0	0
1	5-G	346	2746	1756	470	507	13	0	0
1	6-G	346	2746	1756	470	507	13	0	0

There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	5	GLU	SER	engineered mutation	UNP P28327
G	488	GLU	SER	engineered mutation	UNP P28327
G	489	GLU	THR	engineered mutation	UNP P28327
G	536	VAL	-	expression tag	UNP P28327
G	537	ASP	-	expression tag	UNP P28327
G	538	HIS	-	expression tag	UNP P28327
G	539	HIS	-	expression tag	UNP P28327
G	540	HIS	-	expression tag	UNP P28327
G	541	HIS	-	expression tag	UNP P28327
G	542	HIS	-	expression tag	UNP P28327
G	543	HIS	-	expression tag	UNP P28327

- Molecule 2 is a protein called Fab1 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1-H	223	1676	1064	276	331	5	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	2-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	3-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	4-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	5-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		
2	6-H	223	Total	C	N	O	S	0	0
			1676	1064	276	331	5		

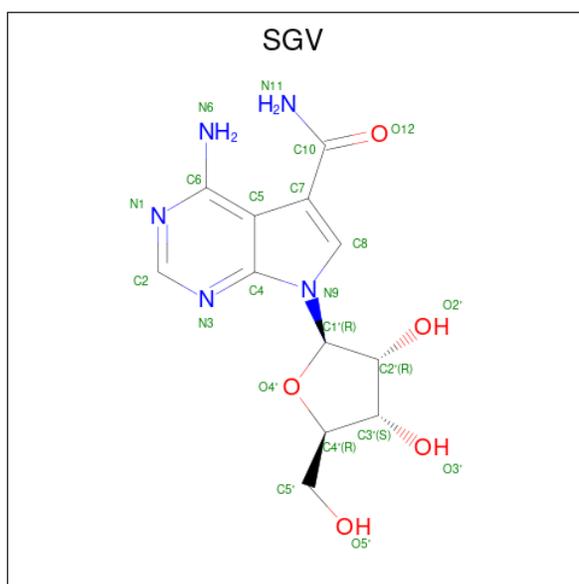
- Molecule 3 is a protein called Fab1 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	1-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	2-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	3-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	4-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	5-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		
3	6-L	215	Total	C	N	O	S	0	0
			1660	1043	276	336	5		

- Molecule 4 is a protein called Rhodopsin.

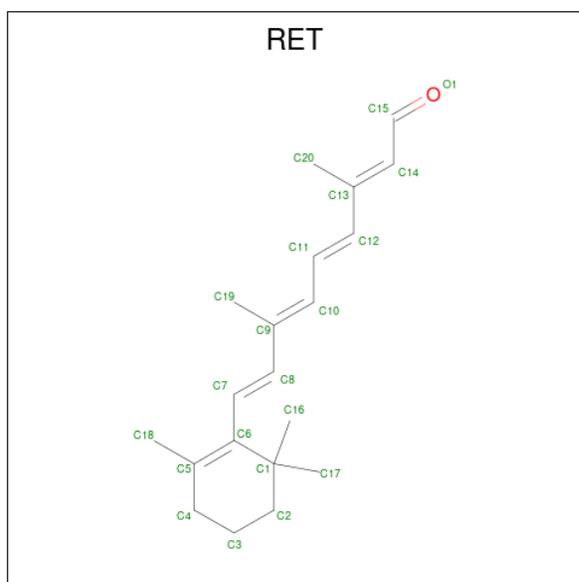
Mol	Chain	Residues	Atoms					AltConf	Trace
4	1-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	2-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	3-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	4-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	5-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		
4	6-R	324	Total	C	N	O	S	0	0
			2575	1715	396	438	26		

- Molecule 5 is SANGIVAMYCIN (three-letter code: SGV) (formula:  $C_{12}H_{15}N_5O_5$ ).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
5	1-G	1	Total	C	N	O	0
			22	12	5	5	
5	2-G	1	Total	C	N	O	0
			22	12	5	5	
5	3-G	1	Total	C	N	O	0
			22	12	5	5	
5	4-G	1	Total	C	N	O	0
			22	12	5	5	
5	5-G	1	Total	C	N	O	0
			22	12	5	5	
5	6-G	1	Total	C	N	O	0
			22	12	5	5	

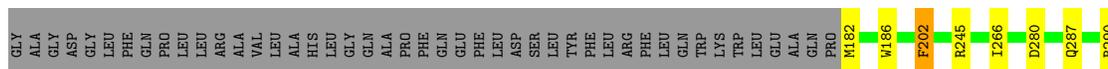
- Molecule 6 is RETINAL (three-letter code: RET) (formula:  $C_{20}H_{28}O$ ).



Mol	Chain	Residues	Atoms	AltConf
6	1-R	1	Total C 20 20	0
6	2-R	1	Total C 20 20	0
6	3-R	1	Total C 20 20	0
6	4-R	1	Total C 20 20	0
6	5-R	1	Total C 20 20	0
6	6-R	1	Total C 20 20	0







• Molecule 2: Fab1 Heavy chain



• Molecule 2: Fab1 Heavy chain



• Molecule 2: Fab1 Heavy chain



• Molecule 2: Fab1 Heavy chain



• Molecule 2: Fab1 Heavy chain



• Molecule 2: Fab1 Heavy chain



• Molecule 3: Fab1 Light chain

Chain 1-L:  92% 6% ..



• Molecule 3: Fab1 Light chain

Chain 2-L:  92% 6% ..



• Molecule 3: Fab1 Light chain

Chain 3-L:  92% 6% ..



• Molecule 3: Fab1 Light chain

Chain 4-L:  91% 7% ..



• Molecule 3: Fab1 Light chain

Chain 5-L:  93% 6% ..



• Molecule 3: Fab1 Light chain

Chain 6-L:  92% 6% .



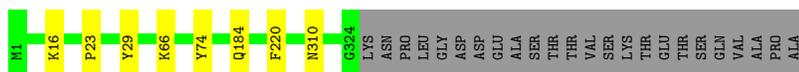
• Molecule 4: Rhodopsin

Chain 1-R:  89% . 7%



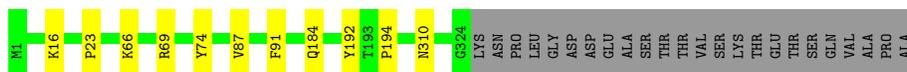
• Molecule 4: Rhodopsin

Chain 2-R:  91% 7%



• Molecule 4: Rhodopsin

Chain 3-R:  90% 7%



• Molecule 4: Rhodopsin

Chain 4-R:  89% 7%



• Molecule 4: Rhodopsin

Chain 5-R:  88% 5% 7%



• Molecule 4: Rhodopsin

Chain 6-R:  89% 7%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	310363	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 ( $e^-/\text{\AA}^2$ )	54	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.583	Depositor
Minimum map value	-2.566	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.49	Depositor
Map size ( $\text{\AA}$ )	432.00003, 432.00003, 432.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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: SGV, RET

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	1-G	0.92	0/2803	1.02	8/3771 (0.2%)
1	2-G	0.92	0/2803	1.00	3/3771 (0.1%)
1	3-G	0.92	0/2803	1.02	4/3771 (0.1%)
1	4-G	0.92	0/2803	1.01	6/3771 (0.2%)
1	5-G	0.92	0/2803	1.00	3/3771 (0.1%)
1	6-G	0.92	0/2803	1.01	6/3771 (0.2%)
2	1-H	0.90	0/1722	1.04	2/2354 (0.1%)
2	2-H	0.90	0/1722	1.04	1/2354 (0.0%)
2	3-H	0.90	0/1722	1.04	2/2354 (0.1%)
2	4-H	0.90	0/1722	1.05	1/2354 (0.0%)
2	5-H	0.90	0/1722	1.03	2/2354 (0.1%)
2	6-H	0.90	0/1722	1.05	3/2354 (0.1%)
3	1-L	0.91	0/1697	1.05	3/2304 (0.1%)
3	2-L	0.91	0/1697	1.08	5/2304 (0.2%)
3	3-L	0.91	0/1697	1.06	2/2304 (0.1%)
3	4-L	0.91	0/1697	1.09	3/2304 (0.1%)
3	5-L	0.91	0/1697	1.07	5/2304 (0.2%)
3	6-L	0.91	0/1697	1.07	2/2304 (0.1%)
4	1-R	0.88	0/2657	0.92	4/3621 (0.1%)
4	2-R	0.88	0/2657	0.91	4/3621 (0.1%)
4	3-R	0.88	0/2657	0.91	2/3621 (0.1%)
4	4-R	0.88	0/2657	0.91	4/3621 (0.1%)
4	5-R	0.87	0/2657	0.91	4/3621 (0.1%)
4	6-R	0.88	0/2657	0.92	4/3621 (0.1%)
All	All	0.90	0/53274	1.00	83/72300 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	1-G	0	1
1	2-G	0	1
1	3-G	0	1
1	4-G	0	1
1	5-G	0	1
1	6-G	0	1
2	1-H	0	1
2	2-H	0	1
2	3-H	0	1
2	4-H	0	1
2	5-H	0	2
2	6-H	0	1
3	1-L	0	1
3	2-L	0	3
3	3-L	0	1
3	4-L	0	2
3	5-L	0	1
3	6-L	0	1
4	4-R	0	1
4	6-R	0	1
All	All	0	24

There are no bond length outliers.

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	4-G	312	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	2-G	312	TYR	CB-CG-CD2	-7.49	116.50	121.00
1	1-G	202	PHE	CB-CG-CD1	7.39	125.98	120.80
1	5-G	312	TYR	CB-CG-CD2	-7.38	116.57	121.00
1	2-G	312	TYR	CB-CG-CD1	7.34	125.41	121.00

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1-G	182	MET	Peptide
2	1-H	102	TYR	Sidechain
3	1-L	95	TRP	Peptide
1	2-G	182	MET	Peptide
2	2-H	102	TYR	Sidechain

## 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	1-G	2746	0	2727	3	0
1	2-G	2746	0	2727	2	0
1	3-G	2746	0	2727	1	0
1	4-G	2746	0	2727	1	0
1	5-G	2746	0	2727	2	0
1	6-G	2746	0	2727	1	0
2	1-H	1676	0	1613	1	0
2	2-H	1676	0	1613	1	0
2	3-H	1676	0	1613	1	0
2	4-H	1676	0	1613	0	0
2	5-H	1676	0	1613	0	0
2	6-H	1676	0	1613	0	0
3	1-L	1660	0	1611	1	0
3	2-L	1660	0	1611	0	0
3	3-L	1660	0	1611	1	0
3	4-L	1660	0	1611	1	0
3	5-L	1660	0	1611	0	0
3	6-L	1660	0	1611	0	0
4	1-R	2575	0	2550	3	0
4	2-R	2575	0	2550	1	0
4	3-R	2575	0	2550	3	0
4	4-R	2575	0	2550	1	0
4	5-R	2575	0	2550	4	0
4	6-R	2575	0	2550	1	0
5	1-G	22	0	15	0	0
5	2-G	22	0	15	0	0
5	3-G	22	0	15	0	0
5	4-G	22	0	15	0	0
5	5-G	22	0	15	0	0
5	6-G	22	0	15	0	0
6	1-R	20	0	27	2	0
6	2-R	20	0	27	2	0
6	3-R	20	0	27	2	0
6	4-R	20	0	27	1	0
6	5-R	20	0	27	2	0
6	6-R	20	0	27	2	0
All	All	52194	0	51258	35	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 0.

The worst 5 of 35 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)
6:R:401:RET:H181	6:R:401:RET:H8	1.78	0.64
6:R:401:RET:H181	6:R:401:RET:C8	2.33	0.57
6:R:401:RET:H181	6:R:401:RET:C8	2.35	0.56
6:R:401:RET:H181	6:R:401:RET:C8	2.35	0.56
6:R:401:RET:H181	6:R:401:RET:C8	2.36	0.55

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	1-G	342/543 (63%)	315 (92%)	17 (5%)	10 (3%)	3	27
1	2-G	342/543 (63%)	314 (92%)	19 (6%)	9 (3%)	4	29
1	3-G	342/543 (63%)	315 (92%)	19 (6%)	8 (2%)	5	31
1	4-G	342/543 (63%)	321 (94%)	16 (5%)	5 (2%)	8	40
1	5-G	342/543 (63%)	320 (94%)	16 (5%)	6 (2%)	7	36
1	6-G	342/543 (63%)	316 (92%)	21 (6%)	5 (2%)	8	40
2	1-H	221/234 (94%)	201 (91%)	17 (8%)	3 (1%)	9	40
2	2-H	221/234 (94%)	203 (92%)	14 (6%)	4 (2%)	7	36
2	3-H	221/234 (94%)	208 (94%)	10 (4%)	3 (1%)	9	40
2	4-H	221/234 (94%)	200 (90%)	16 (7%)	5 (2%)	5	31
2	5-H	221/234 (94%)	202 (91%)	13 (6%)	6 (3%)	4	28
2	6-H	221/234 (94%)	208 (94%)	9 (4%)	4 (2%)	7	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	1-L	213/217 (98%)	191 (90%)	14 (7%)	8 (4%)	2	22
3	2-L	213/217 (98%)	191 (90%)	14 (7%)	8 (4%)	2	22
3	3-L	213/217 (98%)	188 (88%)	15 (7%)	10 (5%)	2	19
3	4-L	213/217 (98%)	194 (91%)	10 (5%)	9 (4%)	2	21
3	5-L	213/217 (98%)	192 (90%)	12 (6%)	9 (4%)	2	21
3	6-L	213/217 (98%)	190 (89%)	16 (8%)	7 (3%)	3	25
4	1-R	322/348 (92%)	290 (90%)	25 (8%)	7 (2%)	5	32
4	2-R	322/348 (92%)	296 (92%)	21 (6%)	5 (2%)	8	39
4	3-R	322/348 (92%)	298 (92%)	19 (6%)	5 (2%)	8	39
4	4-R	322/348 (92%)	294 (91%)	19 (6%)	9 (3%)	4	27
4	5-R	322/348 (92%)	296 (92%)	21 (6%)	5 (2%)	8	39
4	6-R	322/348 (92%)	301 (94%)	15 (5%)	6 (2%)	6	35
All	All	6588/8052 (82%)	6044 (92%)	388 (6%)	156 (2%)	7	30

5 of 156 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-G	280	ASP
1	1-G	315	LEU
1	1-G	483	ASP
2	1-H	111	TYR
2	1-H	127	ALA

### 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	1-G	286/449 (64%)	281 (98%)	5 (2%)	56	72
1	2-G	286/449 (64%)	282 (99%)	4 (1%)	62	76
1	3-G	286/449 (64%)	279 (98%)	7 (2%)	44	63
1	4-G	286/449 (64%)	281 (98%)	5 (2%)	56	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	5-G	286/449 (64%)	279 (98%)	7 (2%)	44	63
1	6-G	286/449 (64%)	279 (98%)	7 (2%)	44	63
2	1-H	184/195 (94%)	183 (100%)	1 (0%)	86	90
2	2-H	184/195 (94%)	181 (98%)	3 (2%)	58	74
2	3-H	184/195 (94%)	180 (98%)	4 (2%)	47	65
2	4-H	184/195 (94%)	183 (100%)	1 (0%)	86	90
2	5-H	184/195 (94%)	183 (100%)	1 (0%)	86	90
2	6-H	184/195 (94%)	182 (99%)	2 (1%)	70	80
3	1-L	190/192 (99%)	184 (97%)	6 (3%)	34	55
3	2-L	190/192 (99%)	187 (98%)	3 (2%)	58	74
3	3-L	190/192 (99%)	185 (97%)	5 (3%)	41	61
3	4-L	190/192 (99%)	185 (97%)	5 (3%)	41	61
3	5-L	190/192 (99%)	187 (98%)	3 (2%)	58	74
3	6-L	190/192 (99%)	183 (96%)	7 (4%)	29	52
4	1-R	276/296 (93%)	275 (100%)	1 (0%)	89	91
4	2-R	276/296 (93%)	276 (100%)	0	100	100
4	3-R	276/296 (93%)	275 (100%)	1 (0%)	89	91
4	4-R	276/296 (93%)	274 (99%)	2 (1%)	81	86
4	5-R	276/296 (93%)	273 (99%)	3 (1%)	70	80
4	6-R	276/296 (93%)	272 (99%)	4 (1%)	62	76
All	All	5616/6792 (83%)	5529 (98%)	87 (2%)	60	75

5 of 87 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	5-G	390	ARG
1	6-G	349	TYR
1	5-G	431	ASP
4	5-R	192	TYR
2	6-H	225	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	5-G	275	HIS
3	5-L	192	HIS
1	6-G	275	HIS
4	2-R	100	HIS
4	2-R	55	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

12 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
6	RET	2-R	401	-	20,20,21	2.65	4 (20%)	27,27,28	0.98	1 (3%)
5	SGV	1-G	601	-	22,24,24	1.45	4 (18%)	22,36,36	1.11	2 (9%)
5	SGV	4-G	601	-	22,24,24	1.38	4 (18%)	22,36,36	1.00	1 (4%)
6	RET	1-R	401	-	20,20,21	2.66	3 (15%)	27,27,28	0.88	0
5	SGV	5-G	601	-	22,24,24	1.39	4 (18%)	22,36,36	1.18	3 (13%)
6	RET	3-R	401	-	20,20,21	2.67	4 (20%)	27,27,28	0.86	0
6	RET	4-R	401	-	20,20,21	2.63	4 (20%)	27,27,28	0.89	0
5	SGV	2-G	601	-	22,24,24	1.37	4 (18%)	22,36,36	1.14	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	SGV	6-G	601	-	22,24,24	1.46	4 (18%)	22,36,36	1.07	2 (9%)
6	RET	6-R	401	-	20,20,21	2.66	4 (20%)	27,27,28	0.93	0
6	RET	5-R	401	-	20,20,21	2.64	3 (15%)	27,27,28	0.92	0
5	SGV	3-G	601	-	22,24,24	1.35	4 (18%)	22,36,36	1.11	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RET	2-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	1-G	601	-	-	1/3/26/26	0/3/3/3
5	SGV	4-G	601	-	-	1/3/26/26	0/3/3/3
6	RET	1-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	5-G	601	-	-	1/3/26/26	0/3/3/3
6	RET	3-R	401	-	-	0/13/30/31	0/1/1/1
6	RET	4-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	2-G	601	-	-	1/3/26/26	0/3/3/3
5	SGV	6-G	601	-	-	1/3/26/26	0/3/3/3
6	RET	6-R	401	-	-	0/13/30/31	0/1/1/1
6	RET	5-R	401	-	-	0/13/30/31	0/1/1/1
5	SGV	3-G	601	-	-	1/3/26/26	0/3/3/3

The worst 5 of 46 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	1-R	401	RET	C14-C13	10.45	1.40	1.33
6	3-R	401	RET	C14-C13	10.43	1.40	1.33
6	6-R	401	RET	C14-C13	10.39	1.40	1.33
6	5-R	401	RET	C14-C13	10.34	1.40	1.33
6	2-R	401	RET	C14-C13	10.28	1.40	1.33

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	1-G	601	SGV	C4'-O4'-C1'	-2.84	107.32	109.92
5	6-G	601	SGV	C4'-O4'-C1'	-2.67	107.48	109.92
5	5-G	601	SGV	C5'-C4'-C3'	-2.25	109.78	115.10
6	2-R	401	RET	C2-C1-C6	2.19	113.62	110.44
5	1-G	601	SGV	C7-C10-N11	-2.15	114.94	118.27

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

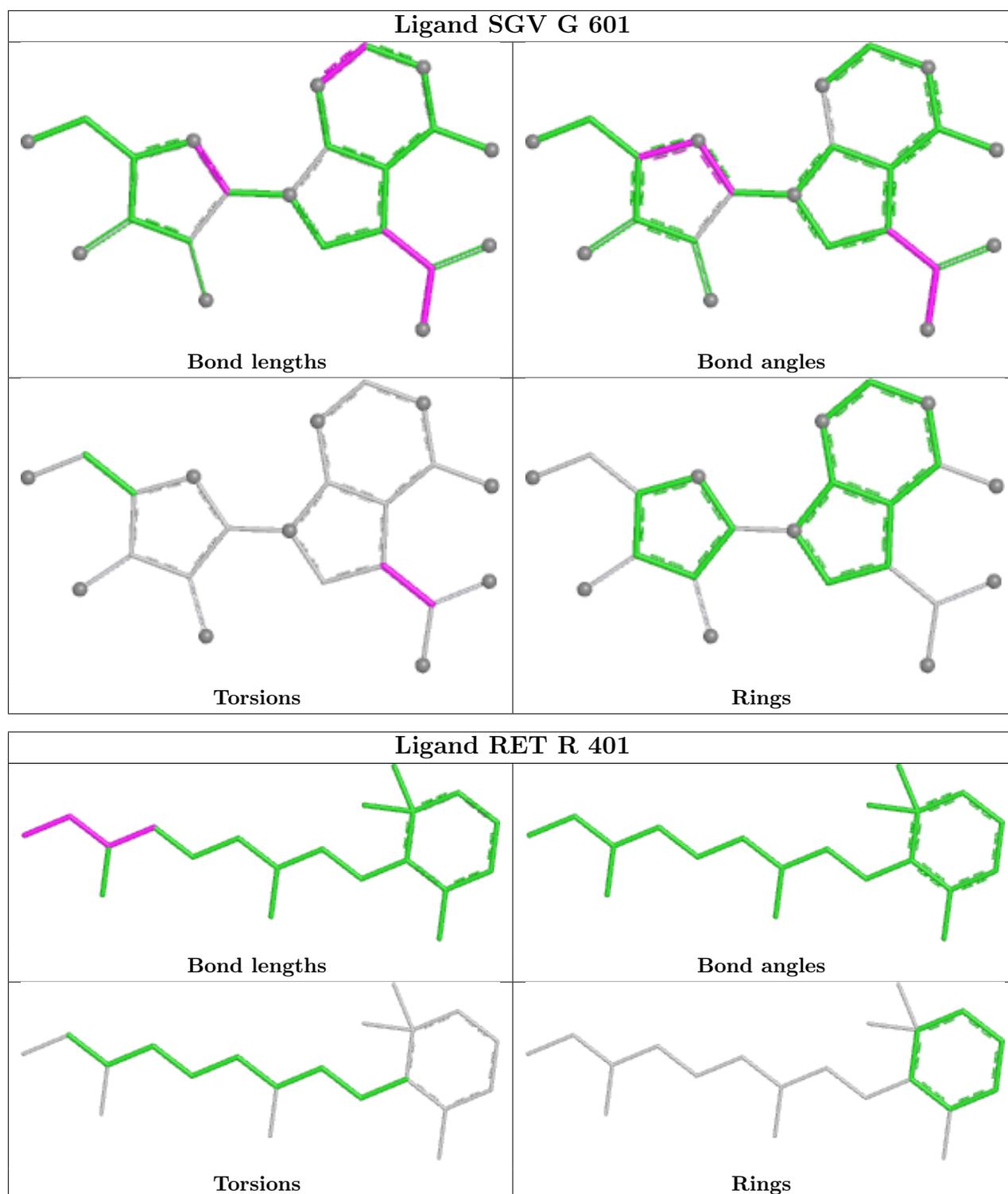
Mol	Chain	Res	Type	Atoms
5	1-G	601	SGV	O12-C10-C7-C8
5	4-G	601	SGV	O12-C10-C7-C8
5	5-G	601	SGV	O12-C10-C7-C8
5	6-G	601	SGV	O12-C10-C7-C8
5	2-G	601	SGV	O12-C10-C7-C8

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	2-R	401	RET	2	0
6	1-R	401	RET	2	0
6	3-R	401	RET	2	0
6	4-R	401	RET	1	0
6	6-R	401	RET	2	0
6	5-R	401	RET	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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

There are no chain breaks in this entry.

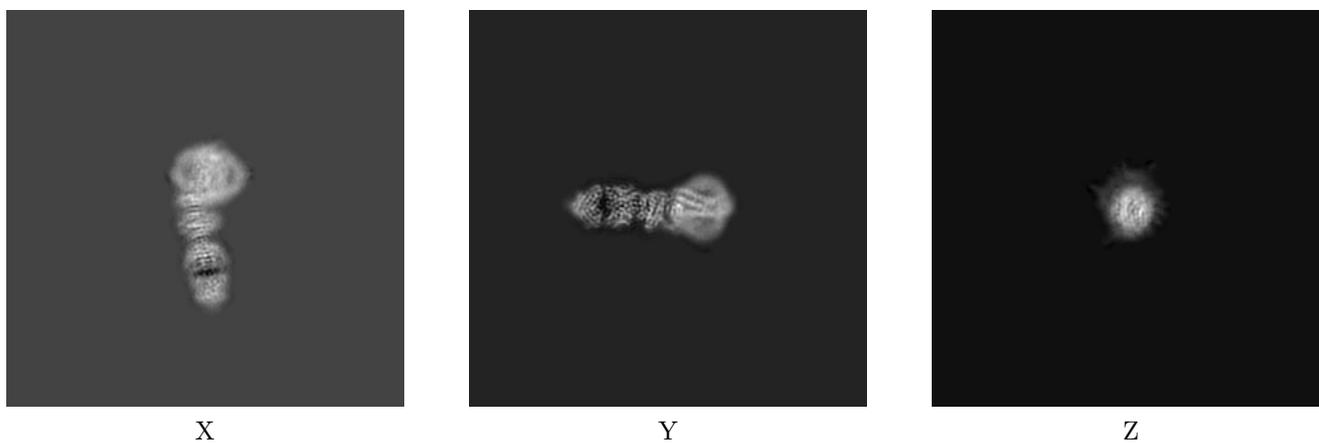
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-23979. 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](#)

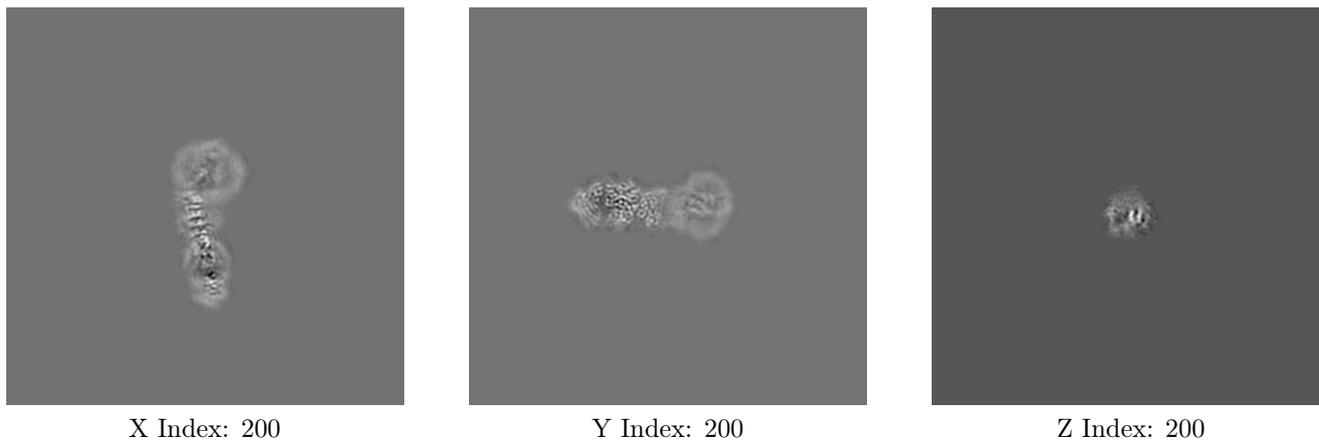
#### 6.1.1 Primary map



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

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

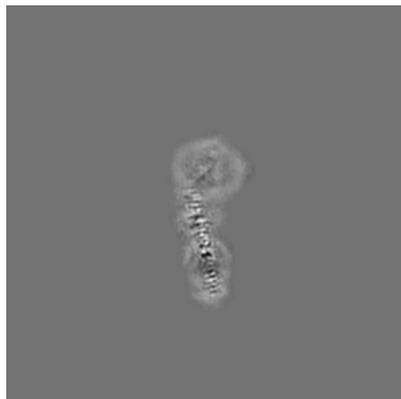
#### 6.2.1 Primary map



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

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

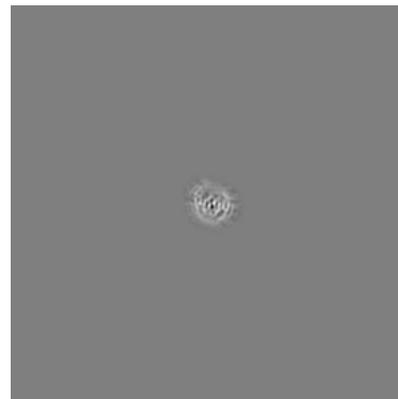
### 6.3.1 Primary map



X Index: 199



Y Index: 197

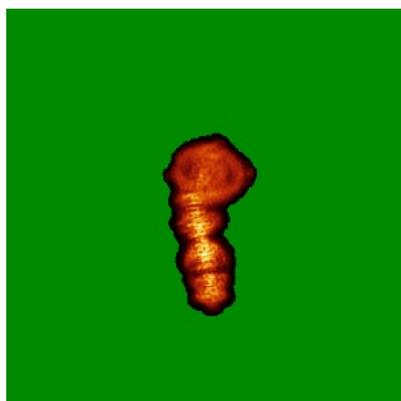


Z Index: 152

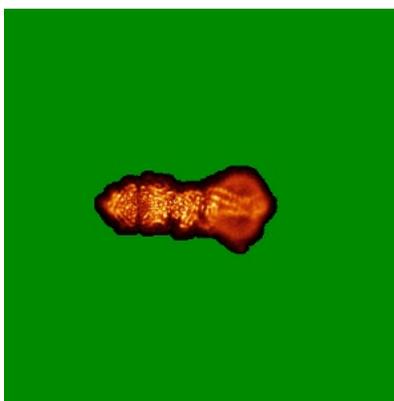
The images above show the largest variance slices of the map in three orthogonal directions.

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

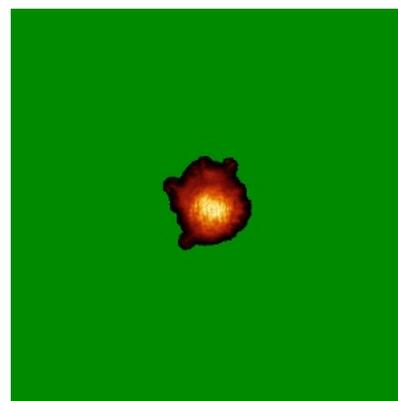
### 6.4.1 Primary map



X



Y



Z

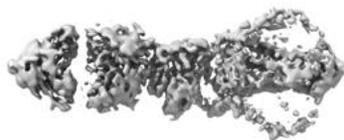
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.49. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

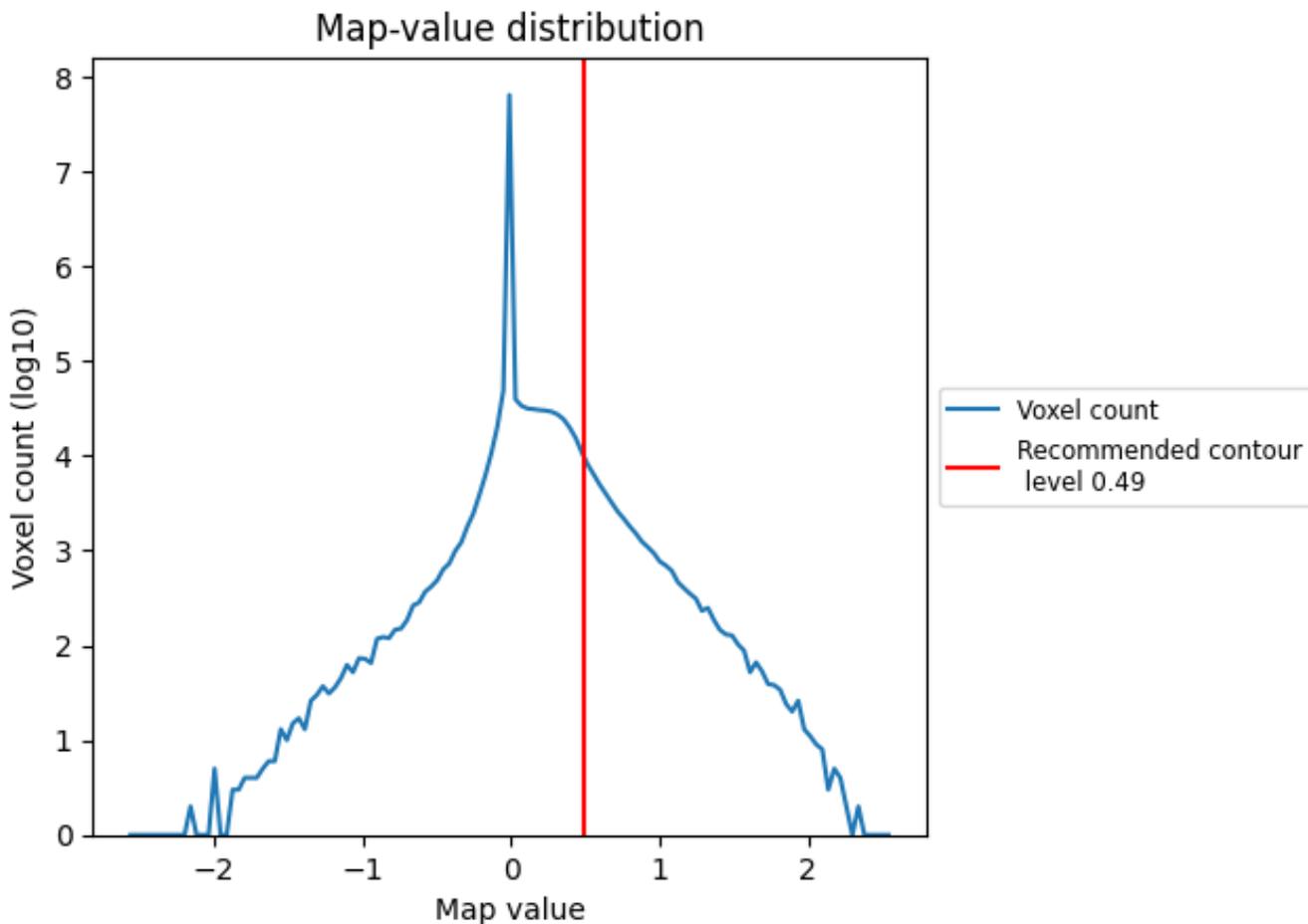
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

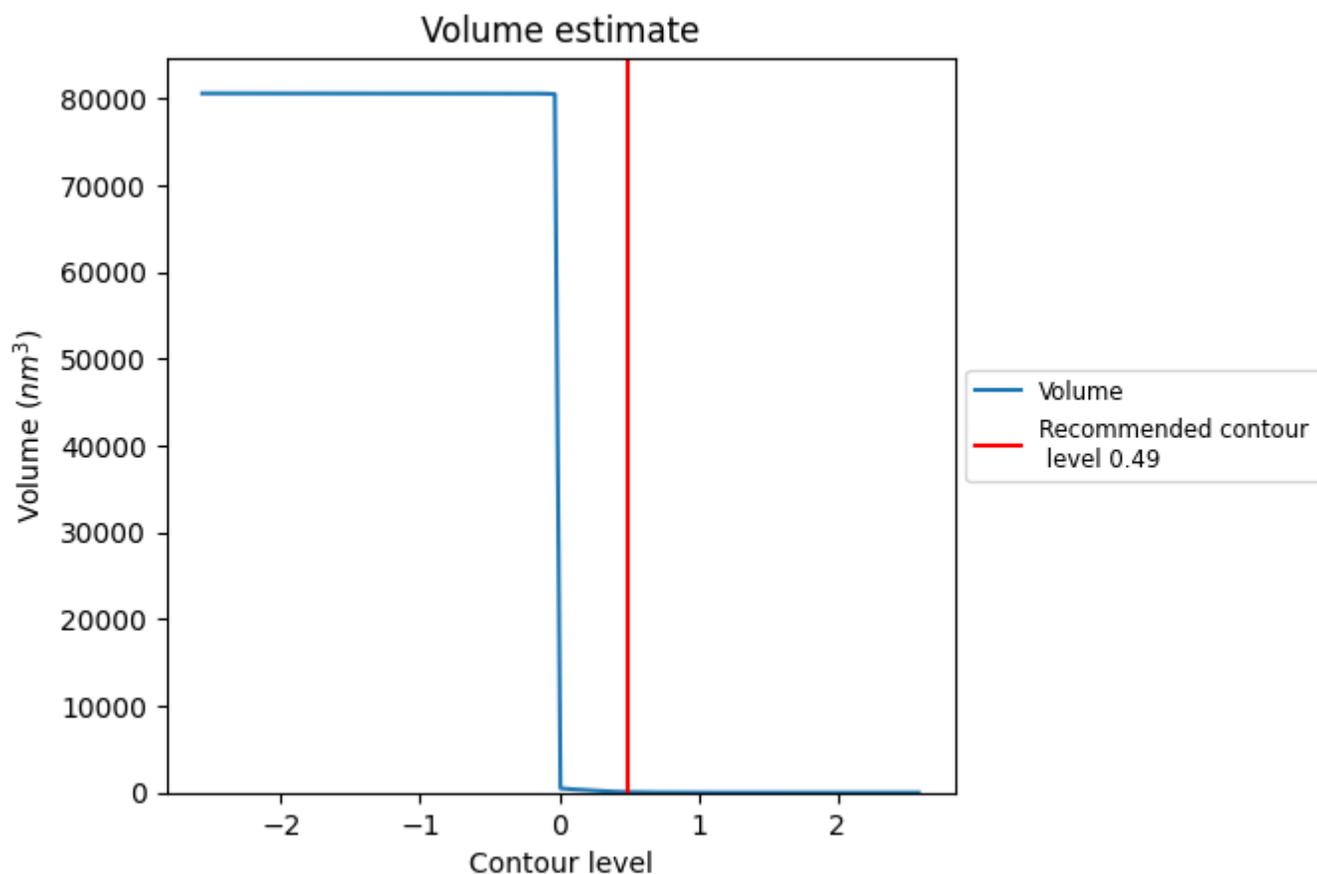
This section contains the results of statistical analysis of the map.

### 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.

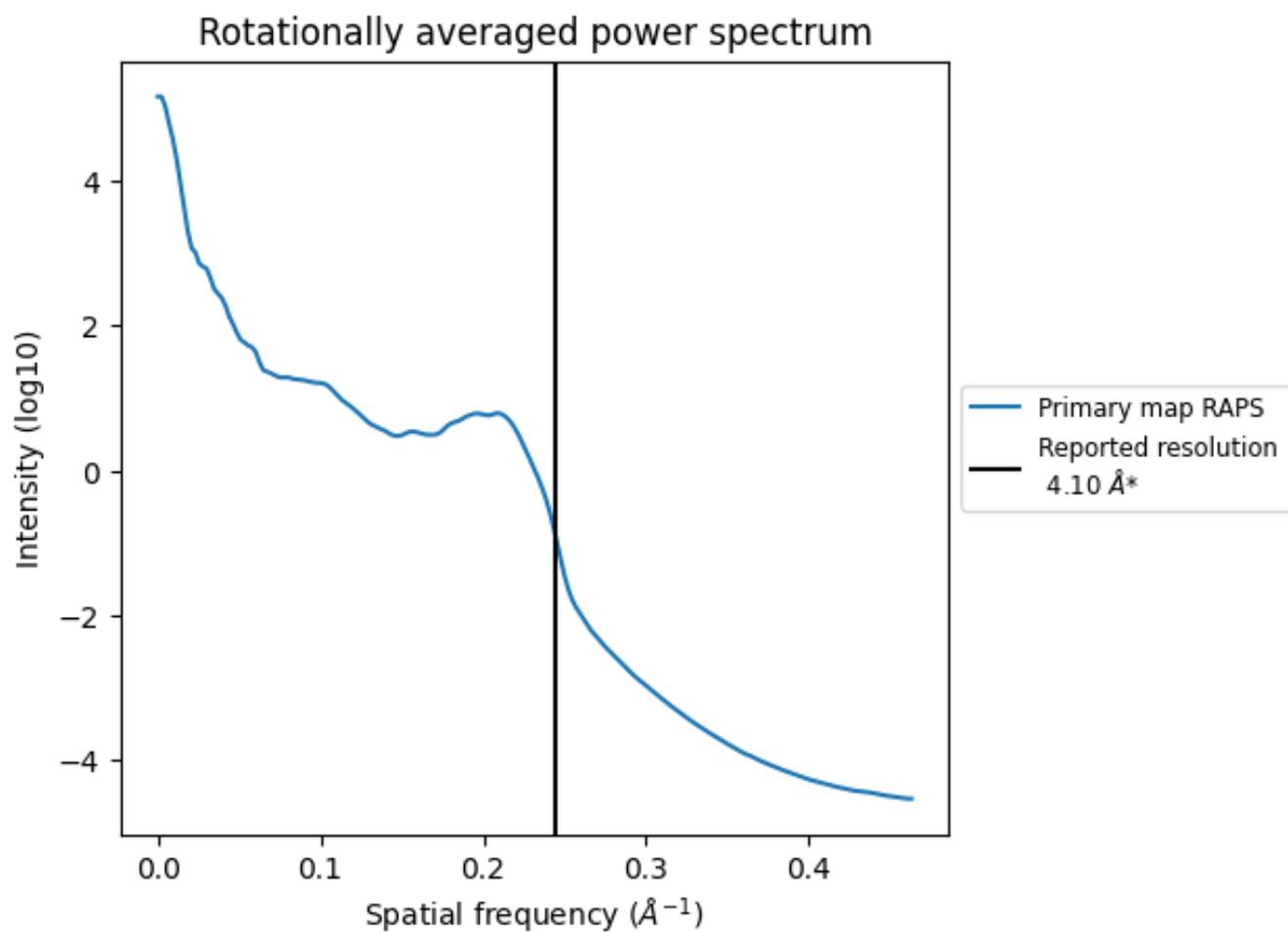
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 62 nm<sup>3</sup>; this corresponds to an approximate mass of 56 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

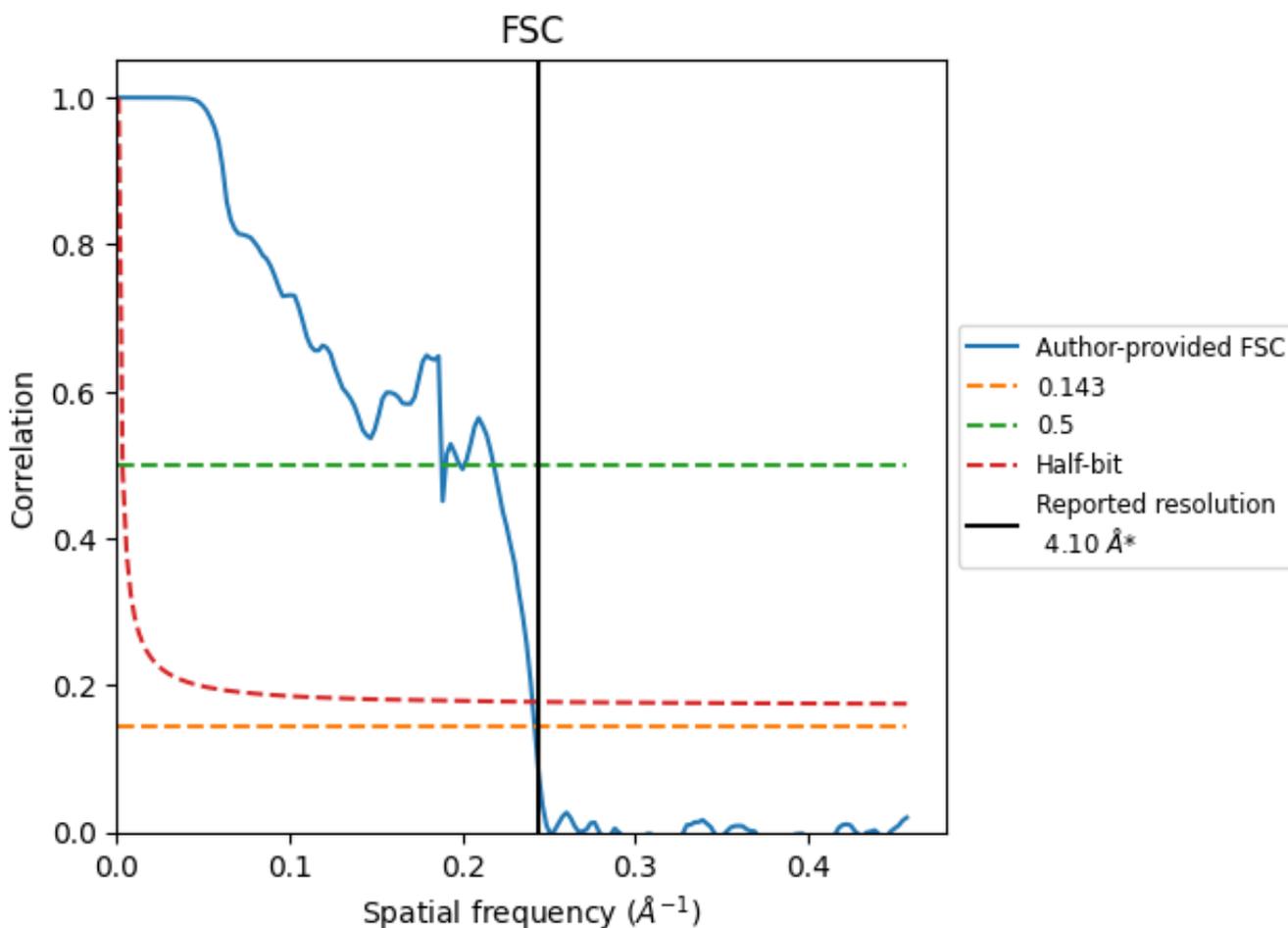


\*Reported resolution corresponds to spatial frequency of  $0.244 \text{\AA}^{-1}$

## 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 0.244 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.14	5.32	4.16
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit

This section was not generated.