



# wwPDB EM Validation Summary Report ⓘ

Oct 21, 2024 – 03:35 PM JST

PDB ID : 7F58  
EMDB ID : EMD-31461  
Title : Cryo-EM structure of THIQ-MC4R-Gs\_Nb35 complex  
Authors : Zhang, H.; Chen, L.; Mao, C.; Shen, Q.; Yang, D.; Shen, D.; Qin, J.  
Deposited on : 2021-06-21  
Resolution : 3.10 Å(reported)

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<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

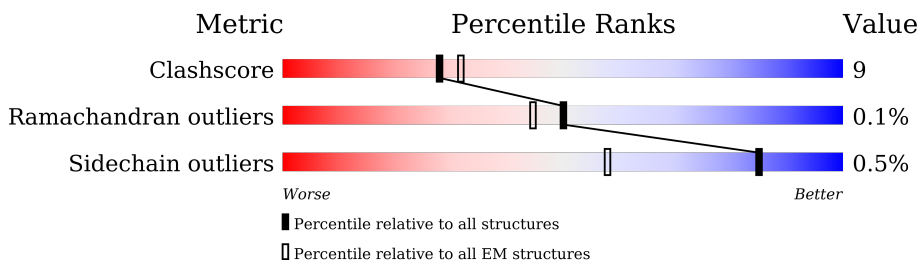
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.10 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  $\leq 5\%$ . 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	R	507	
2	A	380	
3	B	384	
4	G	71	
5	N	126	

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8065 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 Melanocortin receptor 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	273	Total	C	N	O	S	0	0
			2133	1414	329	365	25		

There are 175 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-1	GLY	-	expression tag	UNP P32245
R	0	PRO	-	expression tag	UNP P32245
R	333	GLY	-	expression tag	UNP P32245
R	334	GLY	-	expression tag	UNP P32245
R	335	SER	-	expression tag	UNP P32245
R	336	GLY	-	expression tag	UNP P32245
R	337	GLY	-	expression tag	UNP P32245
R	338	SER	-	expression tag	UNP P32245
R	339	VAL	-	expression tag	UNP P32245
R	340	PHE	-	expression tag	UNP P32245
R	341	THR	-	expression tag	UNP P32245
R	342	LEU	-	expression tag	UNP P32245
R	343	GLU	-	expression tag	UNP P32245
R	344	ASP	-	expression tag	UNP P32245
R	345	PHE	-	expression tag	UNP P32245
R	346	VAL	-	expression tag	UNP P32245
R	347	GLY	-	expression tag	UNP P32245
R	348	ASP	-	expression tag	UNP P32245
R	349	TRP	-	expression tag	UNP P32245
R	350	GLU	-	expression tag	UNP P32245
R	351	GLN	-	expression tag	UNP P32245
R	352	THR	-	expression tag	UNP P32245
R	353	ALA	-	expression tag	UNP P32245
R	354	ALA	-	expression tag	UNP P32245
R	355	TYR	-	expression tag	UNP P32245
R	356	ASN	-	expression tag	UNP P32245
R	357	LEU	-	expression tag	UNP P32245
R	358	ASP	-	expression tag	UNP P32245

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Chain	Residue	Modelled	Actual	Comment	Reference
R	359	GLN	-	expression tag	UNP P32245
R	360	VAL	-	expression tag	UNP P32245
R	361	LEU	-	expression tag	UNP P32245
R	362	GLU	-	expression tag	UNP P32245
R	363	GLN	-	expression tag	UNP P32245
R	364	GLY	-	expression tag	UNP P32245
R	365	GLY	-	expression tag	UNP P32245
R	366	VAL	-	expression tag	UNP P32245
R	367	SER	-	expression tag	UNP P32245
R	368	SER	-	expression tag	UNP P32245
R	369	LEU	-	expression tag	UNP P32245
R	370	LEU	-	expression tag	UNP P32245
R	371	GLN	-	expression tag	UNP P32245
R	372	ASN	-	expression tag	UNP P32245
R	373	LEU	-	expression tag	UNP P32245
R	374	ALA	-	expression tag	UNP P32245
R	375	VAL	-	expression tag	UNP P32245
R	376	SER	-	expression tag	UNP P32245
R	377	VAL	-	expression tag	UNP P32245
R	378	THR	-	expression tag	UNP P32245
R	379	PRO	-	expression tag	UNP P32245
R	380	ILE	-	expression tag	UNP P32245
R	381	GLN	-	expression tag	UNP P32245
R	382	ARG	-	expression tag	UNP P32245
R	383	ILE	-	expression tag	UNP P32245
R	384	VAL	-	expression tag	UNP P32245
R	385	ARG	-	expression tag	UNP P32245
R	386	SER	-	expression tag	UNP P32245
R	387	GLY	-	expression tag	UNP P32245
R	388	GLU	-	expression tag	UNP P32245
R	389	ASN	-	expression tag	UNP P32245
R	390	ALA	-	expression tag	UNP P32245
R	391	LEU	-	expression tag	UNP P32245
R	392	LYS	-	expression tag	UNP P32245
R	393	ILE	-	expression tag	UNP P32245
R	394	ASP	-	expression tag	UNP P32245
R	395	ILE	-	expression tag	UNP P32245
R	396	HIS	-	expression tag	UNP P32245
R	397	VAL	-	expression tag	UNP P32245
R	398	ILE	-	expression tag	UNP P32245
R	399	ILE	-	expression tag	UNP P32245
R	400	PRO	-	expression tag	UNP P32245

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Chain	Residue	Modelled	Actual	Comment	Reference
R	401	TYR	-	expression tag	UNP P32245
R	402	GLU	-	expression tag	UNP P32245
R	403	GLY	-	expression tag	UNP P32245
R	404	LEU	-	expression tag	UNP P32245
R	405	SER	-	expression tag	UNP P32245
R	406	ALA	-	expression tag	UNP P32245
R	407	ASP	-	expression tag	UNP P32245
R	408	GLN	-	expression tag	UNP P32245
R	409	MET	-	expression tag	UNP P32245
R	410	ALA	-	expression tag	UNP P32245
R	411	GLN	-	expression tag	UNP P32245
R	412	ILE	-	expression tag	UNP P32245
R	413	GLU	-	expression tag	UNP P32245
R	414	GLU	-	expression tag	UNP P32245
R	415	VAL	-	expression tag	UNP P32245
R	416	PHE	-	expression tag	UNP P32245
R	417	LYS	-	expression tag	UNP P32245
R	418	VAL	-	expression tag	UNP P32245
R	419	VAL	-	expression tag	UNP P32245
R	420	TYR	-	expression tag	UNP P32245
R	421	PRO	-	expression tag	UNP P32245
R	422	VAL	-	expression tag	UNP P32245
R	423	ASP	-	expression tag	UNP P32245
R	424	ASP	-	expression tag	UNP P32245
R	425	HIS	-	expression tag	UNP P32245
R	426	HIS	-	expression tag	UNP P32245
R	427	PHE	-	expression tag	UNP P32245
R	428	LYS	-	expression tag	UNP P32245
R	429	VAL	-	expression tag	UNP P32245
R	430	ILE	-	expression tag	UNP P32245
R	431	LEU	-	expression tag	UNP P32245
R	432	PRO	-	expression tag	UNP P32245
R	433	TYR	-	expression tag	UNP P32245
R	434	GLY	-	expression tag	UNP P32245
R	435	THR	-	expression tag	UNP P32245
R	436	LEU	-	expression tag	UNP P32245
R	437	VAL	-	expression tag	UNP P32245
R	438	ILE	-	expression tag	UNP P32245
R	439	ASP	-	expression tag	UNP P32245
R	440	GLY	-	expression tag	UNP P32245
R	441	VAL	-	expression tag	UNP P32245
R	442	THR	-	expression tag	UNP P32245

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Chain	Residue	Modelled	Actual	Comment	Reference
R	443	PRO	-	expression tag	UNP P32245
R	444	ASN	-	expression tag	UNP P32245
R	445	MET	-	expression tag	UNP P32245
R	446	LEU	-	expression tag	UNP P32245
R	447	ASN	-	expression tag	UNP P32245
R	448	TYR	-	expression tag	UNP P32245
R	449	PHE	-	expression tag	UNP P32245
R	450	GLY	-	expression tag	UNP P32245
R	451	ARG	-	expression tag	UNP P32245
R	452	PRO	-	expression tag	UNP P32245
R	453	TYR	-	expression tag	UNP P32245
R	454	GLU	-	expression tag	UNP P32245
R	455	GLY	-	expression tag	UNP P32245
R	456	ILE	-	expression tag	UNP P32245
R	457	ALA	-	expression tag	UNP P32245
R	458	VAL	-	expression tag	UNP P32245
R	459	PHE	-	expression tag	UNP P32245
R	460	ASP	-	expression tag	UNP P32245
R	461	GLY	-	expression tag	UNP P32245
R	462	LYS	-	expression tag	UNP P32245
R	463	LYS	-	expression tag	UNP P32245
R	464	ILE	-	expression tag	UNP P32245
R	465	THR	-	expression tag	UNP P32245
R	466	VAL	-	expression tag	UNP P32245
R	467	THR	-	expression tag	UNP P32245
R	468	GLY	-	expression tag	UNP P32245
R	469	THR	-	expression tag	UNP P32245
R	470	LEU	-	expression tag	UNP P32245
R	471	TRP	-	expression tag	UNP P32245
R	472	ASN	-	expression tag	UNP P32245
R	473	GLY	-	expression tag	UNP P32245
R	474	ASN	-	expression tag	UNP P32245
R	475	LYS	-	expression tag	UNP P32245
R	476	ILE	-	expression tag	UNP P32245
R	477	ILE	-	expression tag	UNP P32245
R	478	ASP	-	expression tag	UNP P32245
R	479	GLU	-	expression tag	UNP P32245
R	480	ARG	-	expression tag	UNP P32245
R	481	LEU	-	expression tag	UNP P32245
R	482	ILE	-	expression tag	UNP P32245
R	483	THR	-	expression tag	UNP P32245
R	484	PRO	-	expression tag	UNP P32245

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Chain	Residue	Modelled	Actual	Comment	Reference
R	485	ASP	-	expression tag	UNP P32245
R	486	GLY	-	expression tag	UNP P32245
R	487	SER	-	expression tag	UNP P32245
R	488	MET	-	expression tag	UNP P32245
R	489	LEU	-	expression tag	UNP P32245
R	490	PHE	-	expression tag	UNP P32245
R	491	ARG	-	expression tag	UNP P32245
R	492	VAL	-	expression tag	UNP P32245
R	493	THR	-	expression tag	UNP P32245
R	494	ILE	-	expression tag	UNP P32245
R	495	ASN	-	expression tag	UNP P32245
R	496	SER	-	expression tag	UNP P32245
R	497	GLY	-	expression tag	UNP P32245
R	498	GLY	-	expression tag	UNP P32245
R	499	SER	-	expression tag	UNP P32245
R	500	LEU	-	expression tag	UNP P32245
R	501	GLU	-	expression tag	UNP P32245
R	502	VAL	-	expression tag	UNP P32245
R	503	LEU	-	expression tag	UNP P32245
R	504	PHE	-	expression tag	UNP P32245
R	505	GLN	-	expression tag	UNP P32245

- Molecule 2 is a protein called Isoform Gnas-2 of Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	227	Total	C	N	O	S	0	0
			1885	1189	342	347	7		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P63092-2
A	226	ALA	GLY	engineered mutation	UNP P63092-2
A	268	ALA	GLU	engineered mutation	UNP P63092-2
A	271	LYS	ASN	engineered mutation	UNP P63092-2
A	274	ASP	LYS	engineered mutation	UNP P63092-2
A	280	LYS	ARG	engineered mutation	UNP P63092-2
A	284	ASP	THR	engineered mutation	UNP P63092-2
A	285	THR	ILE	engineered mutation	UNP P63092-2

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit

beta-1.

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

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	initiating methionine	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	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
B	341	GLY	-	expression tag	UNP P62873
B	342	SER	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	GLY	-	expression tag	UNP P62873
B	352	GLY	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	SER	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	VAL	-	expression tag	UNP P62873
B	357	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
B	358	GLY	-	expression tag	UNP P62873
B	359	TRP	-	expression tag	UNP P62873
B	360	ARG	-	expression tag	UNP P62873
B	361	LEU	-	expression tag	UNP P62873
B	362	PHE	-	expression tag	UNP P62873
B	363	LYS	-	expression tag	UNP P62873
B	364	LYS	-	expression tag	UNP P62873
B	365	ILE	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873

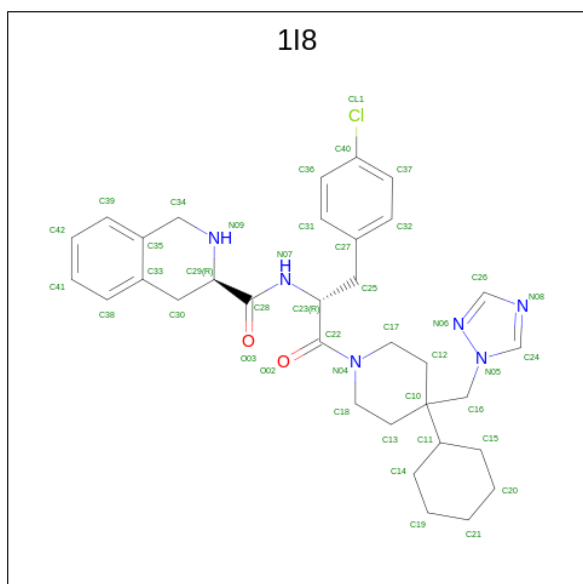
- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	57	Total	C	N	O	S	0	0
			436	273	77	83	3		

- Molecule 5 is a protein called Nanobody35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	126	Total	C	N	O	S	0	0
			961	599	168	188	6		

- Molecule 6 is (3R)-N-[(2R)-3-(4-chlorophenyl)-1-[4-cyclohexyl-4-(1,2,4-triazol-1-ylmethyl)piperidin-1-yl]-1-oxidanylidene-propan-2-yl]-1,2,3,4-tetrahydroisoquinoline-3-carboxamide (three-letter code: 1I8) (formula: C<sub>33</sub>H<sub>41</sub>ClN<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					AltConf
6	R	1	Total	C	Cl	N	O	0
			42	33	1	6	2	

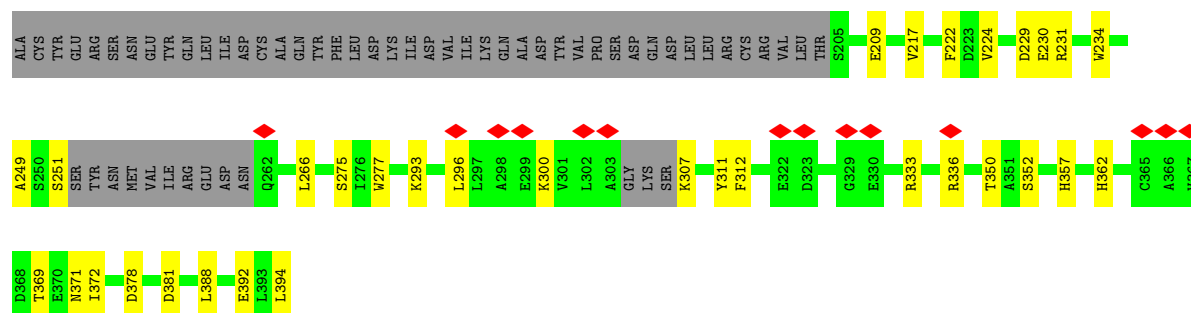
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
7	R	1	Total	Ca	0
			1	1	

- Molecule 8 is water.

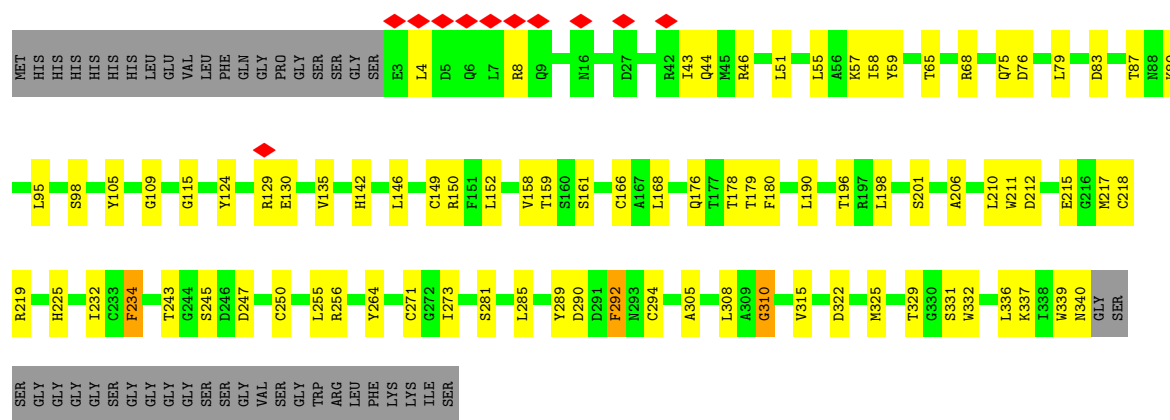
Mol	Chain	Residues	Atoms		AltConf
8	R	6	Total	O	0
			6	6	
8	A	1	Total	O	0
			1	1	





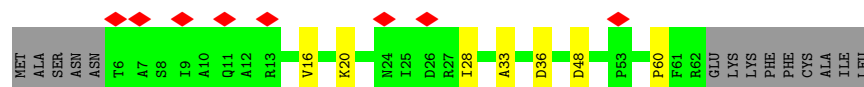
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B: 66% 21% 12%



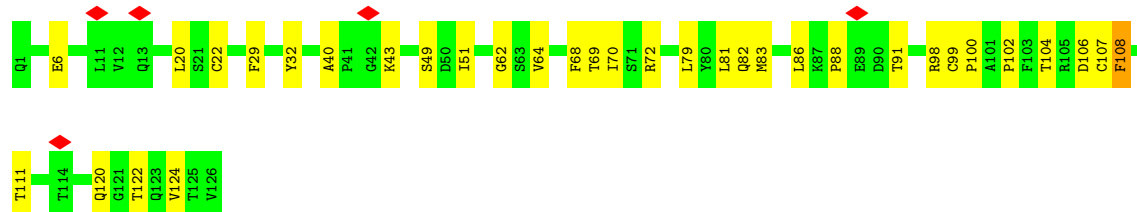
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G: 11% 70% 10% 20%



- Molecule 5: Nanobody35

Chain N: 73% 26%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	269832	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 ( $e^-/\text{\AA}^2$ )	62	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.203	Depositor
Minimum map value	-0.138	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	194.68802, 194.68802, 194.68802	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.014, 1.014, 1.014	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: 1I8, CA

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	R	0.28	0/2177	0.49	0/2960
2	A	0.28	0/1919	0.47	0/2577
3	B	0.29	0/2647	0.54	0/3589
4	G	0.26	0/442	0.40	0/597
5	N	0.28	0/981	0.53	0/1329
All	All	0.28	0/8166	0.50	0/11052

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	R	2133	0	2221	43	0
2	A	1885	0	1862	35	0
3	B	2600	0	2505	58	0
4	G	436	0	448	5	0
5	N	961	0	928	24	0
6	R	42	0	0	0	0
7	R	1	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	R	6	0	0	0	0
All	All	8065	0	7964	150	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.

The worst 5 of 150 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)
5:N:32:TYR:CE2	5:N:98:ARG:NH1	2.43	0.86
2:A:23:ASN:HD21	3:B:89:LYS:H	1.30	0.78
1:R:258:TRP:HE1	1:R:294:ASN:ND2	1.82	0.76
5:N:20:LEU:HD12	5:N:81:LEU:HD23	1.68	0.76
5:N:100:PRO:HD2	5:N:107:CYS:HB2	1.69	0.75

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	R	267/507 (53%)	256 (96%)	11 (4%)	0	100	100
2	A	219/380 (58%)	217 (99%)	2 (1%)	0	100	100
3	B	336/384 (88%)	326 (97%)	9 (3%)	1 (0%)	37	68
4	G	55/71 (78%)	55 (100%)	0	0	100	100
5	N	124/126 (98%)	121 (98%)	3 (2%)	0	100	100
All	All	1001/1468 (68%)	975 (97%)	25 (2%)	1 (0%)	50	79

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	310	GLY

### 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	R	246/443 (56%)	245 (100%)	1 (0%)	89	94
2	A	203/340 (60%)	203 (100%)	0	100	100
3	B	281/313 (90%)	279 (99%)	2 (1%)	81	90
4	G	46/58 (79%)	46 (100%)	0	100	100
5	N	104/104 (100%)	103 (99%)	1 (1%)	73	86
All	All	880/1258 (70%)	876 (100%)	4 (0%)	85	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	R	183	LEU
3	B	234	PHE
3	B	292	PHE
5	N	108	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 13 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	32	GLN
3	B	132	ASN
5	N	13	GLN
3	B	176	GLN
5	N	3	GLN

### 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](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	1I8	R	601	7	43,47,47	4.99	24 (55%)	53,66,66	1.58	10 (18%)

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	1I8	R	601	7	-	6/31/60/60	0/6/6/6

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	601	1I8	C22-N04	11.89	1.52	1.34
6	R	601	1I8	C38-C33	10.69	1.57	1.39
6	R	601	1I8	C39-C35	10.09	1.56	1.39
6	R	601	1I8	C36-C31	9.14	1.55	1.38
6	R	601	1I8	C37-C32	8.89	1.54	1.38

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	R	601	1I8	C24-N08-C26	5.15	108.14	102.34
6	R	601	1I8	N08-C24-N05	-3.43	108.09	112.24
6	R	601	1I8	C33-C30-C29	-3.35	107.15	111.29
6	R	601	1I8	C30-C33-C35	-3.34	113.14	120.30
6	R	601	1I8	C15-C11-C10	-2.99	110.05	114.70

There are no chirality outliers.

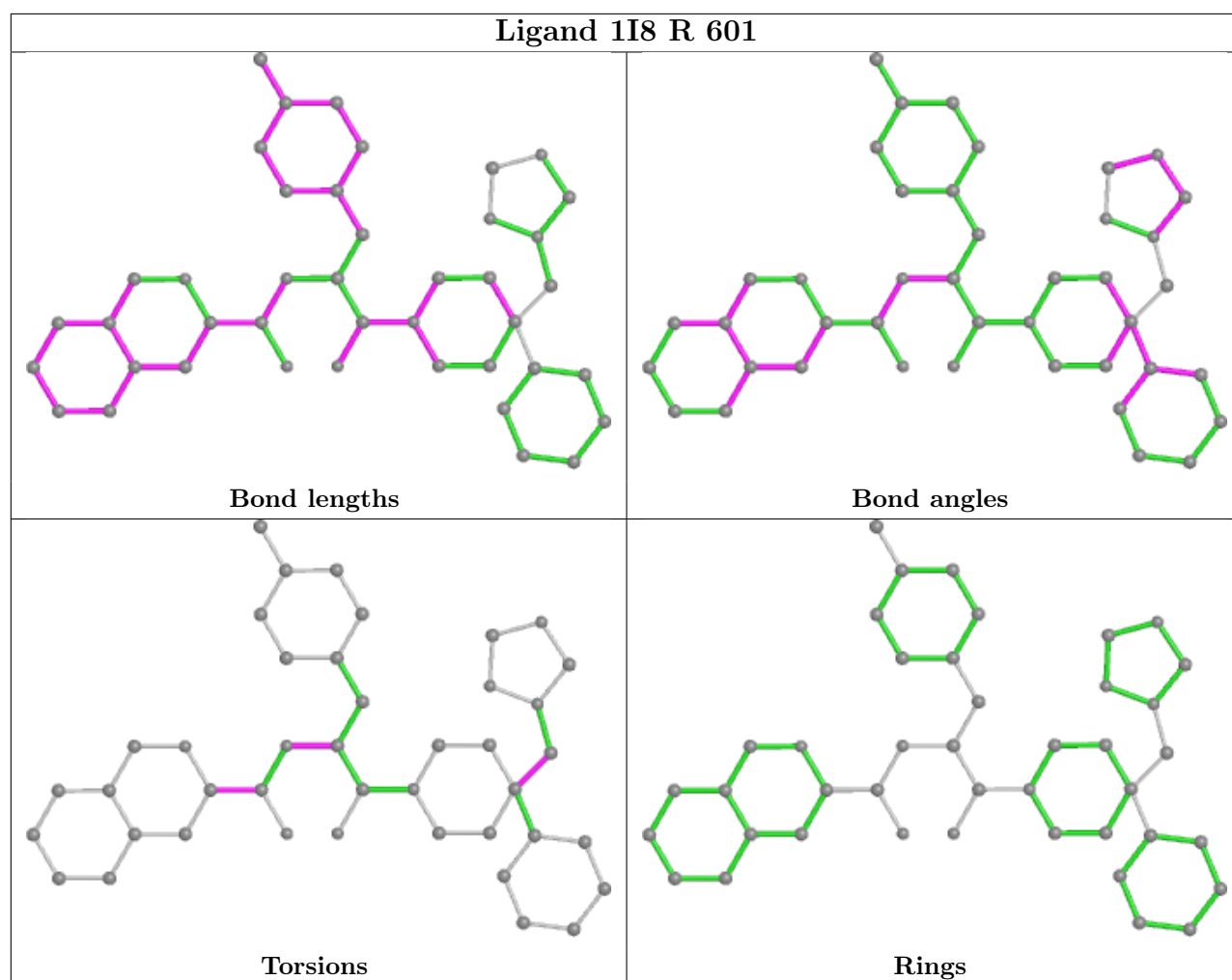
5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	601	1I8	N07-C28-C29-C30
6	R	601	1I8	N07-C28-C29-N09
6	R	601	1I8	O03-C28-C29-C30
6	R	601	1I8	O03-C28-C29-N09
6	R	601	1I8	C25-C23-N07-C28

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.

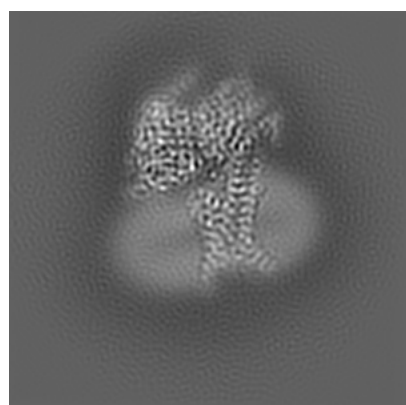
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31461. These allow visual inspection of the internal detail of the map and identification of artifacts.

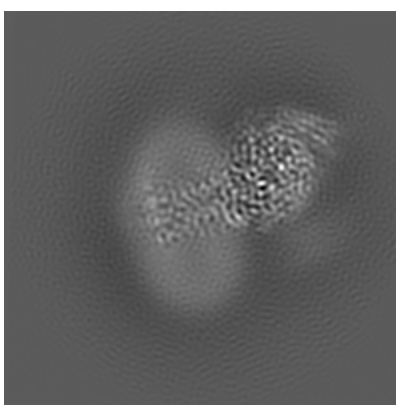
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

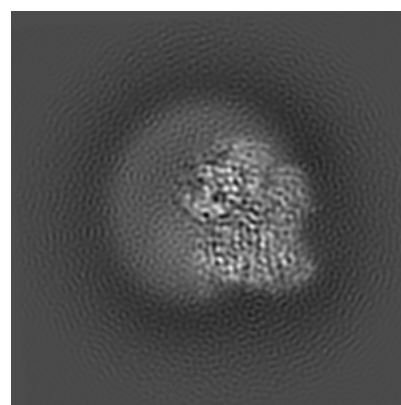
#### 6.1.1 Primary map



X



Y

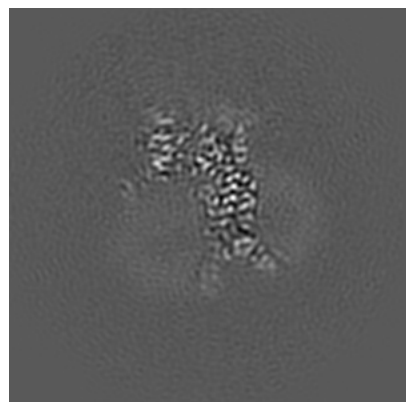


Z

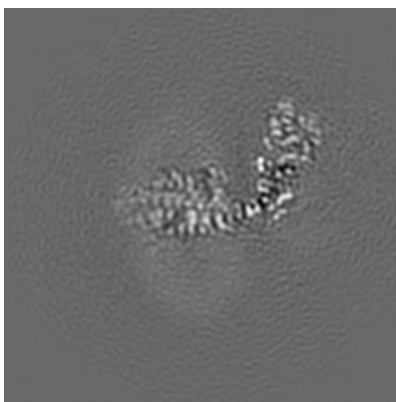
The images above show the map projected in three orthogonal directions.

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

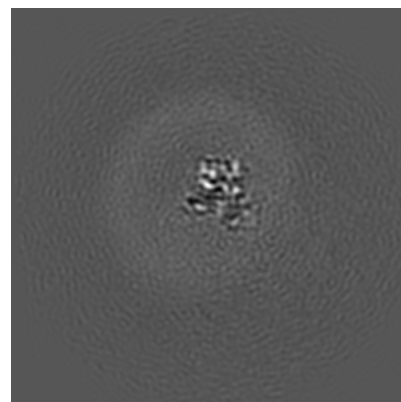
#### 6.2.1 Primary map



X Index: 96



Y Index: 96

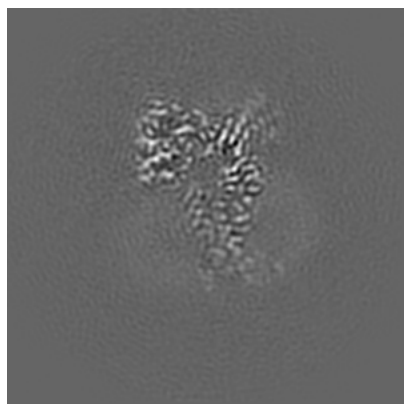


Z Index: 96

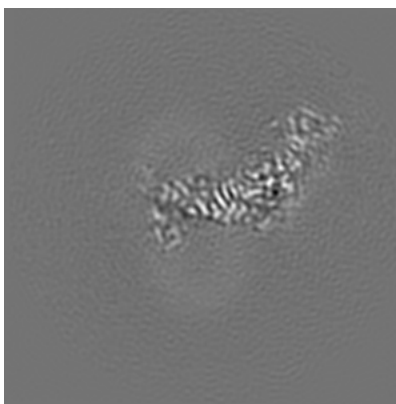
The images above show central slices of the map in three orthogonal directions.

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

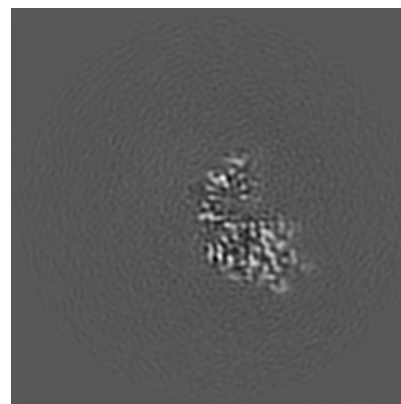
### 6.3.1 Primary map



X Index: 105



Y Index: 106

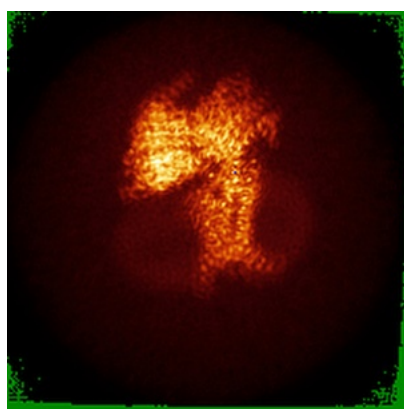


Z Index: 119

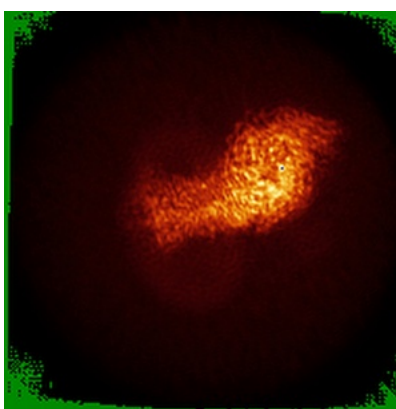
The images above show the largest variance slices of the map in three orthogonal directions.

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

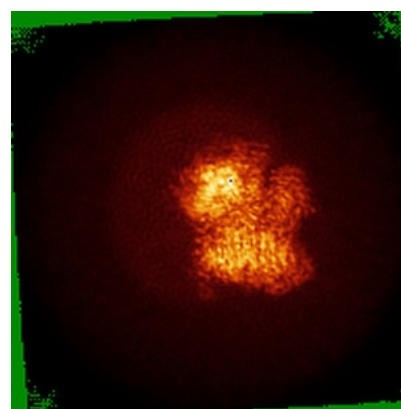
### 6.4.1 Primary map



X



Y

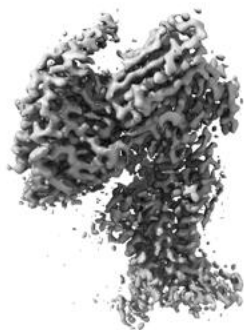


Z

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](#)

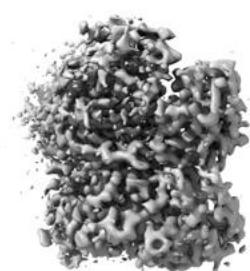
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

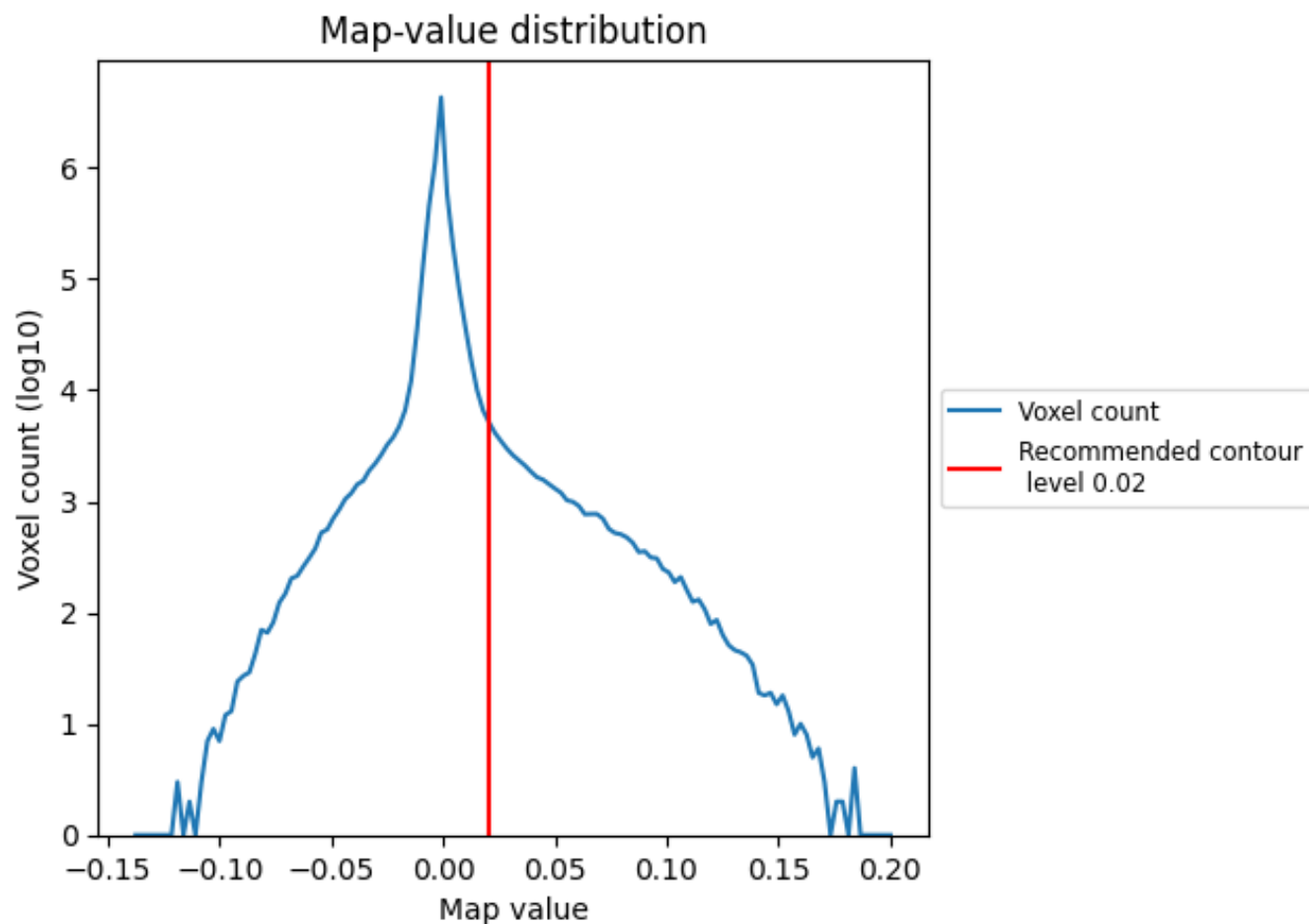
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

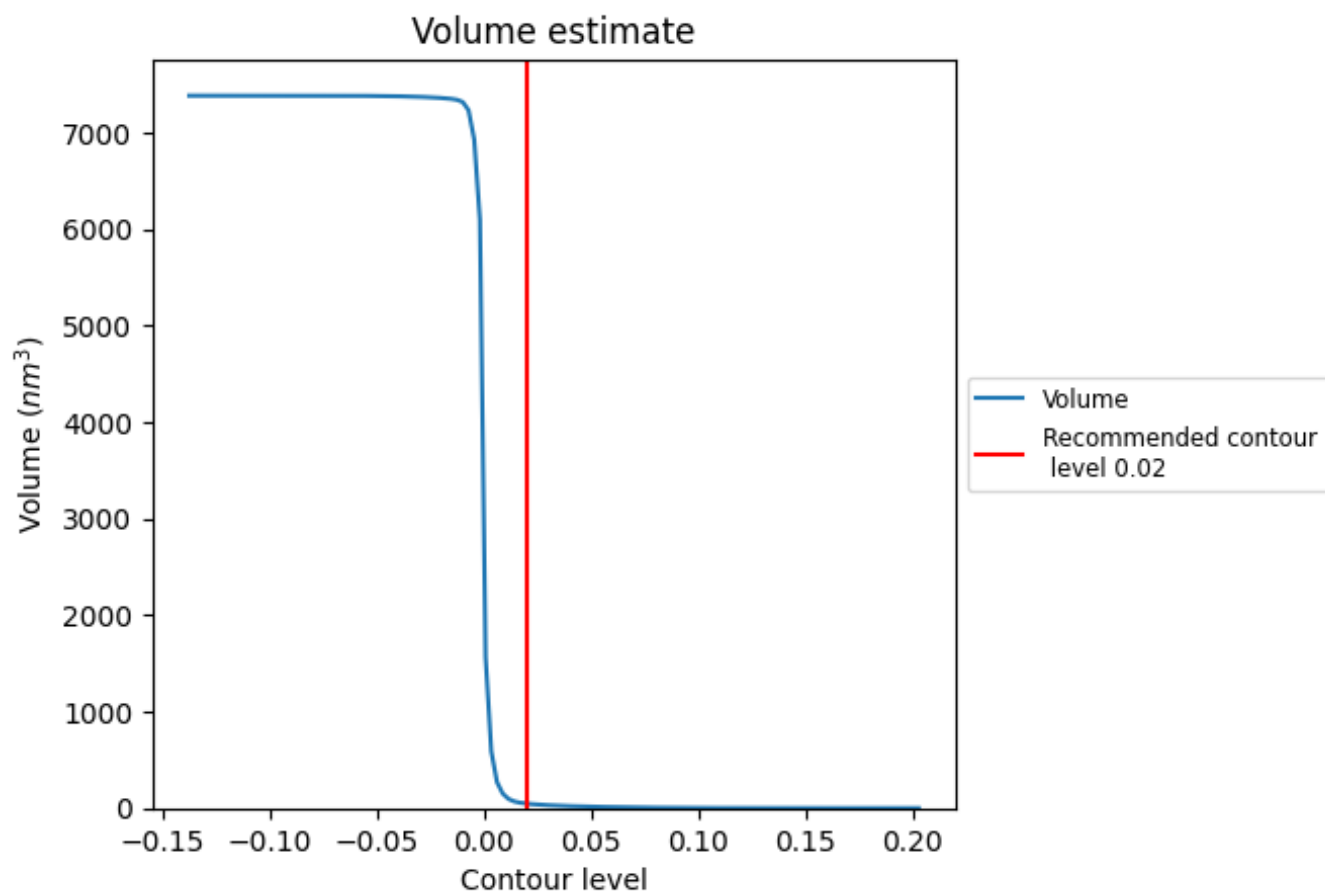
This section contains the results of statistical analysis of the map.

### 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.

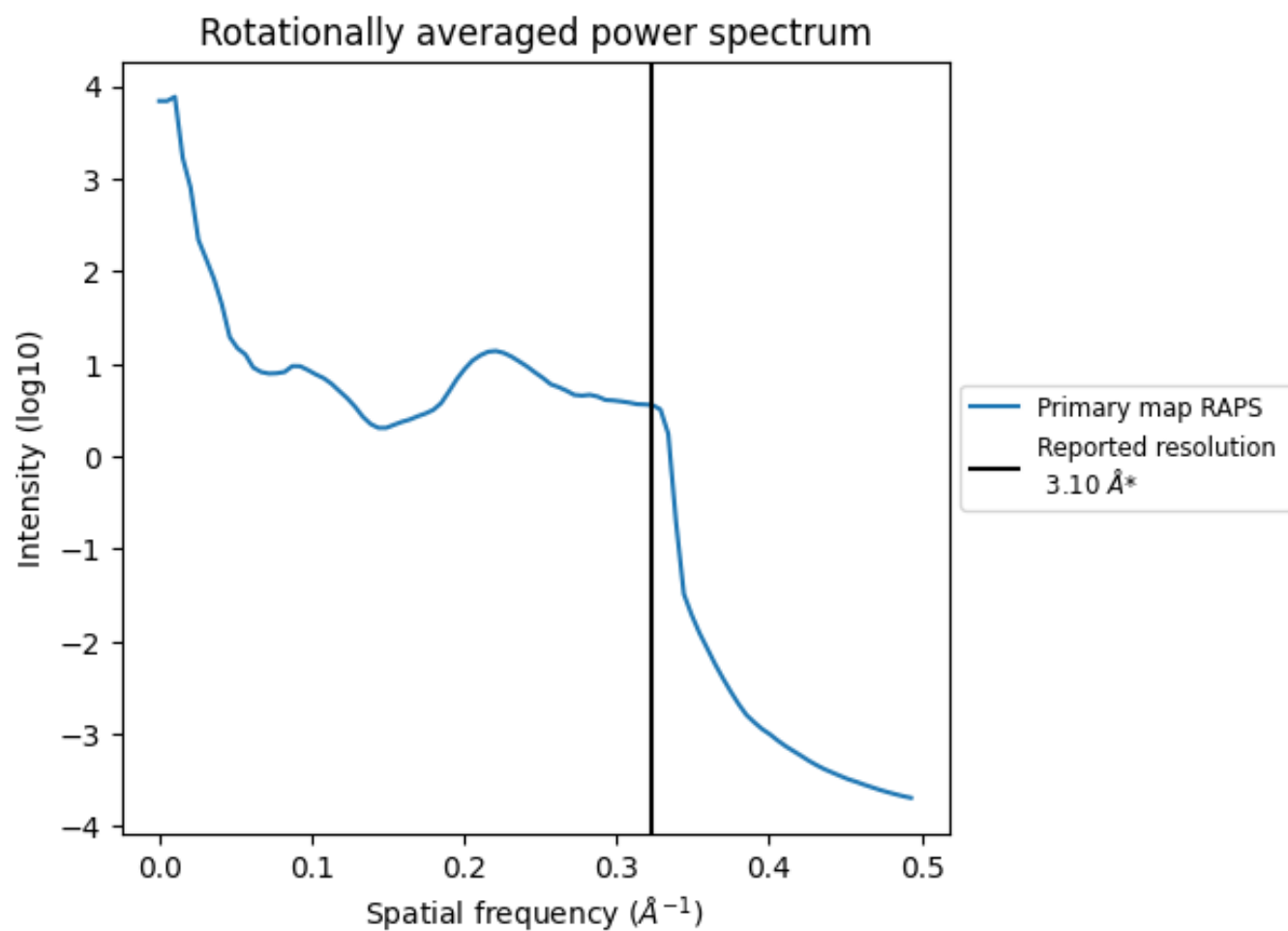
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47 nm<sup>3</sup>; this corresponds to an approximate mass of 42 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 0.323 Å<sup>-1</sup>

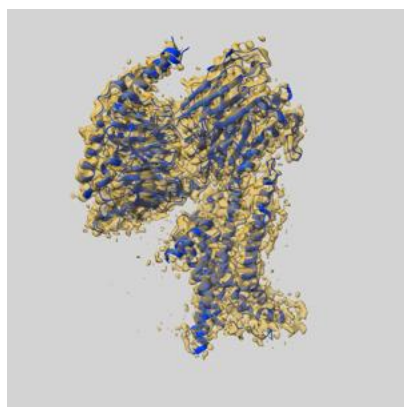
## 8 Fourier-Shell correlation

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

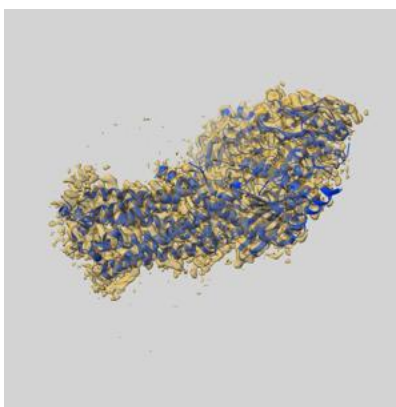
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31461 and PDB model 7F58. Per-residue inclusion information can be found in section 3 on page 11.

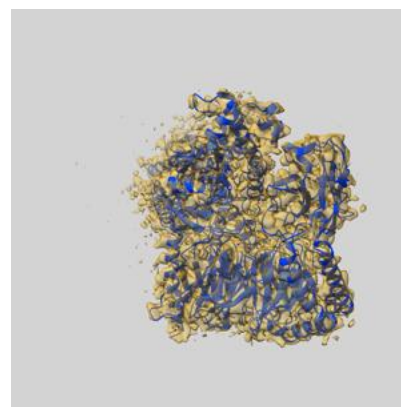
### 9.1 Map-model overlay [i](#)



X



Y



Z

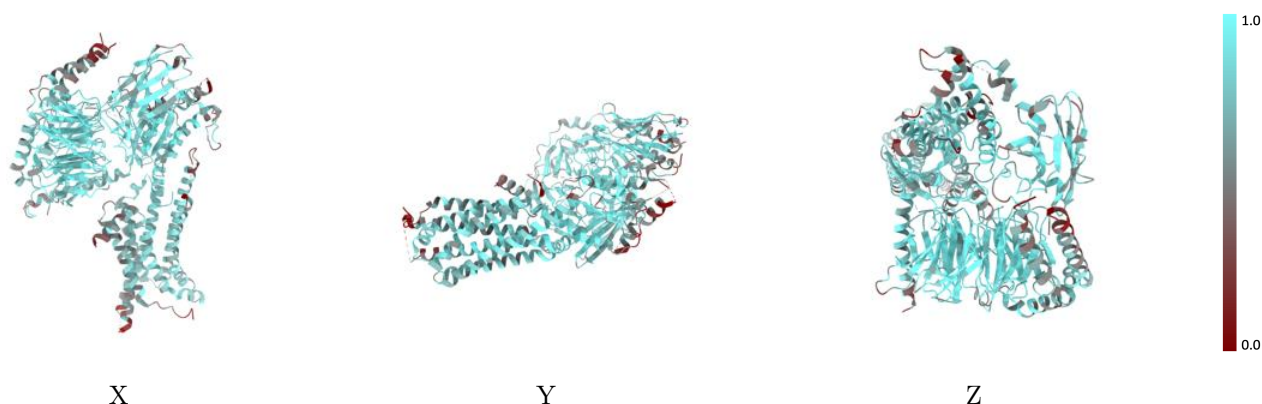
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



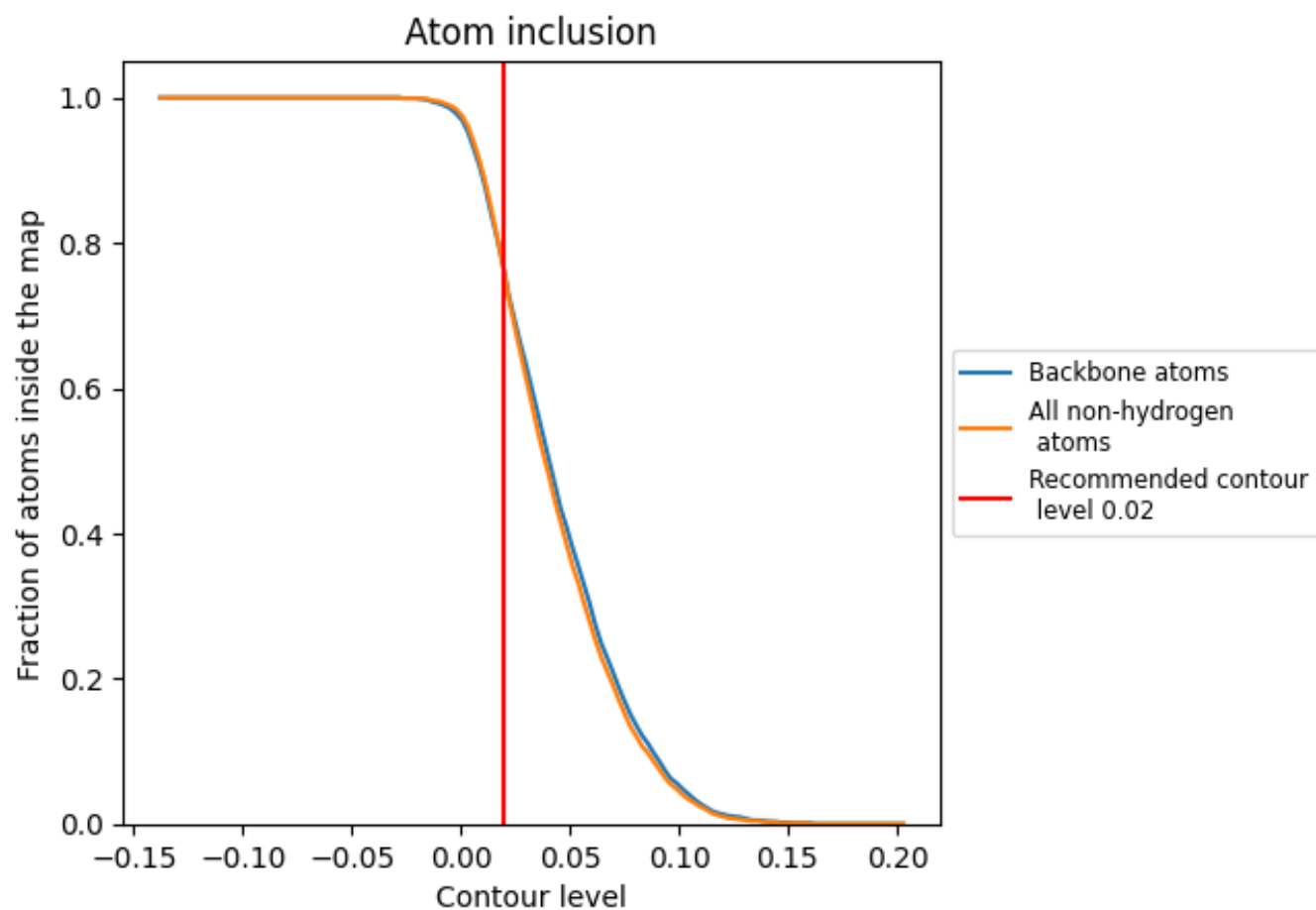
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 76% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7600	<div></div> 0.5160
A	<div></div> 0.7510	<div></div> 0.5050
B	<div></div> 0.8450	<div></div> 0.5580
G	<div></div> 0.6390	<div></div> 0.4600
N	<div></div> 0.7840	<div></div> 0.5420
R	<div></div> 0.7010	<div></div> 0.4730

