



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 06:03 AM UTC

PDB ID : 8JSR / pdb_00008jsr
EMDB ID : EMD-36627
Title : Cryo-EM structure of the anamorelin-bound ghrelin receptor and Gq complex
Authors : Im, D.; Shiimura, Y.; Asada, H.; Iwata, S.
Deposited on : 2023-06-20
Resolution : 2.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

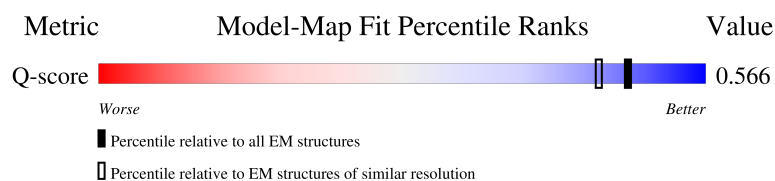
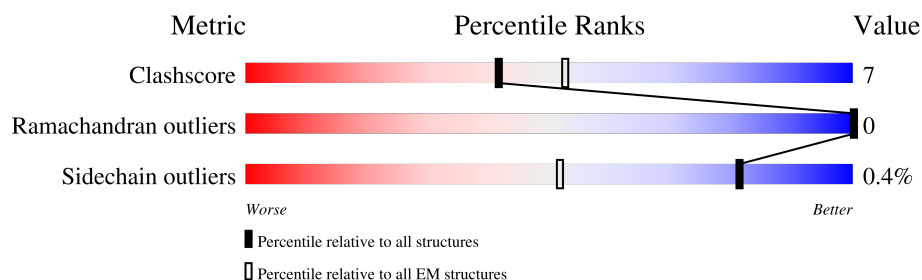
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.90 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.



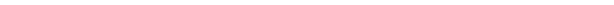
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13054 (2.40 - 3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	R	523	
2	A	361	
3	B	388	
4	C	259	

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Mol	Chain	Length	Quality of chain
5	G	71	 79%20%
6	N	129	 79%19%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 10001 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 Growth hormone secretagogue receptor type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	282	Total	C	N	O	S	0	0
			2209	1486	352	355	16		

There are 158 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	367	VAL	-	expression tag	UNP Q92847
R	368	PHE	-	expression tag	UNP Q92847
R	369	THR	-	expression tag	UNP Q92847
R	370	LEU	-	expression tag	UNP Q92847
R	371	GLU	-	expression tag	UNP Q92847
R	372	ASP	-	expression tag	UNP Q92847
R	373	PHE	-	expression tag	UNP Q92847
R	374	VAL	-	expression tag	UNP Q92847
R	375	GLY	-	expression tag	UNP Q92847
R	376	ASP	-	expression tag	UNP Q92847
R	377	TRP	-	expression tag	UNP Q92847
R	378	GLU	-	expression tag	UNP Q92847
R	379	GLN	-	expression tag	UNP Q92847
R	380	THR	-	expression tag	UNP Q92847
R	381	ALA	-	expression tag	UNP Q92847
R	382	ALA	-	expression tag	UNP Q92847
R	383	TYR	-	expression tag	UNP Q92847
R	384	ASN	-	expression tag	UNP Q92847
R	385	LEU	-	expression tag	UNP Q92847
R	386	ASP	-	expression tag	UNP Q92847
R	387	GLN	-	expression tag	UNP Q92847
R	388	VAL	-	expression tag	UNP Q92847
R	389	LEU	-	expression tag	UNP Q92847
R	390	GLU	-	expression tag	UNP Q92847
R	391	GLN	-	expression tag	UNP Q92847
R	392	GLY	-	expression tag	UNP Q92847
R	393	GLY	-	expression tag	UNP Q92847
R	394	VAL	-	expression tag	UNP Q92847

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Chain	Residue	Modelled	Actual	Comment	Reference
R	395	SER	-	expression tag	UNP Q92847
R	396	SER	-	expression tag	UNP Q92847
R	397	LEU	-	expression tag	UNP Q92847
R	398	LEU	-	expression tag	UNP Q92847
R	399	GLN	-	expression tag	UNP Q92847
R	400	ASN	-	expression tag	UNP Q92847
R	401	LEU	-	expression tag	UNP Q92847
R	402	ALA	-	expression tag	UNP Q92847
R	403	VAL	-	expression tag	UNP Q92847
R	404	SER	-	expression tag	UNP Q92847
R	405	VAL	-	expression tag	UNP Q92847
R	406	THR	-	expression tag	UNP Q92847
R	407	PRO	-	expression tag	UNP Q92847
R	408	ILE	-	expression tag	UNP Q92847
R	409	GLN	-	expression tag	UNP Q92847
R	410	ARG	-	expression tag	UNP Q92847
R	411	ILE	-	expression tag	UNP Q92847
R	412	VAL	-	expression tag	UNP Q92847
R	413	ARG	-	expression tag	UNP Q92847
R	414	SER	-	expression tag	UNP Q92847
R	415	GLY	-	expression tag	UNP Q92847
R	416	GLU	-	expression tag	UNP Q92847
R	417	ASN	-	expression tag	UNP Q92847
R	418	ALA	-	expression tag	UNP Q92847
R	419	LEU	-	expression tag	UNP Q92847
R	420	LYS	-	expression tag	UNP Q92847
R	421	ILE	-	expression tag	UNP Q92847
R	422	ASP	-	expression tag	UNP Q92847
R	423	ILE	-	expression tag	UNP Q92847
R	424	HIS	-	expression tag	UNP Q92847
R	425	VAL	-	expression tag	UNP Q92847
R	426	ILE	-	expression tag	UNP Q92847
R	427	ILE	-	expression tag	UNP Q92847
R	428	PRO	-	expression tag	UNP Q92847
R	429	TYR	-	expression tag	UNP Q92847
R	430	GLU	-	expression tag	UNP Q92847
R	431	GLY	-	expression tag	UNP Q92847
R	432	LEU	-	expression tag	UNP Q92847
R	433	SER	-	expression tag	UNP Q92847
R	434	ALA	-	expression tag	UNP Q92847
R	435	ASP	-	expression tag	UNP Q92847
R	436	GLN	-	expression tag	UNP Q92847

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Chain	Residue	Modelled	Actual	Comment	Reference
R	437	MET	-	expression tag	UNP Q92847
R	438	ALA	-	expression tag	UNP Q92847
R	439	GLN	-	expression tag	UNP Q92847
R	440	ILE	-	expression tag	UNP Q92847
R	441	GLU	-	expression tag	UNP Q92847
R	442	GLU	-	expression tag	UNP Q92847
R	443	VAL	-	expression tag	UNP Q92847
R	444	PHE	-	expression tag	UNP Q92847
R	445	LYS	-	expression tag	UNP Q92847
R	446	VAL	-	expression tag	UNP Q92847
R	447	VAL	-	expression tag	UNP Q92847
R	448	TYR	-	expression tag	UNP Q92847
R	449	PRO	-	expression tag	UNP Q92847
R	450	VAL	-	expression tag	UNP Q92847
R	451	ASP	-	expression tag	UNP Q92847
R	452	ASP	-	expression tag	UNP Q92847
R	453	HIS	-	expression tag	UNP Q92847
R	454	HIS	-	expression tag	UNP Q92847
R	455	PHE	-	expression tag	UNP Q92847
R	456	LYS	-	expression tag	UNP Q92847
R	457	VAL	-	expression tag	UNP Q92847
R	458	ILE	-	expression tag	UNP Q92847
R	459	LEU	-	expression tag	UNP Q92847
R	460	PRO	-	expression tag	UNP Q92847
R	461	TYR	-	expression tag	UNP Q92847
R	462	GLY	-	expression tag	UNP Q92847
R	463	THR	-	expression tag	UNP Q92847
R	464	LEU	-	expression tag	UNP Q92847
R	465	VAL	-	expression tag	UNP Q92847
R	466	ILE	-	expression tag	UNP Q92847
R	467	ASP	-	expression tag	UNP Q92847
R	468	GLY	-	expression tag	UNP Q92847
R	469	VAL	-	expression tag	UNP Q92847
R	470	THR	-	expression tag	UNP Q92847
R	471	PRO	-	expression tag	UNP Q92847
R	472	ASN	-	expression tag	UNP Q92847
R	473	MET	-	expression tag	UNP Q92847
R	474	LEU	-	expression tag	UNP Q92847
R	475	ASN	-	expression tag	UNP Q92847
R	476	TYR	-	expression tag	UNP Q92847
R	477	PHE	-	expression tag	UNP Q92847
R	478	GLY	-	expression tag	UNP Q92847

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Chain	Residue	Modelled	Actual	Comment	Reference
R	479	ARG	-	expression tag	UNP Q92847
R	480	PRO	-	expression tag	UNP Q92847
R	481	TYR	-	expression tag	UNP Q92847
R	482	GLU	-	expression tag	UNP Q92847
R	483	GLY	-	expression tag	UNP Q92847
R	484	ILE	-	expression tag	UNP Q92847
R	485	ALA	-	expression tag	UNP Q92847
R	486	VAL	-	expression tag	UNP Q92847
R	487	PHE	-	expression tag	UNP Q92847
R	488	ASP	-	expression tag	UNP Q92847
R	489	GLY	-	expression tag	UNP Q92847
R	490	LYS	-	expression tag	UNP Q92847
R	491	LYS	-	expression tag	UNP Q92847
R	492	ILE	-	expression tag	UNP Q92847
R	493	THR	-	expression tag	UNP Q92847
R	494	VAL	-	expression tag	UNP Q92847
R	495	THR	-	expression tag	UNP Q92847
R	496	GLY	-	expression tag	UNP Q92847
R	497	THR	-	expression tag	UNP Q92847
R	498	LEU	-	expression tag	UNP Q92847
R	499	TRP	-	expression tag	UNP Q92847
R	500	ASN	-	expression tag	UNP Q92847
R	501	GLY	-	expression tag	UNP Q92847
R	502	ASN	-	expression tag	UNP Q92847
R	503	LYS	-	expression tag	UNP Q92847
R	504	ILE	-	expression tag	UNP Q92847
R	505	ILE	-	expression tag	UNP Q92847
R	506	ASP	-	expression tag	UNP Q92847
R	507	GLU	-	expression tag	UNP Q92847
R	508	ARG	-	expression tag	UNP Q92847
R	509	LEU	-	expression tag	UNP Q92847
R	510	ILE	-	expression tag	UNP Q92847
R	511	THR	-	expression tag	UNP Q92847
R	512	PRO	-	expression tag	UNP Q92847
R	513	ASP	-	expression tag	UNP Q92847
R	514	GLY	-	expression tag	UNP Q92847
R	515	SER	-	expression tag	UNP Q92847
R	516	MET	-	expression tag	UNP Q92847
R	517	LEU	-	expression tag	UNP Q92847
R	518	PHE	-	expression tag	UNP Q92847
R	519	ARG	-	expression tag	UNP Q92847
R	520	VAL	-	expression tag	UNP Q92847

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Chain	Residue	Modelled	Actual	Comment	Reference
R	521	THR	-	expression tag	UNP Q92847
R	522	ILE	-	expression tag	UNP Q92847
R	523	ASN	-	expression tag	UNP Q92847
R	524	SER	-	expression tag	UNP Q92847

- Molecule 2 is a protein called Engineered G-alpha-q.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	240	Total	C	N	O	S	0	0
			1974	1248	352	365	9		

- 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	340	Total	C	N	O	S	0	0
			2610	1609	469	511	21		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	initiating methionine	UNP P62873
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	expression tag	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

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	linker	UNP P62873
B	342	SER	-	linker	UNP P62873
B	343	SER	-	linker	UNP P62873
B	344	GLY	-	linker	UNP P62873
B	345	GLY	-	linker	UNP P62873
B	346	GLY	-	linker	UNP P62873
B	347	GLY	-	linker	UNP P62873
B	348	SER	-	linker	UNP P62873
B	349	GLY	-	linker	UNP P62873
B	350	GLY	-	linker	UNP P62873
B	351	GLY	-	linker	UNP P62873
B	352	GLY	-	linker	UNP P62873
B	353	SER	-	linker	UNP P62873
B	354	SER	-	linker	UNP P62873
B	355	GLY	-	linker	UNP P62873

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	230	Total	C	N	O	S	0	0
			1771	1125	293	343	10		

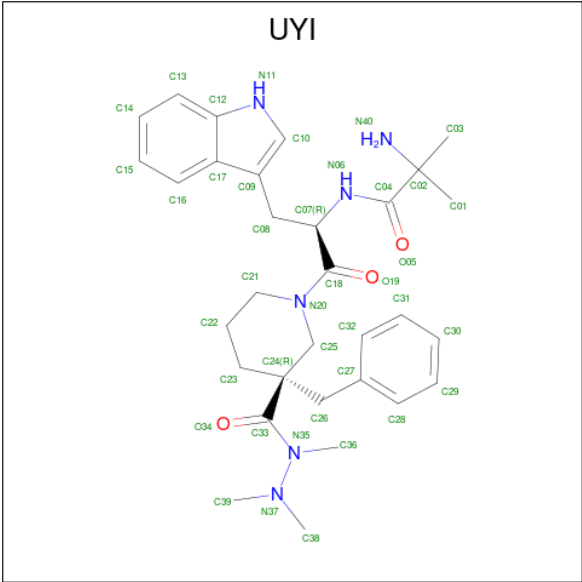
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

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

- Molecule 6 is a protein called Nb35.

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

- Molecule 7 is Anamorelin (CCD ID: UYI) (formula: C₃₁H₄₂N₆O₃).

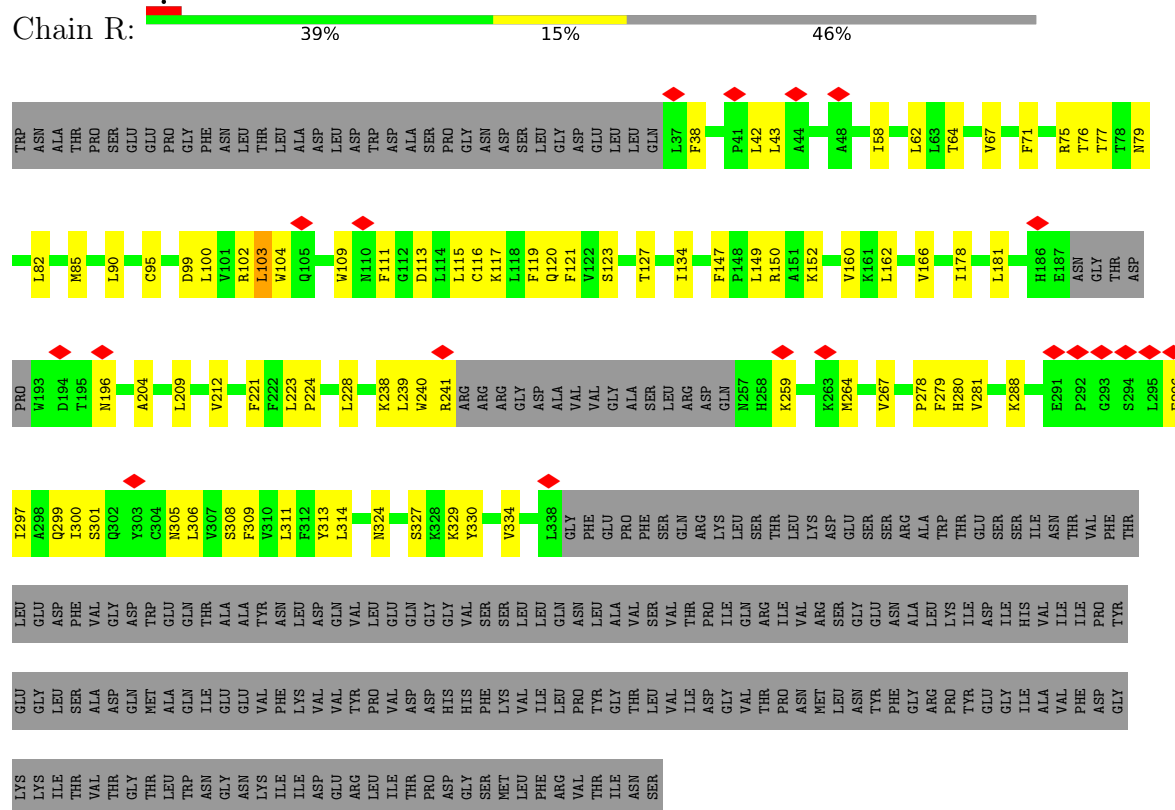


Mol	Chain	Residues	Atoms				AltConf
7	R	1	Total	C	N	O	0
			40	31	6	3	

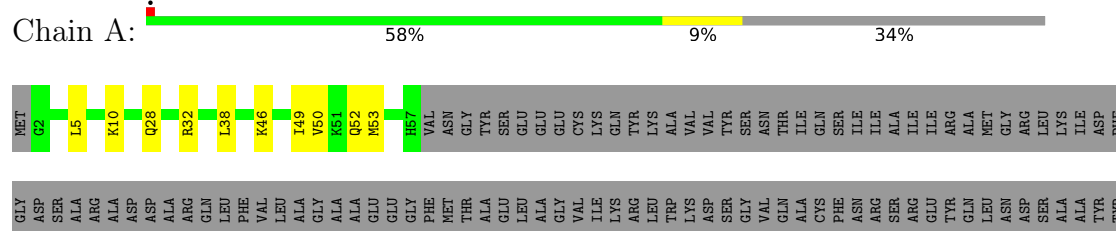
3 Residue-property plots

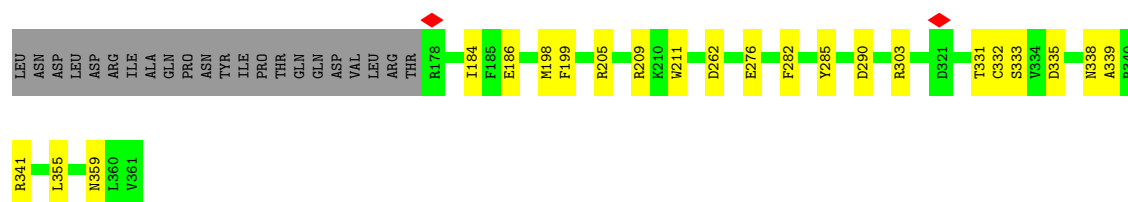
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: Growth hormone secretagogue receptor type 1

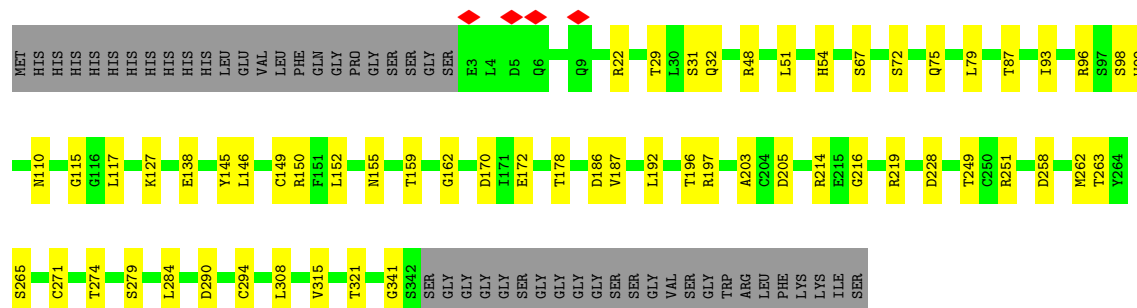


• Molecule 2: Engineered G-alpha-q

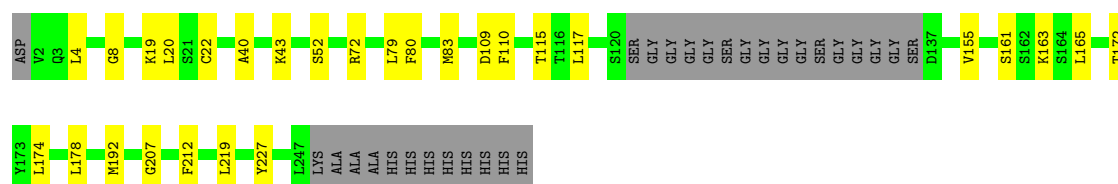
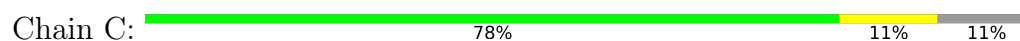




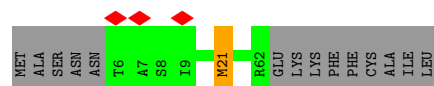
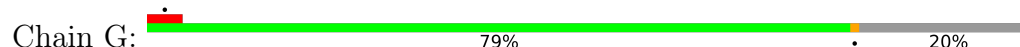
- Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



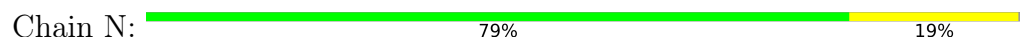
- Molecule 4: scFv16



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



- Molecule 6: Nb35



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	500563	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	63.639	Depositor
Minimum map value	-42.917	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4	Depositor
Map size ($\text{\AA}$)	281.6, 281.6, 281.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.88, 0.88, 0.88	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/2265	0.43	0/3086
2	A	0.12	0/2010	0.24	0/2705
3	B	0.14	0/2657	0.31	0/3602
4	C	0.13	0/1815	0.29	0/2461
5	G	0.10	0/442	0.23	0/597
6	N	0.12	0/981	0.25	0/1329
All	All	0.14	0/10170	0.32	0/13780

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2209	0	2289	51	0
2	A	1974	0	1971	22	0
3	B	2610	0	2513	36	0
4	C	1771	0	1709	16	0
5	G	436	0	448	1	0
6	N	961	0	928	16	0
7	R	40	0	0	0	0
All	All	10001	0	9858	134	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 7.

All (134) 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:R:109:TRP:H	1:R:196:ASN:HB2	1.51	0.76
2:A:205:ARG:NH1	3:B:186:ASP:OD1	2.22	0.71
1:R:278:PRO:HA	1:R:281:VAL:HG12	1.72	0.71
3:B:251:ARG:HG2	3:B:263:THR:HG22	1.73	0.70
1:R:99:ASP:OD1	1:R:102:ARG:NH2	2.24	0.70
2:A:285:TYR:O	2:A:303:ARG:NH1	2.25	0.69
3:B:197:ARG:HH11	3:B:214:ARG:HE	1.42	0.67
1:R:301:SER:O	1:R:305:ASN:ND2	2.27	0.67
4:C:52:SER:O	4:C:72:ARG:NH1	2.28	0.66
3:B:145:TYR:O	3:B:162:GLY:N	2.28	0.66
2:A:335:ASP:OD2	2:A:341:ARG:NH1	2.28	0.66
2:A:332:CYS:SG	2:A:333:SER:N	2.69	0.65
3:B:271:CYS:HB2	3:B:290:ASP:HB2	1.79	0.64
3:B:54:HIS:HE2	3:B:72:SER:HG	1.43	0.64
6:N:52:SER:O	6:N:72:ARG:NH1	2.31	0.63
2:A:52:GLN:NE2	2:A:338:ASN:OD1	2.32	0.63
6:N:91:THR:HG22	6:N:126:VAL:H	1.63	0.63
2:A:209:ARG:HH12	6:N:117:TYR:HE2	1.46	0.62
1:R:111:PHE:HB3	1:R:115:LEU:HD23	1.81	0.62
3:B:155:ASN:HD21	3:B:172:GLU:HG2	1.63	0.61
1:R:181:LEU:HD12	1:R:204:ALA:HB1	1.81	0.61
3:B:115:GLY:HA3	3:B:146:LEU:HD23	1.83	0.61
6:N:72:ARG:HE	6:N:74:ASN:HD21	1.49	0.61
3:B:249:THR:HG23	3:B:265:SER:HB3	1.83	0.60
1:R:327:SER:OG	2:A:359:ASN:ND2	2.35	0.60
1:R:77:THR:HG23	1:R:160:VAL:HG21	1.83	0.59
1:R:147:PHE:HD1	1:R:150:ARG:HH21	1.48	0.59
1:R:100:LEU:HA	1:R:103:LEU:HD23	1.85	0.59
3:B:48:ARG:NH2	3:B:341:GLY:O	2.36	0.58
2:A:50:VAL:HG12	2:A:198:MET:HE3	1.85	0.58
6:N:67:ARG:NH2	6:N:90:ASP:OD2	2.36	0.57
1:R:296:GLU:O	1:R:299:GLN:NE2	2.39	0.56
3:B:279:SER:HB2	3:B:284:LEU:HB2	1.86	0.56
3:B:149:CYS:O	3:B:150:ARG:NH1	2.39	0.56
4:C:8:GLY:O	4:C:115:THR:OG1	2.18	0.55
1:R:38:PHE:HB2	1:R:43:LEU:HD11	1.89	0.54
3:B:155:ASN:ND2	3:B:170:ASP:OD1	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:221:PHE:HB2	1:R:280:HIS:CE1	2.42	0.54
3:B:146:LEU:HD11	3:B:159:THR:HB	1.90	0.54
1:R:113:ASP:OD1	1:R:117:LYS:NZ	2.40	0.53
3:B:96:ARG:NH1	3:B:138:GLU:OE2	2.42	0.53
2:A:53:MET:HG3	2:A:198:MET:HE1	1.91	0.53
3:B:22:ARG:NE	3:B:258:ASP:O	2.38	0.53
1:R:95:CYS:HB3	1:R:119:PHE:CE1	2.44	0.53
2:A:5:LEU:O	2:A:10:LYS:NZ	2.38	0.52
1:R:82:LEU:HD13	1:R:324:ASN:ND2	2.25	0.52
1:R:238:LYS:O	1:R:241:ARG:HD2	2.10	0.52
1:R:223:LEU:HB3	1:R:224:PRO:HD3	1.93	0.51
1:R:58:ILE:HD12	1:R:90:LEU:HD11	1.92	0.51
4:C:83:MET:HE1	4:C:117:LEU:HD22	1.92	0.50
1:R:95:CYS:HB3	1:R:119:PHE:HE1	1.76	0.50
1:R:121:PHE:HA	1:R:178:ILE:HG21	1.93	0.50
4:C:161:SER:OG	4:C:163:LYS:O	2.28	0.50
1:R:43:LEU:HD23	1:R:104:TRP:HA	1.94	0.50
1:R:76:THR:OG1	1:R:79:ASN:OD1	2.29	0.50
3:B:54:HIS:NE2	3:B:72:SER:OG	2.30	0.49
1:R:297:ILE:HG23	1:R:300:ILE:HD11	1.93	0.49
1:R:279:PHE:HA	1:R:308:SER:HB3	1.94	0.49
1:R:102:ARG:HH12	1:R:119:PHE:HE2	1.60	0.49
3:B:79:LEU:HB2	3:B:93:ILE:HB	1.93	0.49
2:A:38:LEU:HD21	2:A:46:LYS:HB2	1.94	0.49
4:C:174:LEU:HB3	4:C:192:MET:HB2	1.95	0.49
4:C:192:MET:HG2	4:C:192:MET:O	2.12	0.48
2:A:290:ASP:OD1	2:A:290:ASP:N	2.39	0.48
1:R:82:LEU:HA	1:R:85:MET:HE2	1.95	0.48
1:R:309:PHE:CE1	1:R:313:TYR:HE2	2.31	0.48
6:N:99:CYS:SG	6:N:100:PRO:HD2	2.54	0.48
4:C:40:ALA:HB3	4:C:43:LYS:HB2	1.96	0.48
1:R:264:MET:O	1:R:267:VAL:HG12	2.13	0.48
1:R:209:LEU:O	1:R:212:VAL:HG22	2.14	0.48
1:R:134:ILE:HG22	1:R:228:LEU:HD11	1.97	0.47
2:A:262:ASP:OD1	2:A:262:ASP:N	2.44	0.47
4:C:165:LEU:HB3	4:C:172:THR:O	2.14	0.47
2:A:276:GLU:HG3	2:A:282:PHE:HB3	1.96	0.47
1:R:162:LEU:O	1:R:166:VAL:HG23	2.15	0.47
4:C:20:LEU:HG	4:C:83:MET:HE2	1.96	0.47
1:R:82:LEU:HD13	1:R:324:ASN:HD21	1.79	0.47
6:N:29:PHE:O	6:N:72:ARG:NH2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:N:83:MET:HB3	6:N:86:LEU:HD21	1.96	0.47
3:B:294:CYS:HB3	3:B:308:LEU:HB2	1.96	0.47
1:R:150:ARG:HD3	1:R:150:ARG:H	1.80	0.46
2:A:184:ILE:HD11	3:B:117:LEU:HD13	1.96	0.46
1:R:67:VAL:HG11	1:R:330:TYR:CE1	2.50	0.46
1:R:123:SER:O	1:R:127:THR:HG23	2.15	0.46
3:B:99:TRP:HB2	3:B:117:LEU:HB2	1.98	0.46
2:A:49:ILE:O	2:A:53:MET:HG2	2.16	0.46
3:B:31:SER:OG	3:B:262:MET:SD	2.74	0.46
3:B:75:GLN:O	3:B:98:SER:OG	2.32	0.46
4:C:4:LEU:HD12	4:C:110:PHE:HD2	1.80	0.46
2:A:53:MET:HE1	2:A:339:ALA:N	2.31	0.45
3:B:152:LEU:HD12	3:B:192:LEU:HD11	1.99	0.45
1:R:327:SER:C	1:R:329:LYS:H	2.24	0.45
1:R:109:TRP:N	1:R:196:ASN:HB2	2.27	0.45
3:B:197:ARG:NH1	3:B:214:ARG:HE	2.11	0.45
1:R:297:ILE:H	1:R:297:ILE:HD12	1.81	0.45
3:B:228:ASP:OD1	6:N:117:TYR:OH	2.33	0.45
2:A:28:GLN:O	2:A:32:ARG:HG2	2.17	0.44
1:R:71:PHE:O	1:R:75:ARG:HG3	2.17	0.44
1:R:150:ARG:HD3	1:R:150:ARG:N	2.32	0.44
6:N:36:TRP:HD1	6:N:70:ILE:HD12	1.83	0.44
3:B:110:ASN:HD22	3:B:127:LYS:HD2	1.82	0.43
1:R:42:LEU:HD21	1:R:306:LEU:HD21	2.01	0.43
3:B:178:THR:HG21	3:B:216:GLY:HA3	2.00	0.43
6:N:83:MET:HE1	6:N:124:VAL:HG11	2.00	0.43
1:R:330:TYR:O	1:R:334:VAL:HG23	2.19	0.43
6:N:22:CYS:HB3	6:N:79:LEU:HB3	2.01	0.43
3:B:67:SER:HB3	3:B:321:THR:HB	2.00	0.43
3:B:29:THR:HB	3:B:32:GLN:HG3	2.01	0.43
4:C:109:ASP:N	4:C:109:ASP:OD1	2.45	0.43
1:R:102:ARG:NH1	1:R:120:GLN:HE21	2.17	0.43
1:R:64:THR:O	1:R:67:VAL:HG12	2.19	0.42
2:A:211:TRP:HB2	3:B:117:LEU:HD21	2.01	0.42
3:B:51:LEU:HD23	3:B:87:THR:HG23	2.01	0.42
6:N:37:VAL:HG12	6:N:47:TRP:HA	2.01	0.42
3:B:219:ARG:HA	5:G:21:MET:HE1	2.00	0.42
4:C:19:LYS:HE3	4:C:80:PHE:CD1	2.55	0.42
3:B:205:ASP:OD1	3:B:205:ASP:N	2.52	0.42
4:C:22:CYS:HB3	4:C:79:LEU:HB3	2.02	0.42
6:N:72:ARG:NE	6:N:74:ASN:HD21	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:109:TRP:NE1	1:R:116:CYS:HB2	2.35	0.42
2:A:331:THR:OG1	2:A:332:CYS:N	2.53	0.42
3:B:274:THR:OG1	3:B:315:VAL:O	2.28	0.41
1:R:288:LYS:HA	1:R:288:LYS:HD3	1.83	0.41
2:A:186:GLU:HG3	2:A:199:PHE:CE1	2.56	0.41
3:B:187:VAL:HA	3:B:203:ALA:HA	2.03	0.41
4:C:155:VAL:HG12	4:C:219:LEU:HD21	2.02	0.41
6:N:3:GLN:HB3	6:N:5:GLN:HE22	1.86	0.41
6:N:33:LYS:HG3	6:N:51:ILE:O	2.20	0.41
1:R:239:LEU:HD21	2:A:355:LEU:HD21	2.04	0.40
4:C:207:GLY:HA3	4:C:212:PHE:HA	2.03	0.40
1:R:311:LEU:HD23	1:R:314:LEU:HD23	2.03	0.40
1:R:149:LEU:O	1:R:152:LYS:HG2	2.21	0.40
1:R:240:TRP:HZ3	1:R:259:LYS:HD3	1.87	0.40
4:C:178:LEU:HD13	4:C:227:TYR:CZ	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	276/523 (53%)	272 (99%)	4 (1%)	0	100	100
2	A	236/361 (65%)	232 (98%)	4 (2%)	0	100	100
3	B	338/388 (87%)	327 (97%)	11 (3%)	0	100	100
4	C	226/259 (87%)	220 (97%)	6 (3%)	0	100	100
5	G	55/71 (78%)	55 (100%)	0	0	100	100
6	N	124/129 (96%)	121 (98%)	3 (2%)	0	100	100
All	All	1255/1731 (72%)	1227 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R	240/459 (52%)	238 (99%)	2 (1%)	73	90
2	A	217/316 (69%)	217 (100%)	0	100	100
3	B	282/317 (89%)	281 (100%)	1 (0%)	84	94
4	C	195/209 (93%)	195 (100%)	0	100	100
5	G	46/58 (79%)	45 (98%)	1 (2%)	45	77
6	N	104/107 (97%)	104 (100%)	0	100	100
All	All	1084/1466 (74%)	1080 (100%)	4 (0%)	81	94

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

Mol	Chain	Res	Type
1	R	62	LEU
1	R	103	LEU
3	B	196	THR
5	G	21	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	R	61	ASN
1	R	280	HIS
1	R	324	ASN
2	A	52	GLN
2	A	213	GLN
2	A	231	ASN
2	A	261	GLN
2	A	338	ASN
2	A	359	ASN
3	B	6	GLN
3	B	75	GLN
3	B	110	ASN
3	B	155	ASN

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Mol	Chain	Res	Type
3	B	156	GLN
3	B	220	GLN
3	B	268	ASN
3	B	293	ASN
4	C	142	GLN
4	C	169	ASN
4	C	171	ASN
6	N	13	GLN
6	N	74	ASN
6	N	84	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](#)

1 ligand is 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	$\# Z > 2$
7	UYI	R	601	-	37,43,43	2.54	14 (37%)	48,63,63	1.99	12 (25%)

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
7	UYI	R	601	-	-	4/41/53/53	0/4/4/4

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	R	601	UYI	C07-C18	7.04	1.66	1.53
7	R	601	UYI	C18-N20	6.14	1.43	1.35
7	R	601	UYI	C39-N37	4.98	1.52	1.46
7	R	601	UYI	C38-N37	4.78	1.52	1.46
7	R	601	UYI	C04-N06	4.46	1.42	1.34
7	R	601	UYI	C08-C07	3.43	1.60	1.53
7	R	601	UYI	C26-C27	2.83	1.55	1.51
7	R	601	UYI	C25-C24	2.48	1.62	1.54
7	R	601	UYI	C26-C24	2.47	1.59	1.55
7	R	601	UYI	C10-N11	2.39	1.41	1.37
7	R	601	UYI	C17-C12	2.35	1.44	1.41
7	R	601	UYI	C17-C09	2.22	1.47	1.44
7	R	601	UYI	C12-N11	2.13	1.41	1.37
7	R	601	UYI	C10-C09	2.01	1.39	1.36

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	R	601	UYI	C07-C18-N20	6.34	128.40	118.85
7	R	601	UYI	C02-C04-N06	4.78	125.84	116.63
7	R	601	UYI	C39-N37-C38	-3.90	105.36	112.52
7	R	601	UYI	O19-C18-C07	-3.86	112.54	119.61
7	R	601	UYI	C08-C07-C18	3.79	117.78	109.71
7	R	601	UYI	C08-C07-N06	3.38	117.08	110.64
7	R	601	UYI	C16-C17-C12	-2.86	115.88	118.84
7	R	601	UYI	C22-C23-C24	2.61	116.13	112.40
7	R	601	UYI	O05-C04-N06	-2.53	117.62	122.71
7	R	601	UYI	O19-C18-N20	-2.14	119.05	121.61
7	R	601	UYI	O05-C04-C02	-2.14	116.53	120.58
7	R	601	UYI	C23-C22-C21	2.07	114.14	110.75

There are no chirality outliers.

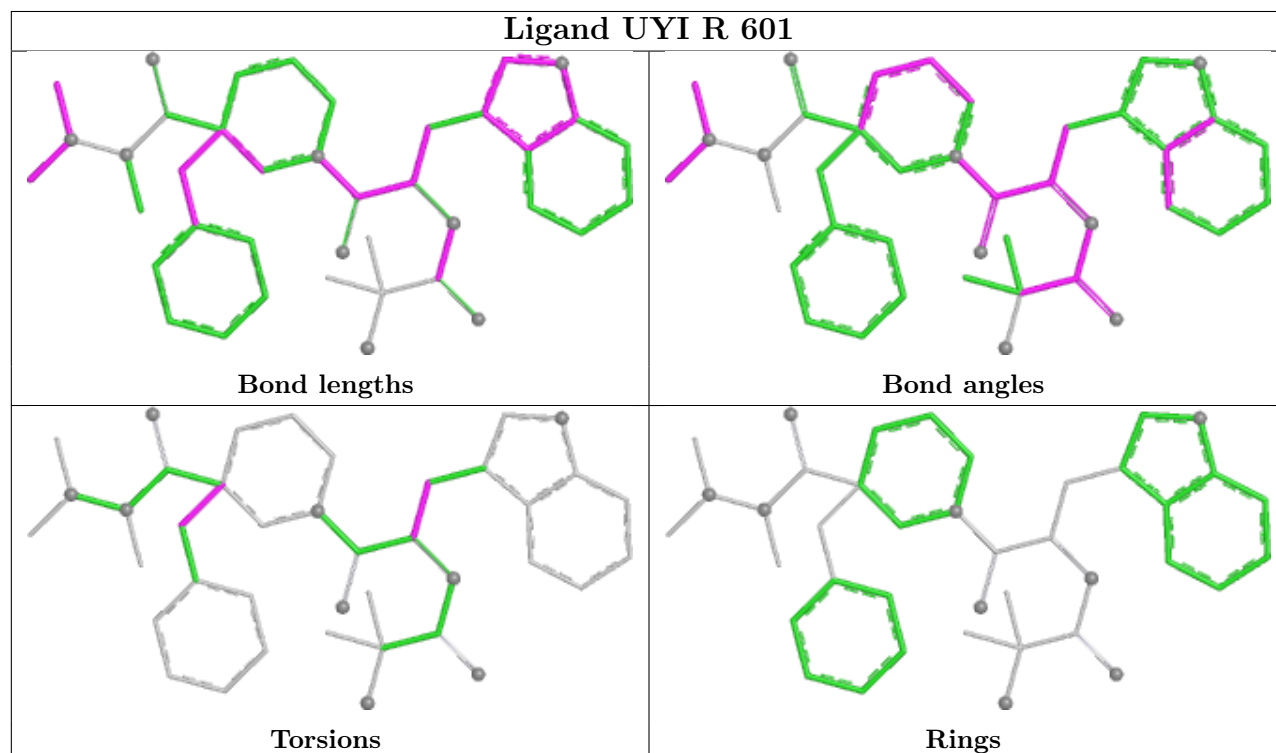
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	R	601	UYI	C23-C24-C26-C27
7	R	601	UYI	C25-C24-C26-C27
7	R	601	UYI	C33-C24-C26-C27
7	R	601	UYI	C18-C07-C08-C09

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

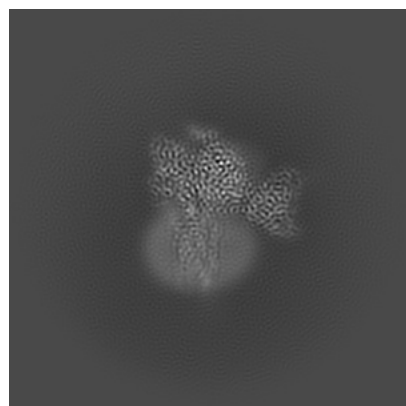
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36627. These allow visual inspection of the internal detail of the map and identification of artifacts.

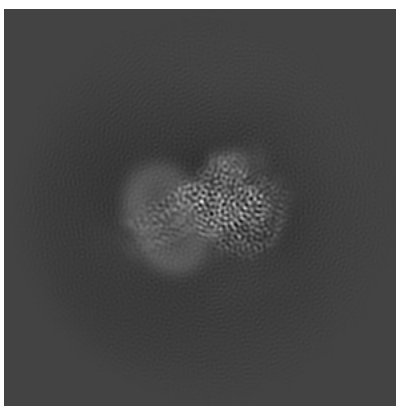
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

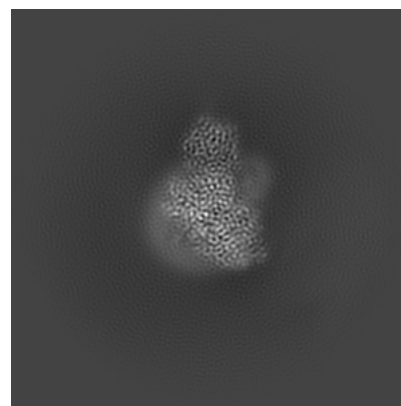
6.1.1 Primary map



X

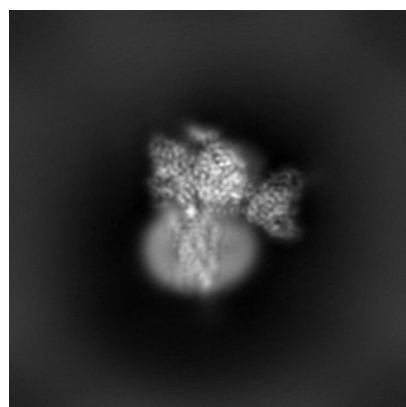


Y

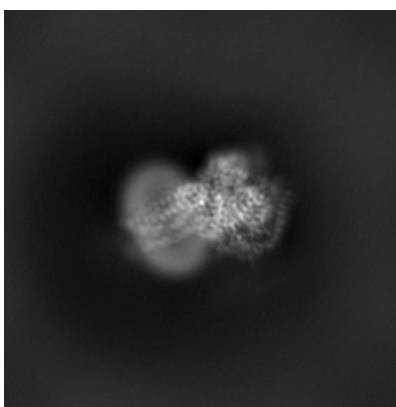


Z

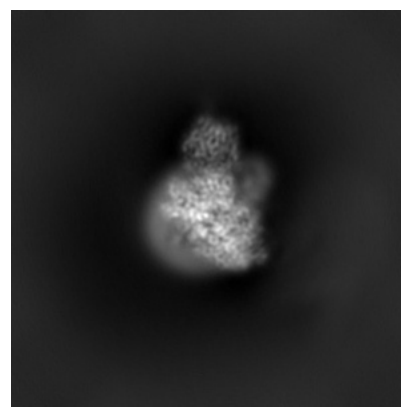
6.1.2 Raw map



X



Y

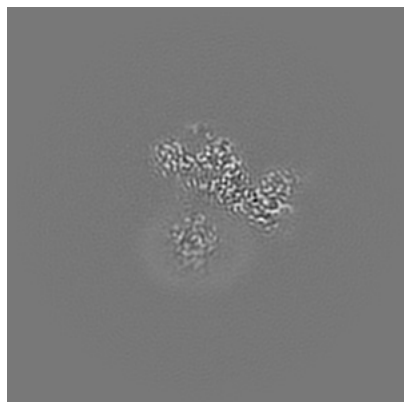


Z

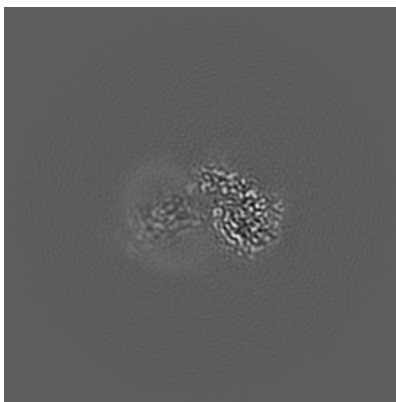
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

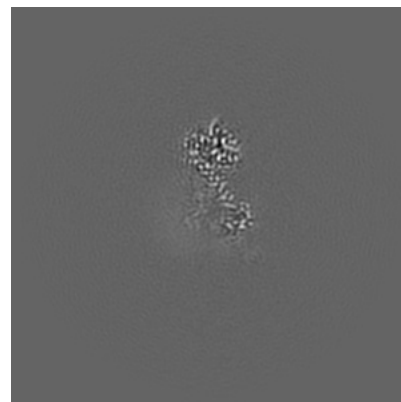
6.2.1 Primary map



X Index: 160

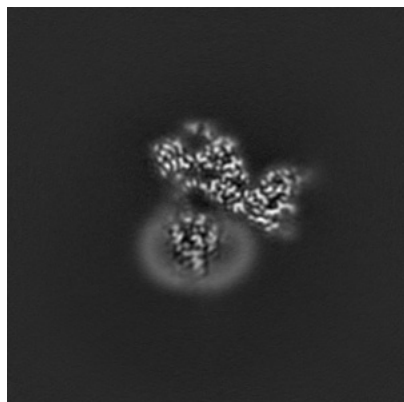


Y Index: 160

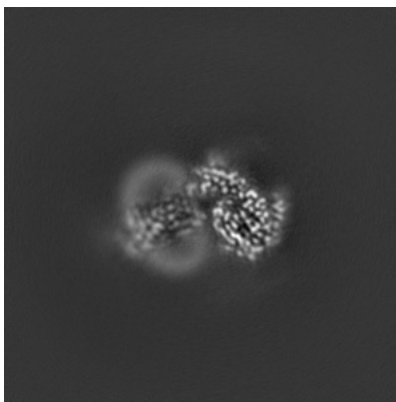


Z Index: 160

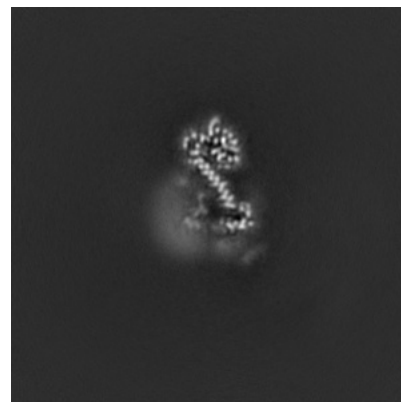
6.2.2 Raw map



X Index: 160



Y Index: 160

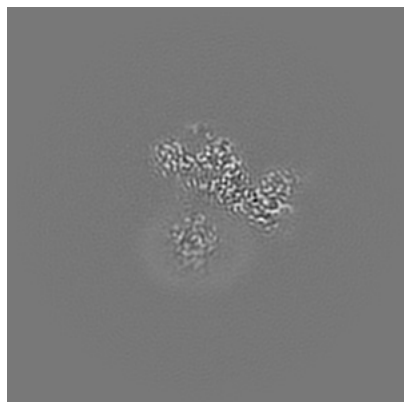


Z Index: 160

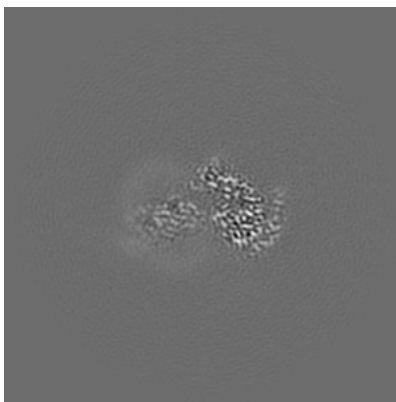
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

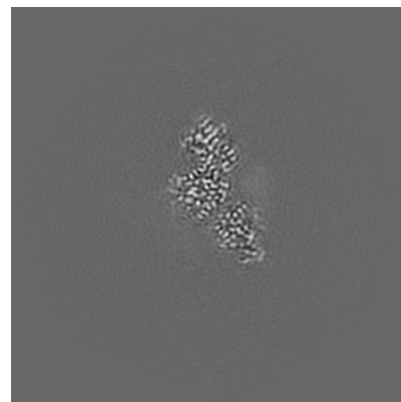
6.3.1 Primary map



X Index: 160

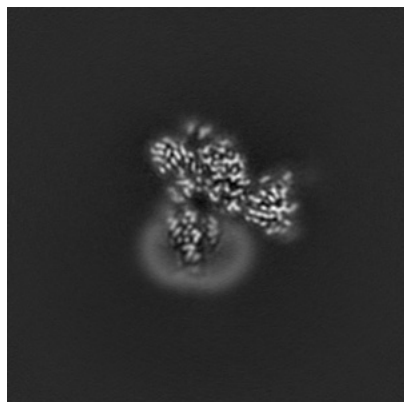


Y Index: 156

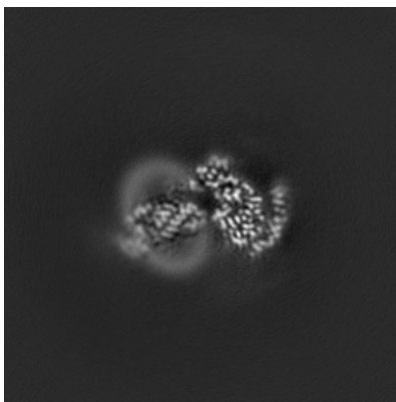


Z Index: 172

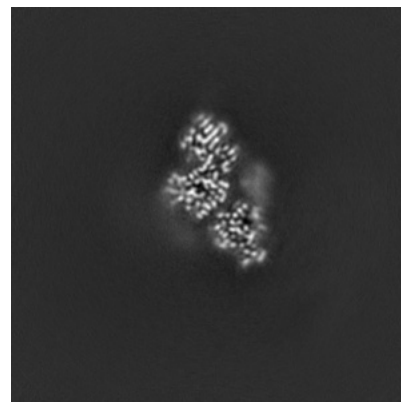
6.3.2 Raw map



X Index: 164



Y Index: 155

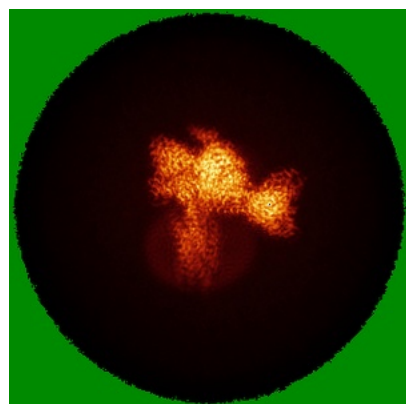


Z Index: 172

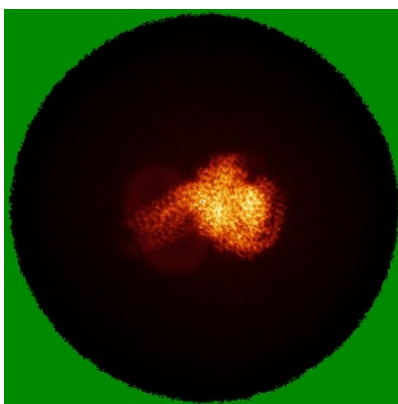
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

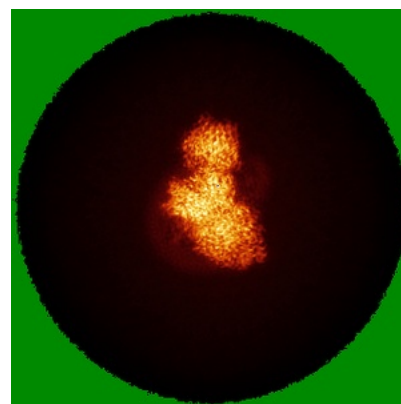
6.4.1 Primary map



X

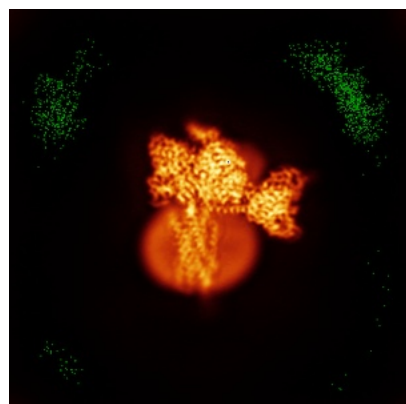


Y

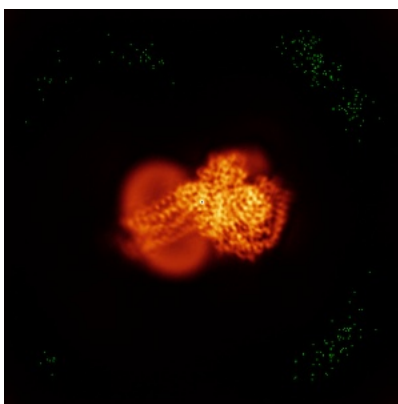


Z

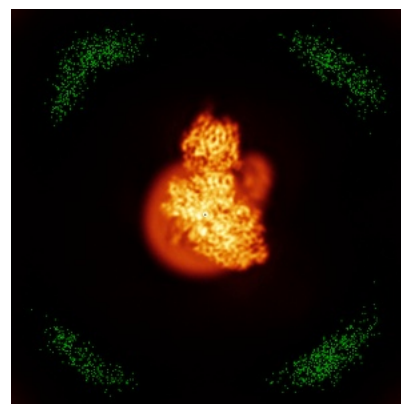
6.4.2 Raw map



X



Y

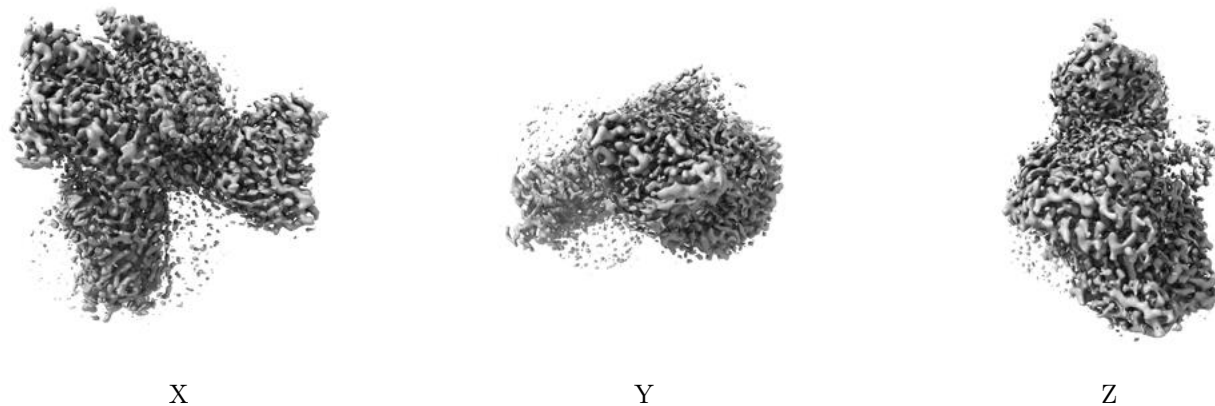


Z

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

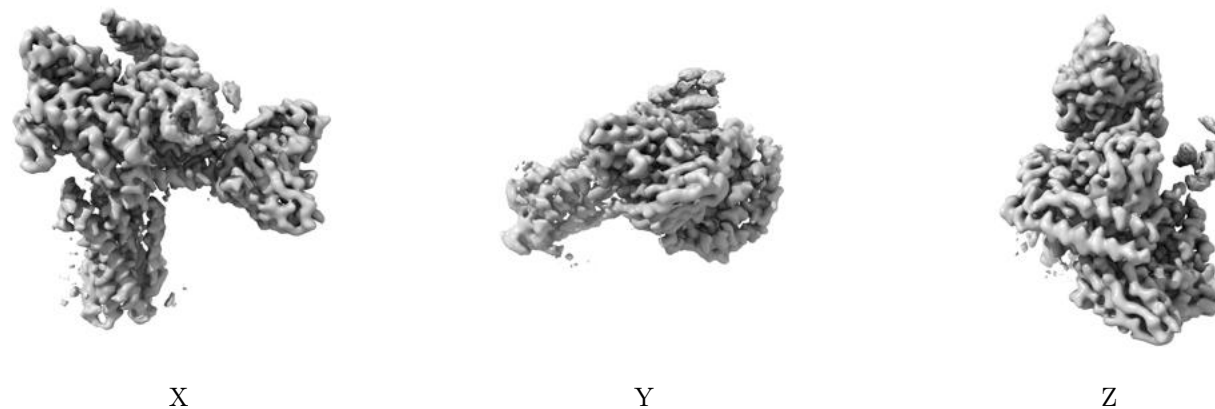
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

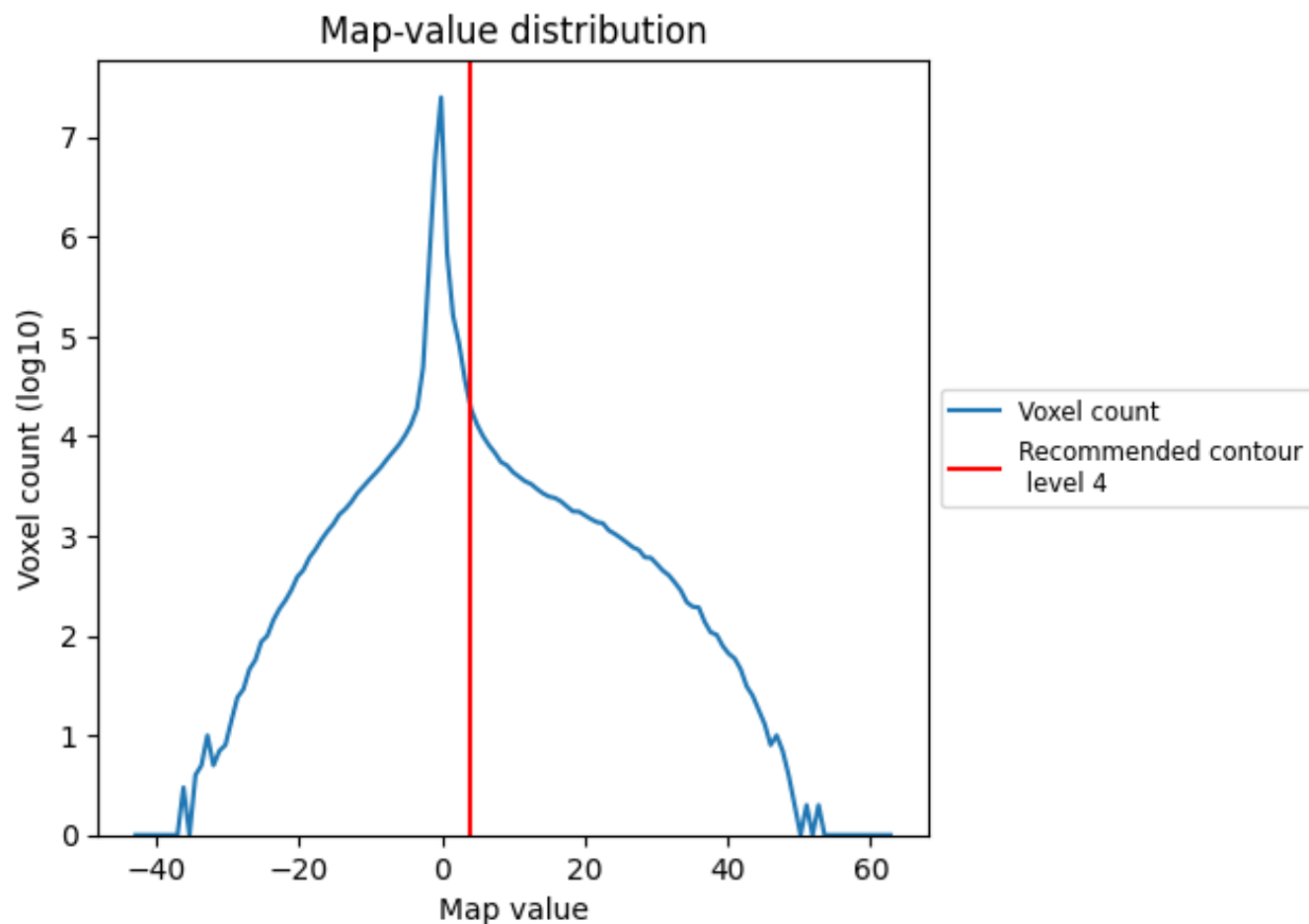
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

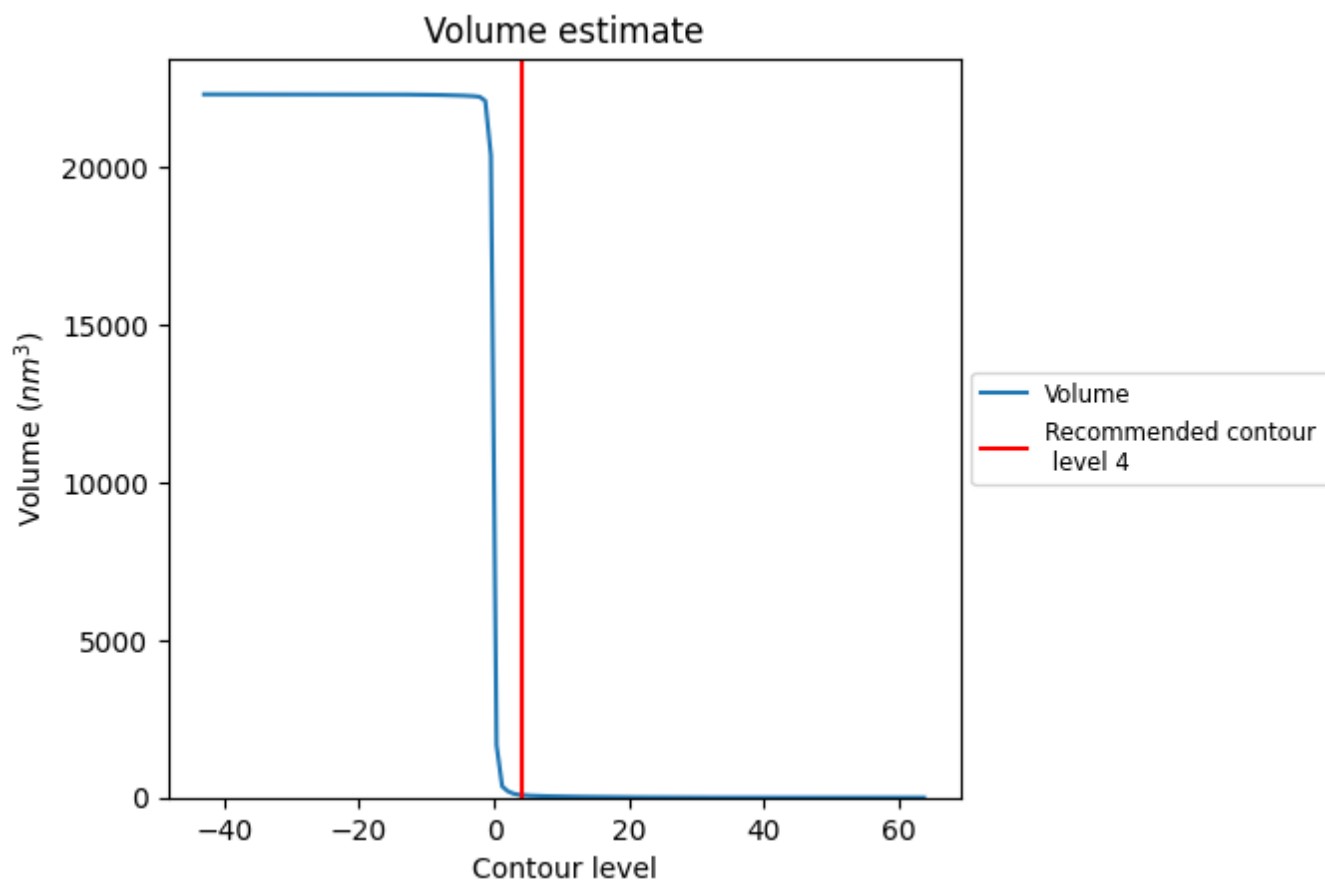
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

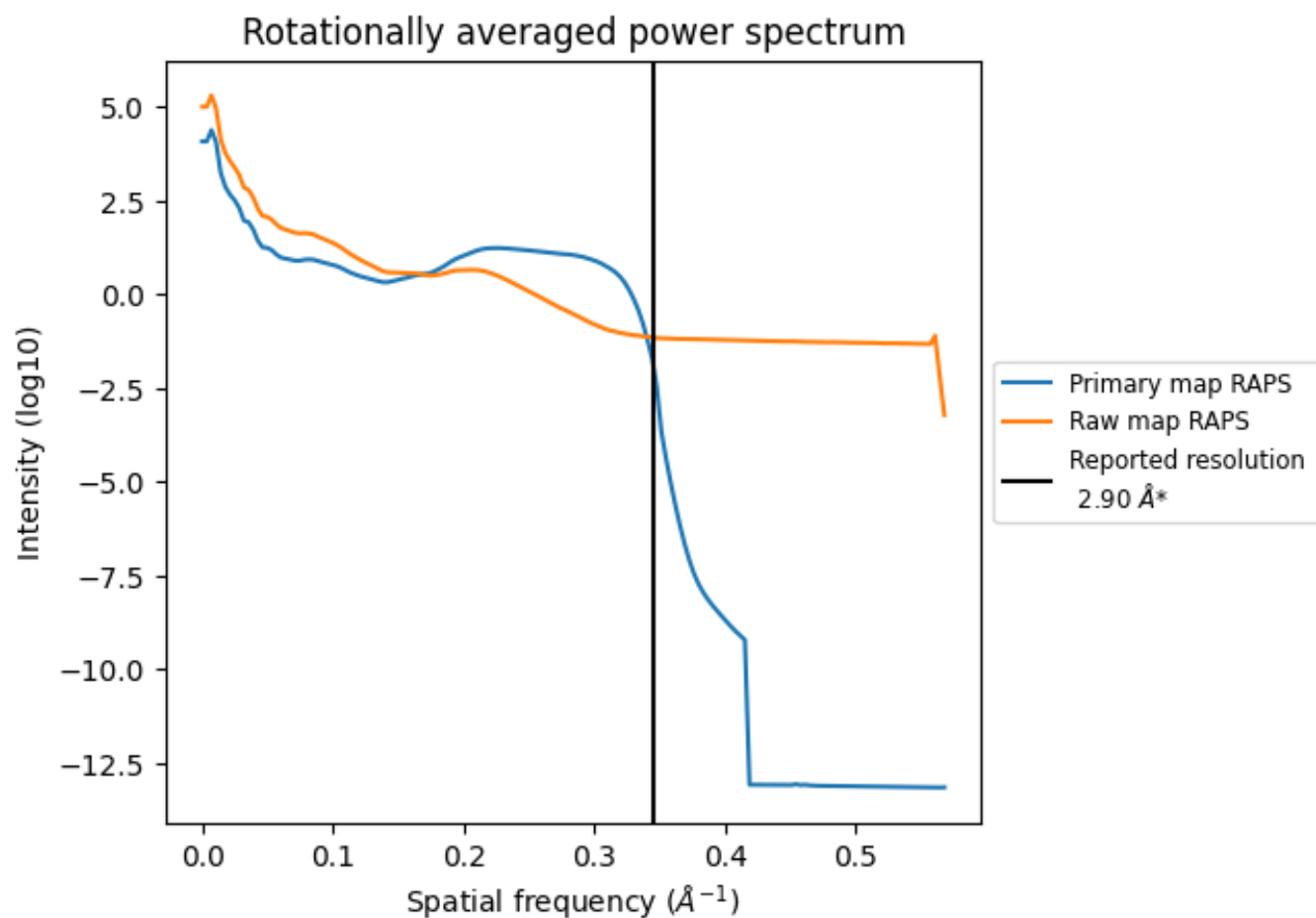
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 82 nm^3 ; this corresponds to an approximate mass of 74 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 ⓘ

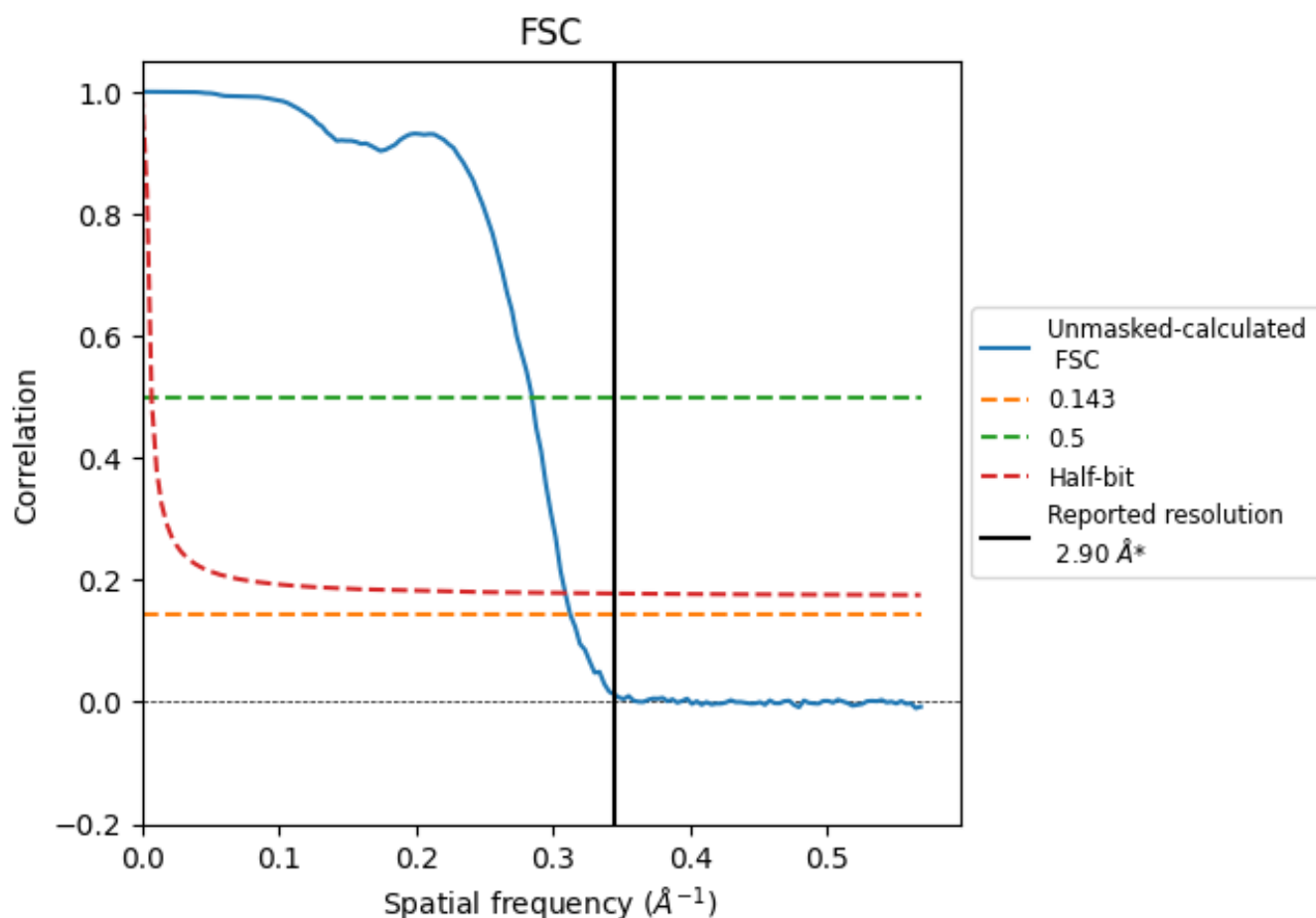


*Reported resolution corresponds to spatial frequency of 0.345 Å⁻¹

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 $0.345 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

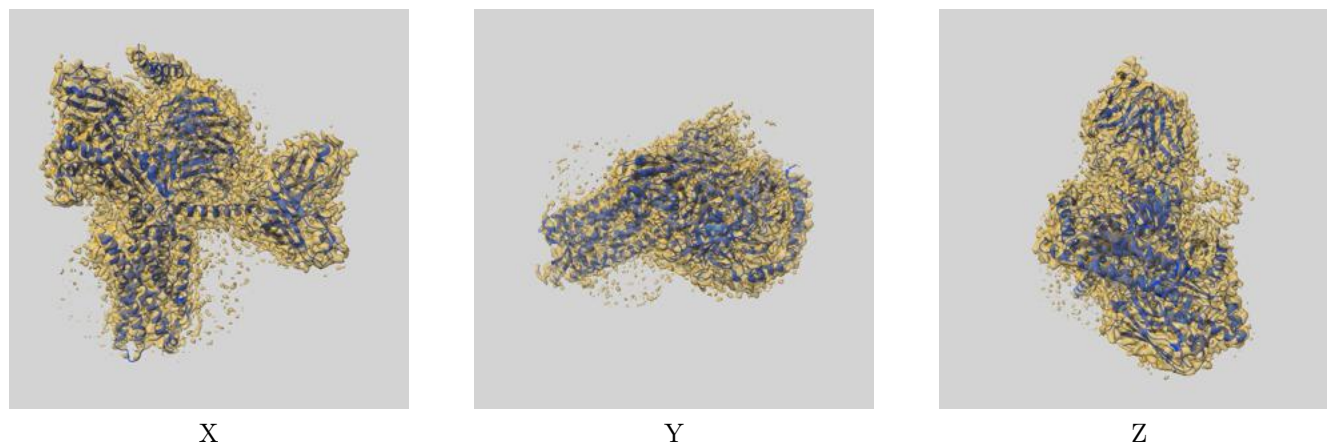
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.90	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.20	3.51	3.24

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.20 differs from the reported value 2.9 by more than 10 %

9 Map-model fit [i](#)

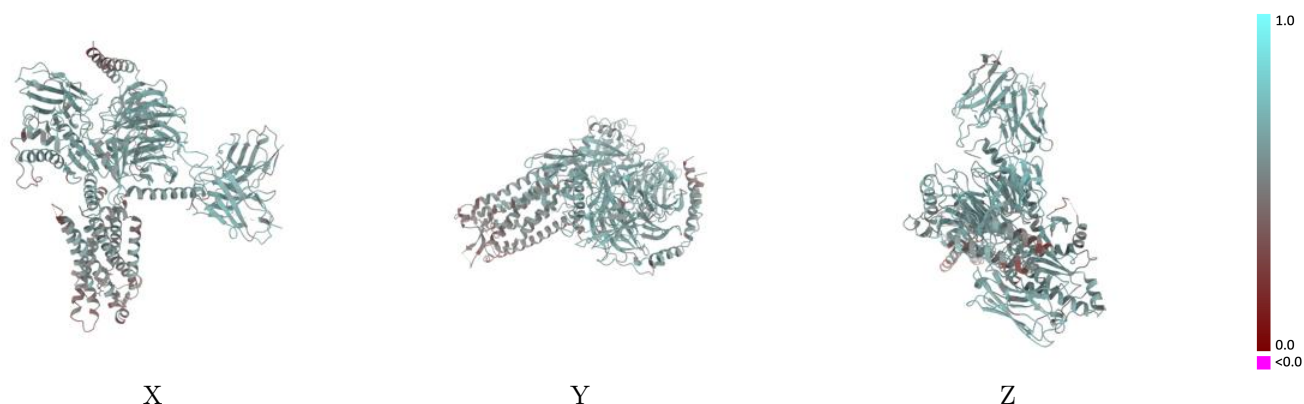
This section contains information regarding the fit between EMDB map EMD-36627 and PDB model 8JSR. Per-residue inclusion information can be found in section [3](#) on page [11](#).

9.1 Map-model overlay [i](#)



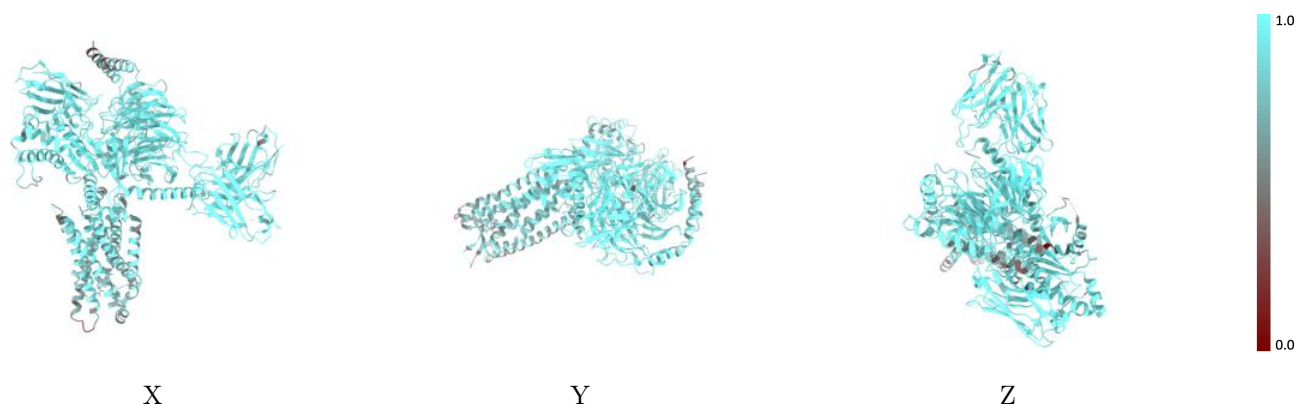
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



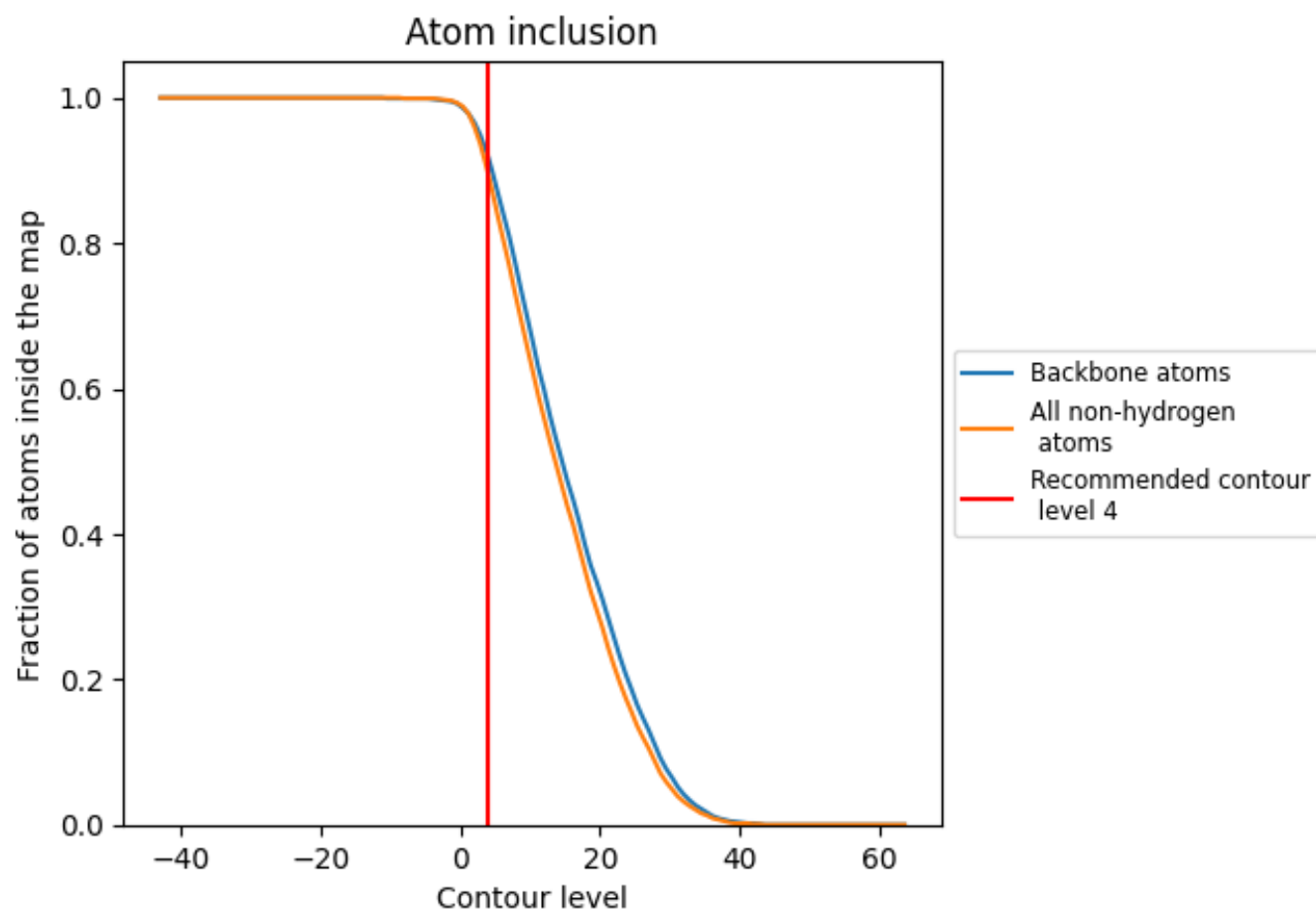
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 90% 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 (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8960	0.5660
A	0.9170	0.5770
B	0.9490	0.6060
C	0.9470	0.6000
G	0.8180	0.5360
N	0.9520	0.6020
R	0.7680	0.4720

1.0

0.0

<0.0