W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

wwPDB EM Validation Summary Report (i)

Nov 18, 2024 – 11:40 AM JST

PDB ID	:	8WYJ
EMDB ID	:	EMD-37930
Title	:	The global map of Omicron Subvariants Spike with two antibodies
Authors	:	Yan, R.H.; Wang, A.J.; Yang, H.N.
Deposited on	:	2023-10-31
Resolution	:	3.10 Å(reported)

This is a wwPDB EM Validation Summary 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 (i) 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 (i)) were used in the production of this report:
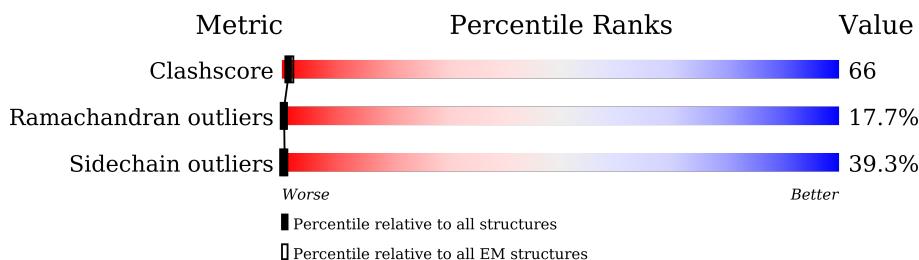
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY
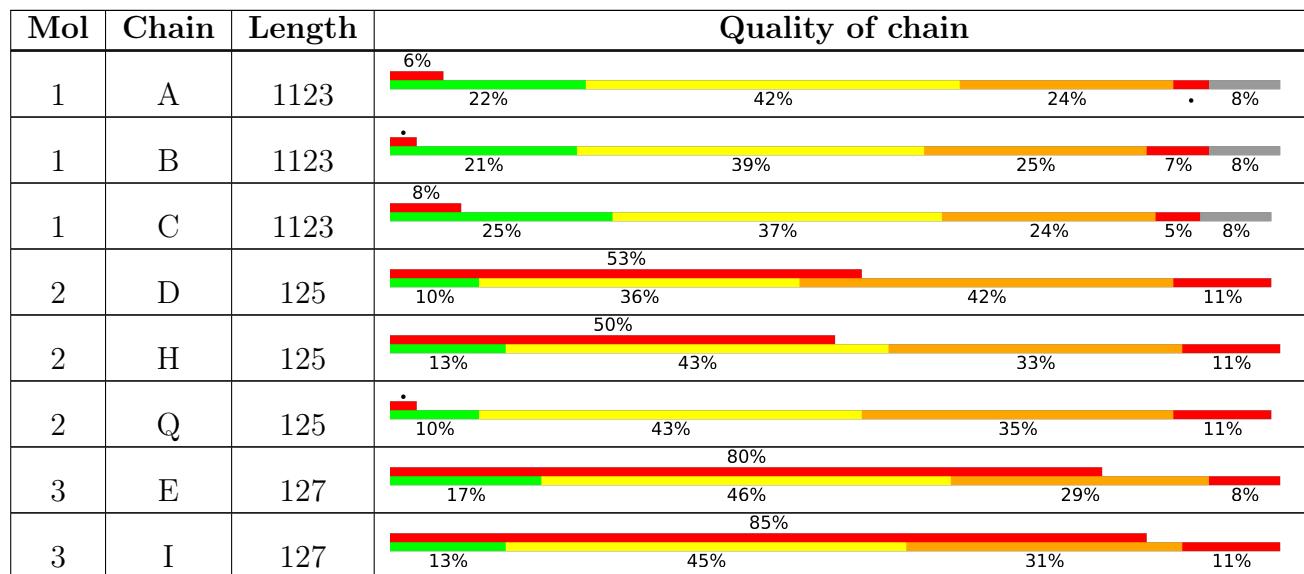
The reported resolution of this entry is 3.10 Å.

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	Percentile Ranks	Value
Clashscore		66
Ramachandran outliers		17.7%
Sidechain outliers		39.3%

Worse ... *Better*

▮ Percentile relative to all structures
▯ Percentile relative to all EM structures

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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1123	6% / 22% 42% 24% • 8%
1	B	1123	• / 21% 39% 25% 7% 8%
1	C	1123	8% / 25% 37% 24% 5% 8%
2	D	125	53% / 10% 36% 42% 11%
2	H	125	50% / 13% 43% 33% 11%
2	Q	125	• / 10% 43% 35% 11%
3	E	127	80% / 17% 46% 29% 8%
3	I	127	85% / 13% 45% 31% 11%

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Mol	Chain	Length	Quality of chain
3	S	127	45% · 14% · 50% · 28% · 8%
4	F	106	84% · 15% · 37% · 41% · 8%
4	J	106	74% · 14% · 42% · 35% · 8%
4	R	106	7% · 11% · 42% · 39% · 8%
5	G	104	95% · 19% · 44% · 22% · 14%
5	K	104	86% · 19% · 45% · 27% · 9%
5	T	104	38% · 15% · 47% · 25% · 12%

2   Entity composition (i)

There are 5 unique types of molecules in this entry. The entry contains 34491 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		
1	B	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		
1	C	1030	Total	C	N	O	S	0	0
			8083	5183	1342	1522	36		

There are 207 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	22	ILE	THR	conflict	UNP P0DTC2
A	24	THR	ARG	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	conflict	UNP P0DTC2
A	50	LEU	SER	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	127	PHE	VAL	conflict	UNP P0DTC2
A	142	ASP	GLY	conflict	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	157	SER	PHE	conflict	UNP P0DTC2
A	158	GLY	ARG	conflict	UNP P0DTC2
A	?	-	ASN	deletion	UNP P0DTC2
A	211	ILE	LEU	conflict	UNP P0DTC2
A	212	GLY	VAL	conflict	UNP P0DTC2
A	215	PHE	LEU	conflict	UNP P0DTC2
A	245	ASN	HIS	conflict	UNP P0DTC2
A	264	ASP	ALA	conflict	UNP P0DTC2
A	332	VAL	ILE	conflict	UNP P0DTC2
A	339	HIS	GLY	conflict	UNP P0DTC2
A	356	THR	LYS	conflict	UNP P0DTC2
A	371	PHE	SER	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	376	ALA	THR	conflict	UNP P0DTC2
A	403	LYS	ARG	conflict	UNP P0DTC2
A	405	ASN	ASP	conflict	UNP P0DTC2
A	408	SER	ARG	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	445	HIS	VAL	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	450	ASP	ASN	conflict	UNP P0DTC2
A	452	TRP	LEU	conflict	UNP P0DTC2
A	460	LYS	ASN	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	481	LYS	ASN	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	483	LYS	GLU	conflict	UNP P0DTC2
A	485	PRO	PHE	conflict	UNP P0DTC2
A	497	ARG	GLN	conflict	UNP P0DTC2
A	500	TYR	ASN	conflict	UNP P0DTC2
A	504	HIS	TYR	conflict	UNP P0DTC2
A	553	LYS	GLU	conflict	UNP P0DTC2
A	569	VAL	ALA	conflict	UNP P0DTC2
A	613	GLY	ASP	conflict	UNP P0DTC2
A	620	SER	PRO	conflict	UNP P0DTC2
A	654	TYR	HIS	conflict	UNP P0DTC2
A	669	VAL	ILE	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	ARG	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	939	PHE	SER	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1143	LEU	PRO	conflict	UNP P0DTC2
B	22	ILE	THR	conflict	UNP P0DTC2
B	24	THR	ARG	conflict	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	conflict	UNP P0DTC2
B	50	LEU	SER	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	127	PHE	VAL	conflict	UNP P0DTC2
B	142	ASP	GLY	conflict	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	157	SER	PHE	conflict	UNP P0DTC2
B	158	GLY	ARG	conflict	UNP P0DTC2
B	?	-	ASN	deletion	UNP P0DTC2
B	211	ILE	LEU	conflict	UNP P0DTC2
B	212	GLY	VAL	conflict	UNP P0DTC2
B	215	PHE	LEU	conflict	UNP P0DTC2
B	245	ASN	HIS	conflict	UNP P0DTC2
B	264	ASP	ALA	conflict	UNP P0DTC2
B	332	VAL	ILE	conflict	UNP P0DTC2
B	339	HIS	GLY	conflict	UNP P0DTC2
B	356	THR	LYS	conflict	UNP P0DTC2
B	371	PHE	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2
B	375	PHE	SER	conflict	UNP P0DTC2
B	376	ALA	THR	conflict	UNP P0DTC2
B	403	LYS	ARG	conflict	UNP P0DTC2
B	405	ASN	ASP	conflict	UNP P0DTC2
B	408	SER	ARG	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	445	HIS	VAL	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	450	ASP	ASN	conflict	UNP P0DTC2
B	452	TRP	LEU	conflict	UNP P0DTC2
B	460	LYS	ASN	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	481	LYS	ASN	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	483	LYS	GLU	conflict	UNP P0DTC2
B	485	PRO	PHE	conflict	UNP P0DTC2
B	497	ARG	GLN	conflict	UNP P0DTC2
B	500	TYR	ASN	conflict	UNP P0DTC2
B	504	HIS	TYR	conflict	UNP P0DTC2
B	553	LYS	GLU	conflict	UNP P0DTC2
B	569	VAL	ALA	conflict	UNP P0DTC2
B	613	GLY	ASP	conflict	UNP P0DTC2
B	620	SER	PRO	conflict	UNP P0DTC2
B	654	TYR	HIS	conflict	UNP P0DTC2
B	669	VAL	ILE	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	ARG	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	939	PHE	SER	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	986	PRO	LYS	conflict	UNP P0DTC2
B	987	PRO	VAL	conflict	UNP P0DTC2
B	1143	LEU	PRO	conflict	UNP P0DTC2
C	22	ILE	THR	conflict	UNP P0DTC2
C	24	THR	ARG	conflict	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	conflict	UNP P0DTC2
C	50	LEU	SER	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	127	PHE	VAL	conflict	UNP P0DTC2
C	142	ASP	GLY	conflict	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	157	SER	PHE	conflict	UNP P0DTC2
C	158	GLY	ARG	conflict	UNP P0DTC2
C	?	-	ASN	deletion	UNP P0DTC2
C	211	ILE	LEU	conflict	UNP P0DTC2
C	212	GLY	VAL	conflict	UNP P0DTC2
C	215	PHE	LEU	conflict	UNP P0DTC2
C	245	ASN	HIS	conflict	UNP P0DTC2
C	264	ASP	ALA	conflict	UNP P0DTC2
C	332	VAL	ILE	conflict	UNP P0DTC2
C	339	HIS	GLY	conflict	UNP P0DTC2
C	356	THR	LYS	conflict	UNP P0DTC2
C	371	PHE	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	376	ALA	THR	conflict	UNP P0DTC2
C	403	LYS	ARG	conflict	UNP P0DTC2
C	405	ASN	ASP	conflict	UNP P0DTC2
C	408	SER	ARG	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	445	HIS	VAL	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	450	ASP	ASN	conflict	UNP P0DTC2
C	452	TRP	LEU	conflict	UNP P0DTC2
C	460	LYS	ASN	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	481	LYS	ASN	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	483	LYS	GLU	conflict	UNP P0DTC2
C	485	PRO	PHE	conflict	UNP P0DTC2
C	497	ARG	GLN	conflict	UNP P0DTC2
C	500	TYR	ASN	conflict	UNP P0DTC2
C	504	HIS	TYR	conflict	UNP P0DTC2
C	553	LYS	GLU	conflict	UNP P0DTC2
C	569	VAL	ALA	conflict	UNP P0DTC2
C	613	GLY	ASP	conflict	UNP P0DTC2
C	620	SER	PRO	conflict	UNP P0DTC2
C	654	TYR	HIS	conflict	UNP P0DTC2
C	669	VAL	ILE	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	ARG	PRO	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	conflict	UNP P0DTC2
C	892	PRO	ALA	conflict	UNP P0DTC2
C	899	PRO	ALA	conflict	UNP P0DTC2
C	939	PHE	SER	conflict	UNP P0DTC2
C	942	PRO	ALA	conflict	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	986	PRO	LYS	conflict	UNP P0DTC2
C	987	PRO	VAL	conflict	UNP P0DTC2
C	1143	LEU	PRO	conflict	UNP P0DTC2

- Molecule 2 is a protein called SA55-HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Q	125	Total	C	N	O	S	0	0
			924	586	156	177	5		
2	D	125	Total	C	N	O	S	0	0
			924	586	156	177	5		
2	H	125	Total	C	N	O	S	0	0
			924	586	156	177	5		

- Molecule 3 is a protein called S309-HC.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	S	127	Total	C	N	O	S	0	0
			956	605	166	180	5		
3	E	127	Total	C	N	O	S	0	0
			956	605	166	180	5		
3	I	127	Total	C	N	O	S	0	0
			956	605	166	180	5		

- Molecule 4 is a protein called SA55_KC.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	106	Total	C	N	O	S	0	0
			796	505	134	154	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	106	Total 796	C 505	N 134	O 154	S 3	0	0
4	J	106	Total 796	C 505	N 134	O 154	S 3	0	0
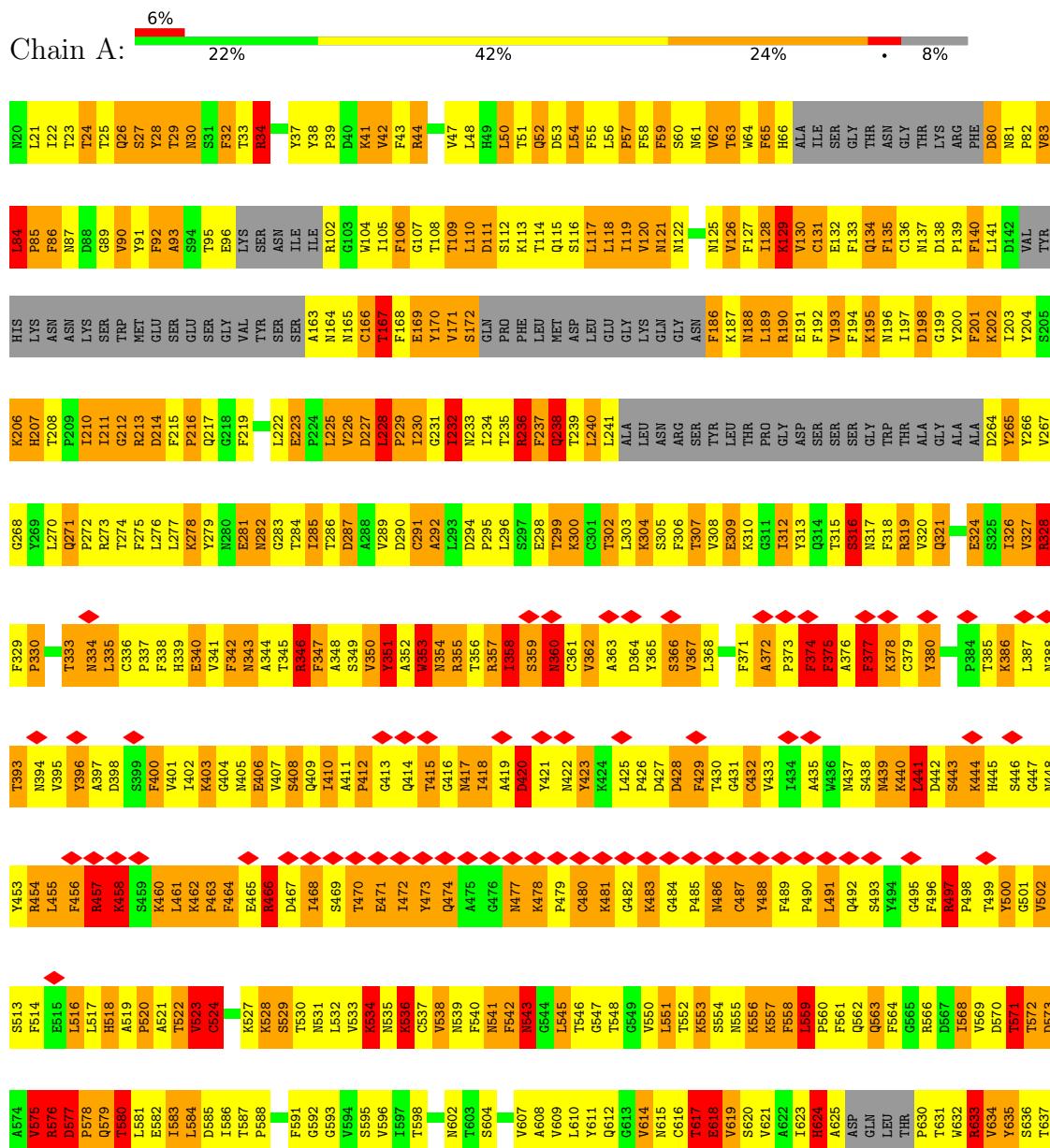
- Molecule 5 is a protein called S309-KC.
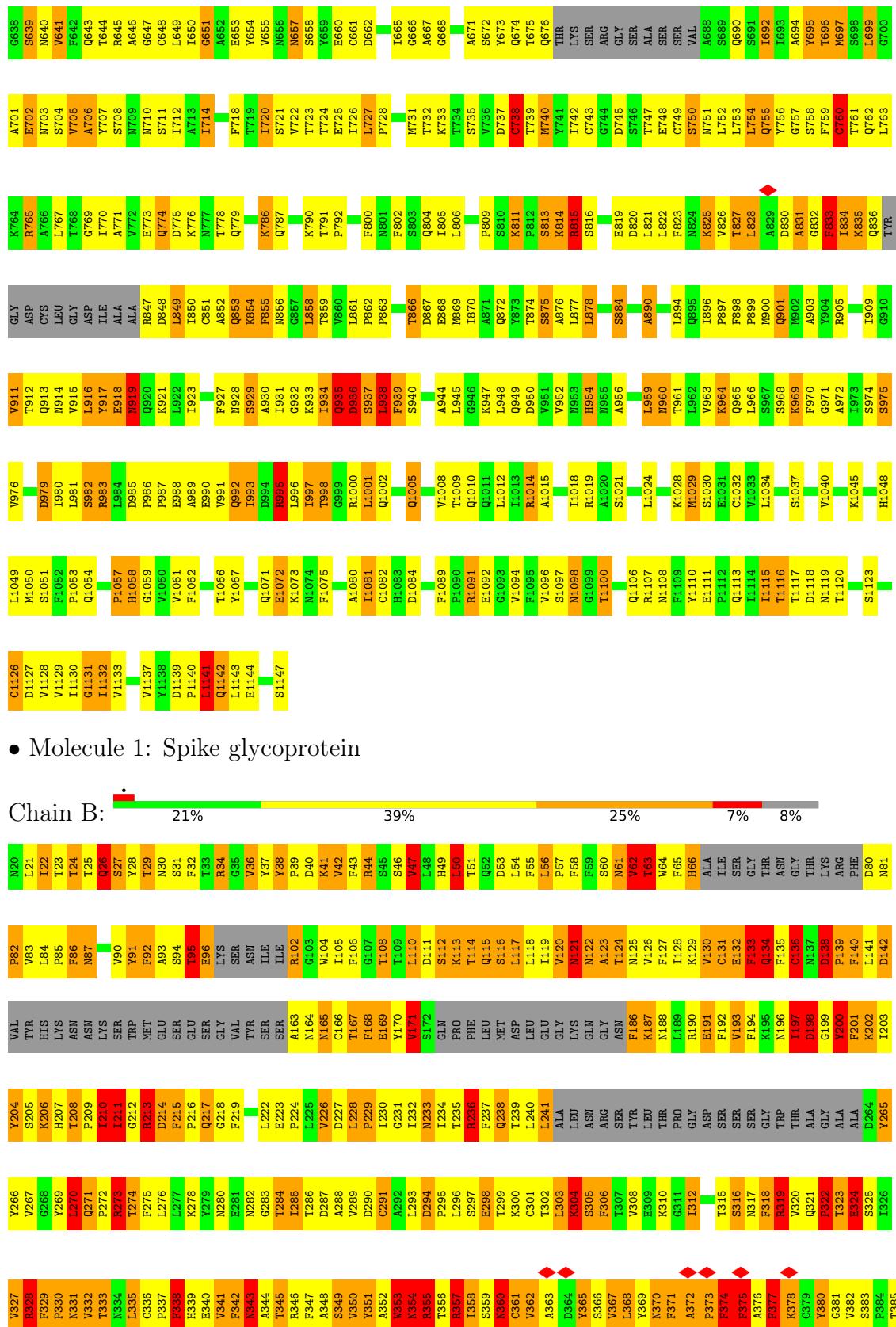
Mol	Chain	Residues	Atoms					AltConf	Trace
5	T	104	Total 738	C 466	N 134	O 136	S 2	0	0
5	G	104	Total 738	C 466	N 134	O 136	S 2	0	0
5	K	104	Total 738	C 466	N 134	O 136	S 2	0	0
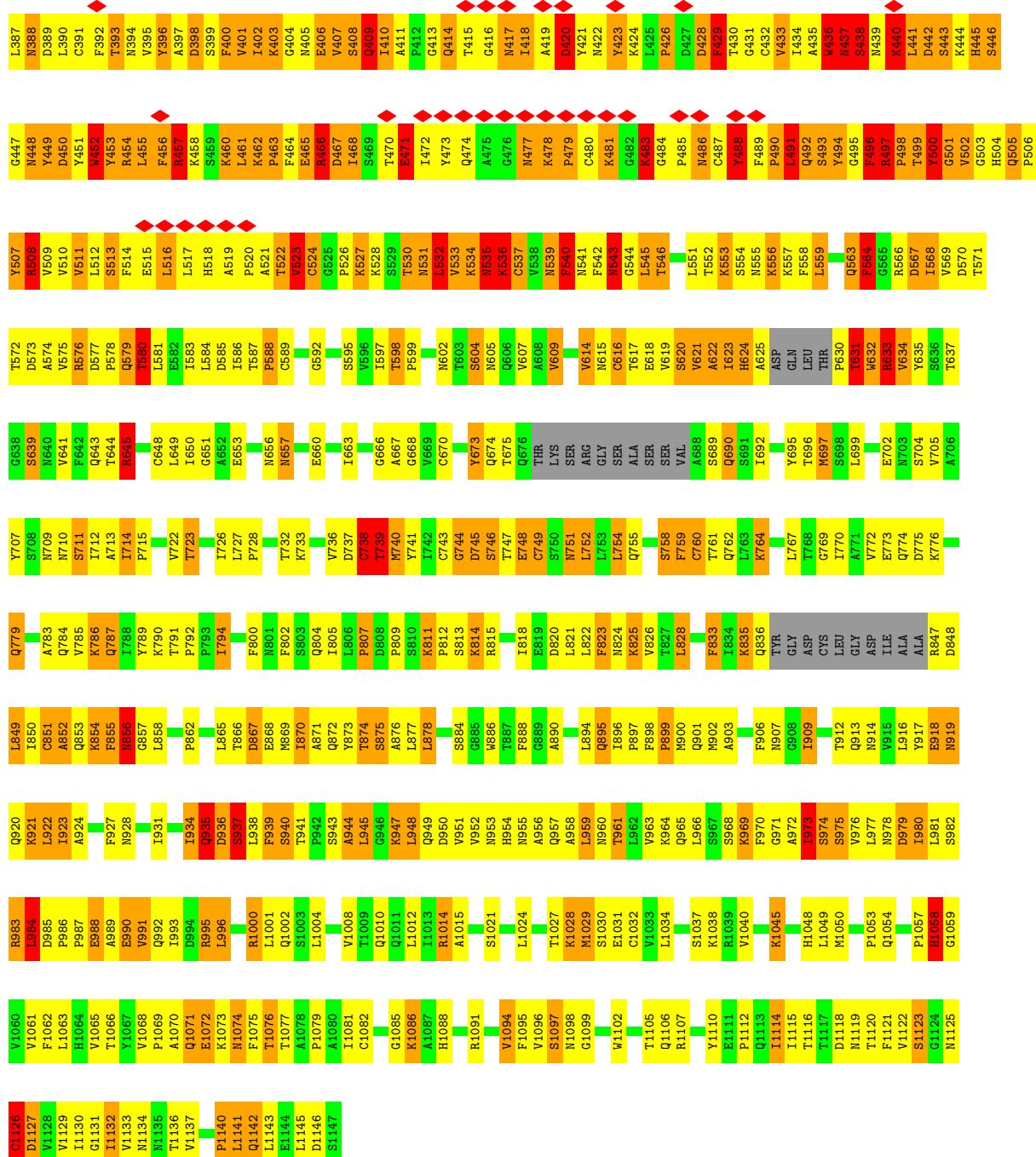
3   Residue-property plots ⓘ

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

• Molecule 1: Spike glycoprotein

• Molecule 1: Spike glycoprotein

Chain B:

• Molecule 1: Spike glycoprotein

Chain C:

• Molecule 2: SA55-HC

Chain Q:

- Molecule 2: SA55-HC

Chain D:

- Molecule 2: SA55-HC

Chain H:

- Molecule 3: S309-HC

Chain S:

K63 F64 Q65 G66 R67 V68 T69 M70 T71 T72 D73 T74 S75 T76 T77 T78 G79 Y80 M81 E82 L83 R84 R85 L86 R87 S88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 Y100 T101 R102 G103 A104 W105 F106 G107 E108 S109 L110 I111 G112 G113 F114 D115 N116 W117 G118 Q119 G120 T121 L122

V123 T124 V125 S126 S127

• Molecule 3: S309-HC

80%

Chain E: 17% 46% 29% 8%

Q1 V2 Q3 L4 V5 Q6 S7 G8 A9 E10 V11 K12 K13 P14 G15 A16 S17 V18 K19 V20 S21 C22 K23 A24 S25 G26 Y27 P28 F29 T30 S31 Y32 G33 I34 S35 W36 V37 R38 Q39 A40 P41 G42 Q43 G44 L45 E46 W47 M48 G49 W50 I51 S52 T53 Y54 N55 G56 N57 T58 N59 Y60

A61 Q62 K63 F64 Q65 G66 R67 V68 T69 M70 T71 T72 D73 T74 S75 T76 T77 T78 G79 Y80 M81 E82 L83 R84 R85 L86 R87 S88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 Y100 T101 R102 G103 A104 W105 F106 G107 E108 S109 L110 I111 G112 G113 F114 D115 N116 W117 Q118 Q119 G120

T121 L122 V123 T124 V125 S126 S127

• Molecule 3: S309-HC

85%

Chain I: 13% 45% 31% 11%

Q1 V2 Q3 L4 V5 Q6 S7 G8 A9 E10 V11 K12 K13 P14 G15 A16 S17 V18 K19 V20 S21 C22 K23 A24 S25 G26 Y27 P28 F29 T30 S31 Y32 G33 I34 S35 W36 V37 R38 Q39 A40 P41 G42 Q43 G44 L45 E46 W47 M48 G49 W50 I51 S52 T53 Y54 N55 G56 N57 T58 N59 Y60

A61 Q62 K63 F64 Q65 G66 R67 V68 T69 M70 T71 T72 D73 T74 S75 T76 T77 T78 G79 Y80 M81 E82 L83 R84 R85 L86 R87 S88 D89 D90 T91 A92 V93 Y94 Y95 C96 A97 R98 D99 Y100 T101 R102 G103 A104 W105 F106 G107 E108 S109 L110 I111 G112 G113 F114 D115 N116 W117 G118 Q119 G120

T121 L122 V123 T124 V125 S126 S127

• Molecule 4: SA55_KC

7%

Chain R: 11% 42% 39% 8%

D2 I3 Q4 M5 T6 Q7 S8 P9 S10 S11 L12 S13 A14 S15 V16 G17 D18 R19 V20 T21 I22 T23 C24 Q25 A26 S27 Q28 D29 I30 G31 N32 Y33 L34 N35 W36 Y37 Q38 Q39 K40 P41 G42 K43 A44 P45 K46 L47 L48 I49 Y50 D51 A52 S53 H54 L55 E56 T57 G58 V59 P60 S61

R62 F63 S64 G65 S66 G67 S68 G69 T70 D71 F72 T73 F74 T75 I76 S77 S78 L79 Q80 P81 E82 D83 I84 A85 T86 Y87 Y88 C89 Q90 R91 Y92 D93 P94 S95 Y96 T97 F98 G99 Q100 Q101 T102 K103 V104 E105 I106 K107

• Molecule 4: SA55_KC

84%

Chain F: 15% 37% 41% 8%

• Molecule 4: SA55_KC

Chain J:

• Molecule 5: S309-KC

Chain T:

• Molecule 5: S309-KC

Chain G:

• Molecule 5: S309-KC

Chain K:

4 Experimental information ⓘ

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	125226	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	1.5625	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.303	Depositor
Minimum map value	-1.180	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.038	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	448.19998, 448.19998, 448.19998	wwPDB
Map dimensions	540, 540, 540	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.64	0/8277	0.81	0/11261
1	B	0.64	0/8277	0.84	0/11261
1	C	0.63	0/8277	0.83	0/11261
2	D	0.65	0/946	0.83	0/1285
2	H	0.64	0/946	0.85	0/1285
2	Q	0.66	0/946	0.85	0/1285
3	E	0.63	0/980	0.74	0/1334
3	I	0.61	0/980	0.78	0/1334
3	S	0.61	0/980	0.73	0/1334
4	F	0.64	0/815	0.84	0/1108
4	J	0.65	0/815	0.84	0/1108
4	R	0.65	0/815	0.84	0/1108
5	G	0.67	0/754	0.75	0/1026
5	K	0.65	0/754	0.74	0/1026
5	T	0.67	0/754	0.73	0/1026
All	All	0.64	0/35316	0.82	0/48042

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	A	0	24
1	B	0	16
1	C	0	28
2	D	0	3
2	H	0	4
2	Q	0	4
3	E	0	5
3	I	0	6
3	S	0	5
4	F	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
4	J	0	2
4	R	0	2
5	G	0	6
5	K	0	6
5	T	0	5
All	All	0	119

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 119 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	190	ARG	Sidechain
1	A	236	ARG	Sidechain
1	A	34	ARG	Sidechain
1	A	44	ARG	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	A	8083	0	7910	911	0
1	B	8083	0	7908	1040	0
1	C	8083	0	7906	842	0
2	D	924	0	881	223	0
2	H	924	0	881	192	0
2	Q	924	0	881	229	0
3	E	956	0	894	140	0
3	I	956	0	894	176	0
3	S	956	0	894	132	0
4	F	796	0	737	146	0
4	J	796	0	737	132	0
4	R	796	0	737	149	0
5	G	738	0	686	137	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	738	0	686	107	0
5	T	738	0	686	142	0
All	All	34491	0	33318	4448	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 66.

The worst 5 of 4448 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:HA	1:A:396:TYR:HA	1.19	1.16
1:A:343:ASN:HA	2:D:53:PRO:HB3	1.30	1.13
1:A:474:GLN:HA	1:A:483:LYS:HA	1.12	1.11
5:T:40:LYS:HD2	5:T:46:ARG:NH1	1.66	1.11
1:B:85:PRO:HA	1:B:236:ARG:HA	1.31	1.09

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1012/1123 (90%)	589 (58%)	291 (29%)	132 (13%)	0	1
1	B	1012/1123 (90%)	597 (59%)	242 (24%)	173 (17%)	0	0
1	C	1012/1123 (90%)	582 (58%)	289 (29%)	141 (14%)	0	1
2	D	123/125 (98%)	47 (38%)	40 (32%)	36 (29%)	0	0
2	H	123/125 (98%)	45 (37%)	46 (37%)	32 (26%)	0	0
2	Q	123/125 (98%)	50 (41%)	45 (37%)	28 (23%)	0	0
3	E	125/127 (98%)	63 (50%)	36 (29%)	26 (21%)	0	0
3	I	125/127 (98%)	65 (52%)	31 (25%)	29 (23%)	0	0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	S	125/127 (98%)	68 (54%)	31 (25%)	26 (21%)	0	0
4	F	104/106 (98%)	48 (46%)	31 (30%)	25 (24%)	0	0
4	J	104/106 (98%)	47 (45%)	32 (31%)	25 (24%)	0	0
4	R	104/106 (98%)	50 (48%)	23 (22%)	31 (30%)	0	0
5	G	102/104 (98%)	48 (47%)	29 (28%)	25 (24%)	0	0
5	K	102/104 (98%)	44 (43%)	34 (33%)	24 (24%)	0	0
5	T	102/104 (98%)	39 (38%)	39 (38%)	24 (24%)	0	0
All	All	4398/4755 (92%)	2382 (54%)	1239 (28%)	777 (18%)	0	0

5 of 777 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	27	SER
1	A	59	PHE
1	A	92	PHE
1	A	226	VAL
1	A	292	ALA

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	A	903/978 (92%)	586 (65%)	317 (35%)	0	0
1	B	903/978 (92%)	555 (62%)	348 (38%)	0	0
1	C	903/978 (92%)	572 (63%)	331 (37%)	0	0
2	D	96/102 (94%)	47 (49%)	49 (51%)	0	0
2	H	96/102 (94%)	53 (55%)	43 (45%)	0	0
2	Q	96/102 (94%)	51 (53%)	45 (47%)	0	0
3	E	94/103 (91%)	52 (55%)	42 (45%)	0	0
3	I	94/103 (91%)	51 (54%)	43 (46%)	0	0
3	S	94/103 (91%)	52 (55%)	42 (45%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	F	81/92 (88%)	41 (51%)	40 (49%)	0	0
4	J	81/92 (88%)	43 (53%)	38 (47%)	0	0
4	R	81/92 (88%)	47 (58%)	34 (42%)	0	0
5	G	69/86 (80%)	37 (54%)	32 (46%)	0	0
5	K	69/86 (80%)	41 (59%)	28 (41%)	0	0
5	T	69/86 (80%)	35 (51%)	34 (49%)	0	0
All	All	3729/4083 (91%)	2263 (61%)	1466 (39%)	0	0

5 of 1466 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	861	LEU
5	T	93	ASP
1	C	980	ILE
1	C	859	THR
2	Q	120	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 146 such sidechains are listed below:

Mol	Chain	Res	Type
2	Q	39	GLN
5	K	27	GLN
4	R	28	GLN
4	F	4	GLN
1	B	334	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6   Ligand geometry ⓘ

There are no ligands in this entry.

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.
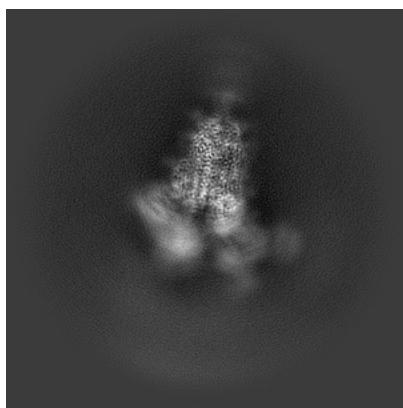
6   Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-37930. These allow visual inspection of the internal detail of the map and identification of artifacts.
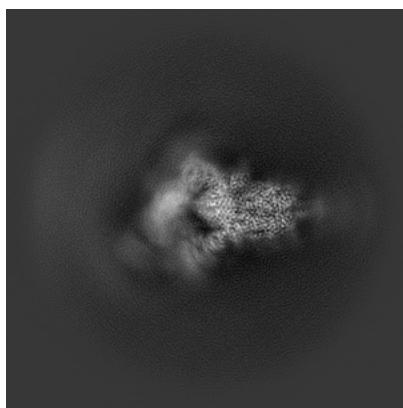
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1   Orthogonal projections ⓘ
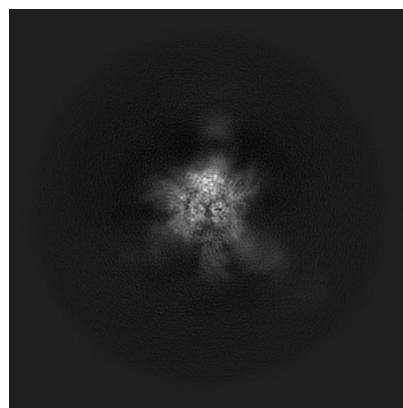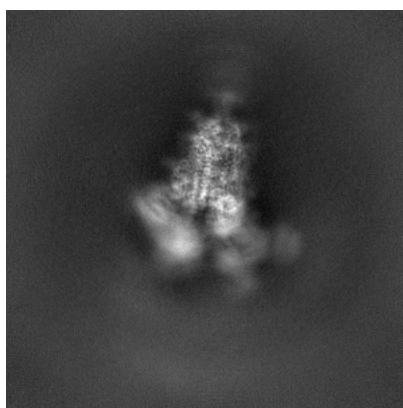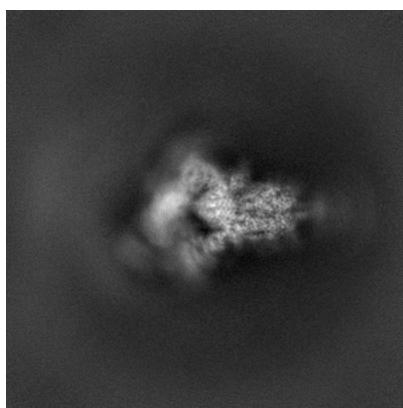
6.1.1   Primary map

X   Y   Z
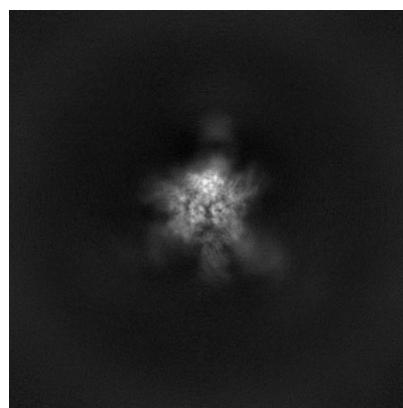
6.1.2   Raw map

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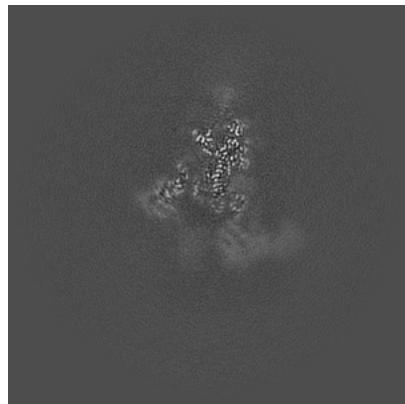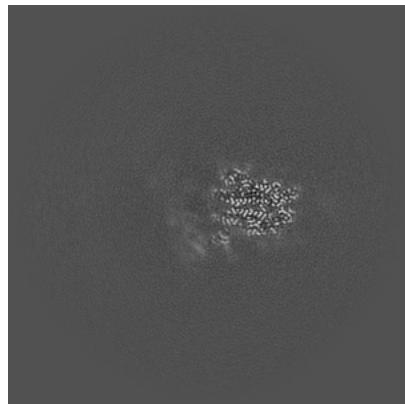
The images above show the map projected in three orthogonal directions.

6.2   Central slices ⓘ
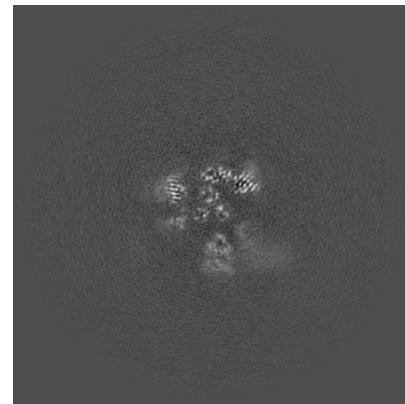
6.2.1   Primary map
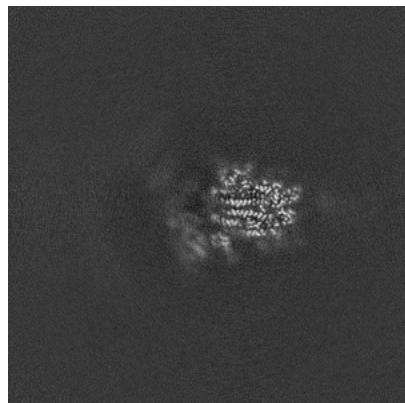
X Index: 270   Y Index: 270   Z Index: 270
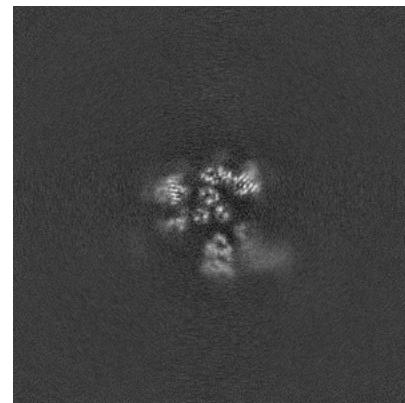
6.2.2   Raw map

X Index: 270   Y Index: 270   Z Index: 270
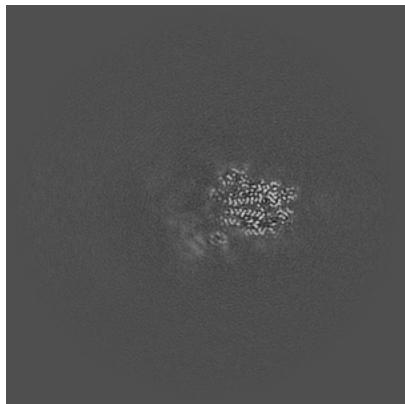
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ
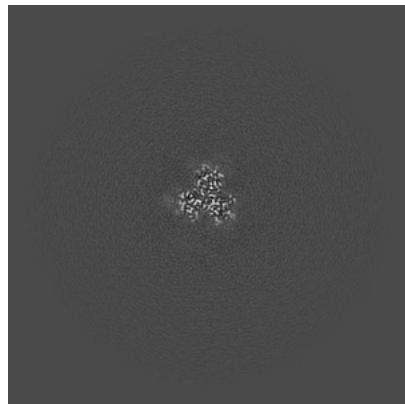
6.3.1 Primary map

X Index: 278   Y Index: 271   Z Index: 343
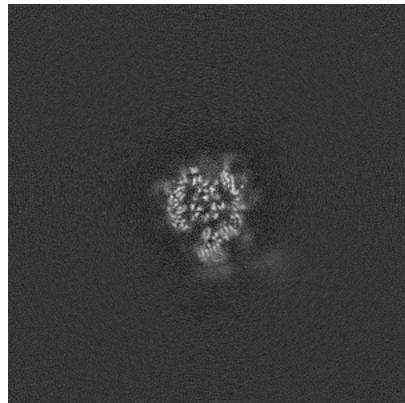
6.3.2 Raw map

X Index: 277   Y Index: 275   Z Index: 288
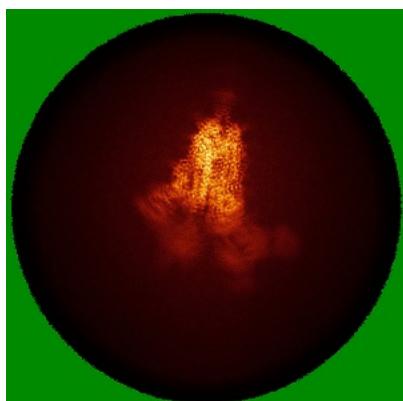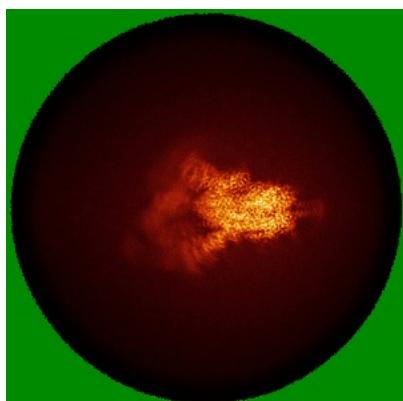
The images above show the largest variance slices of the map in three orthogonal directions.

6.4   Orthogonal standard-deviation projections (False-color) ⓘ
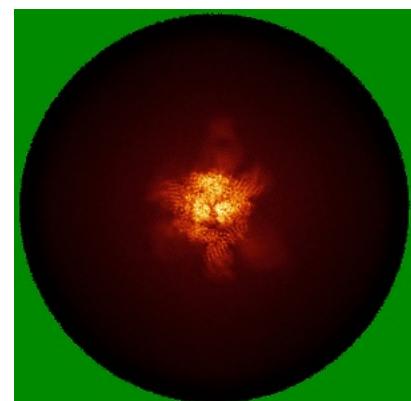
6.4.1   Primary map
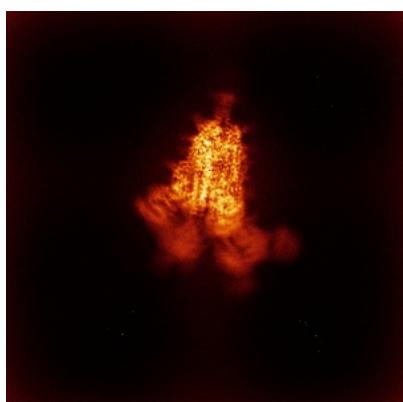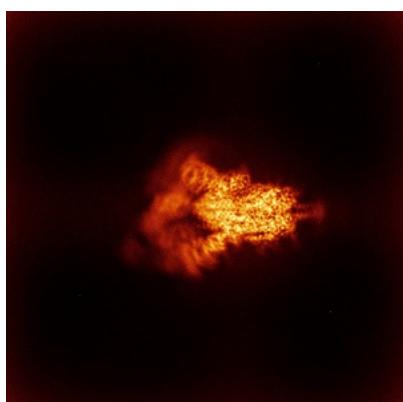
X   Y   Z
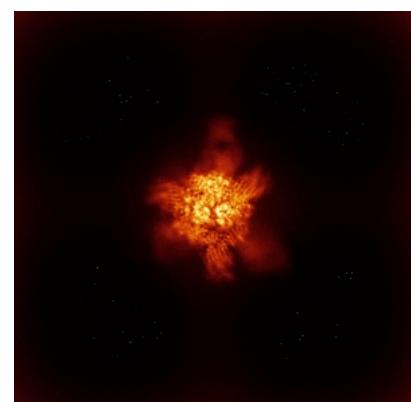
6.4.2   Raw map

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.
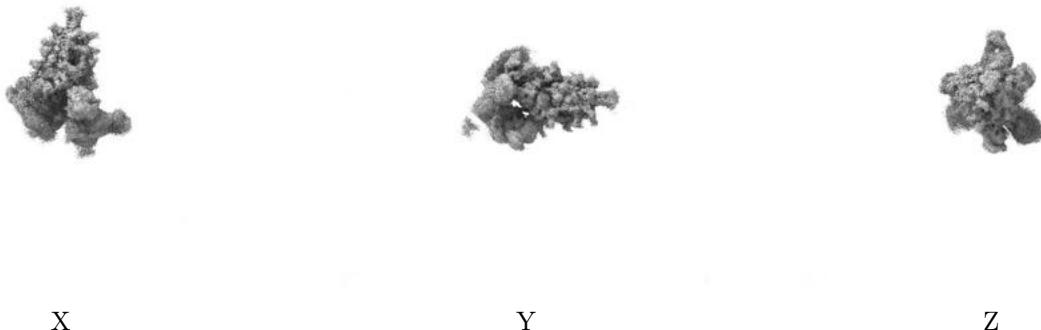
6.5 Orthogonal surface views ⓘ

6.5.1 Primary map

| X | Y | Z |

The images above show the 3D surface view of the map at the recommended contour level 0.15. 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

| X | Y | Z |

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.
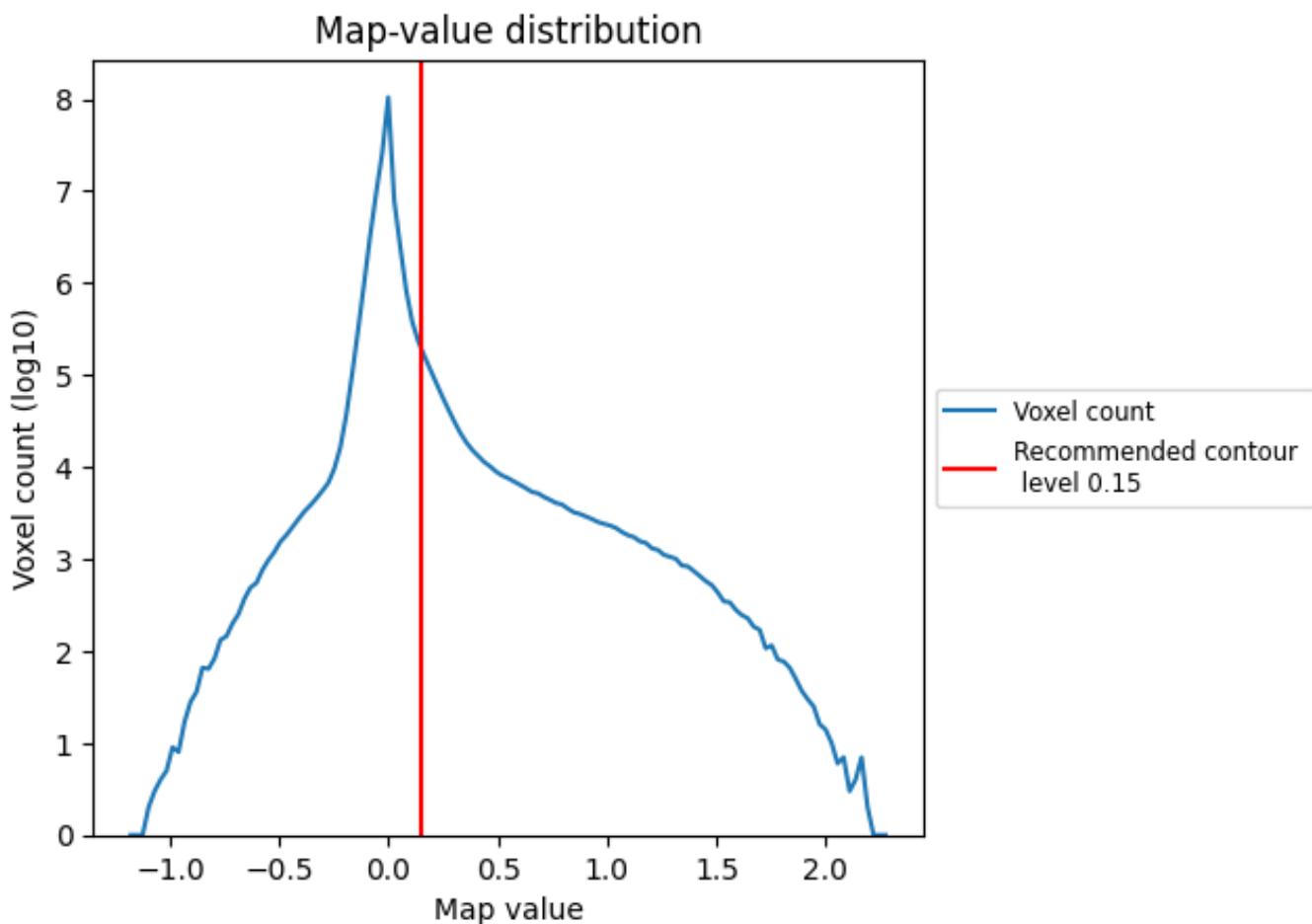
6.6 Mask visualisation ⓘ

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

7 Map analysis ⓘ
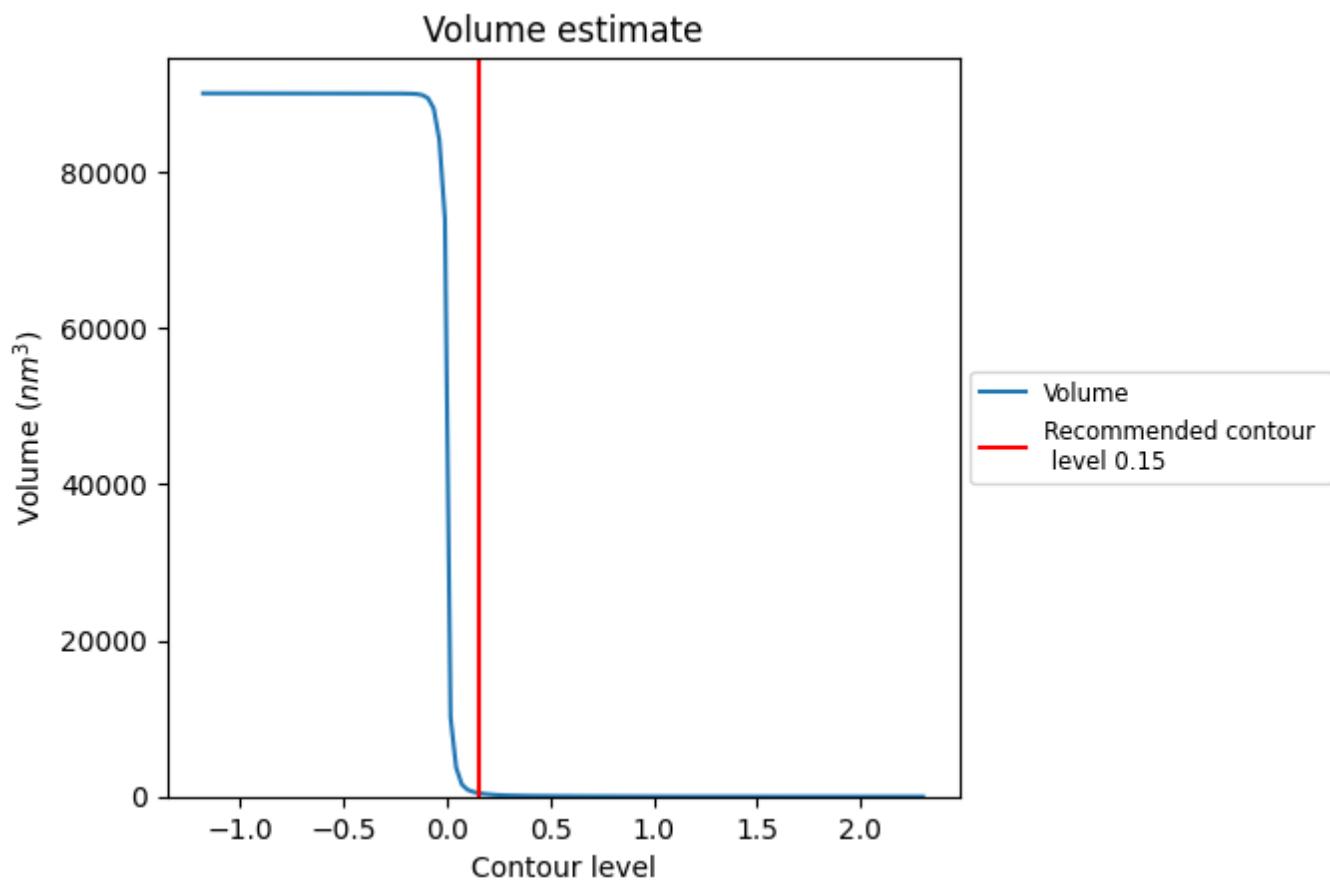
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

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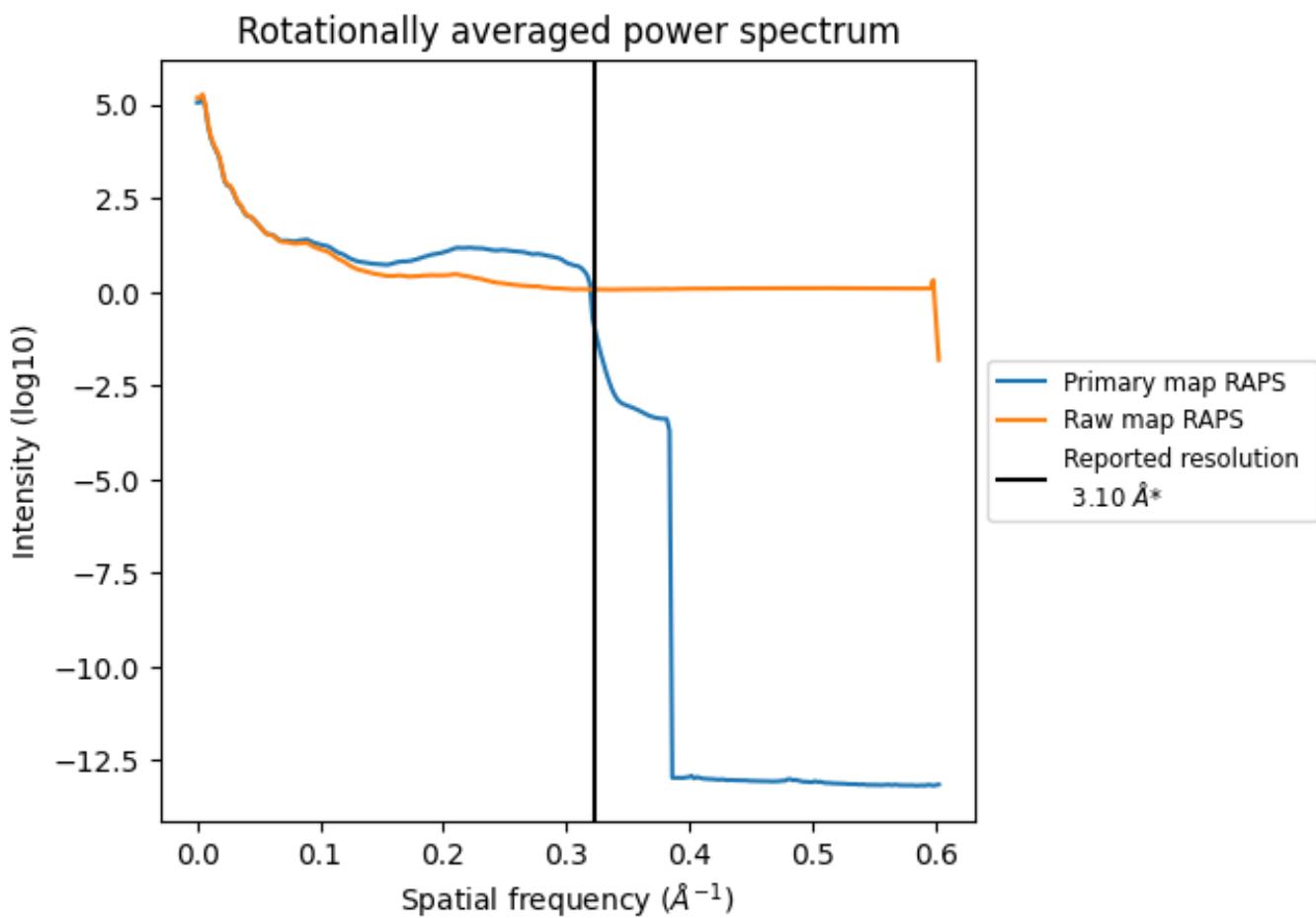
7.2 Volume estimate ⓘ

The volume at the recommended contour level is 464 nm^3; this corresponds to an approximate mass of 419 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 ⓘ
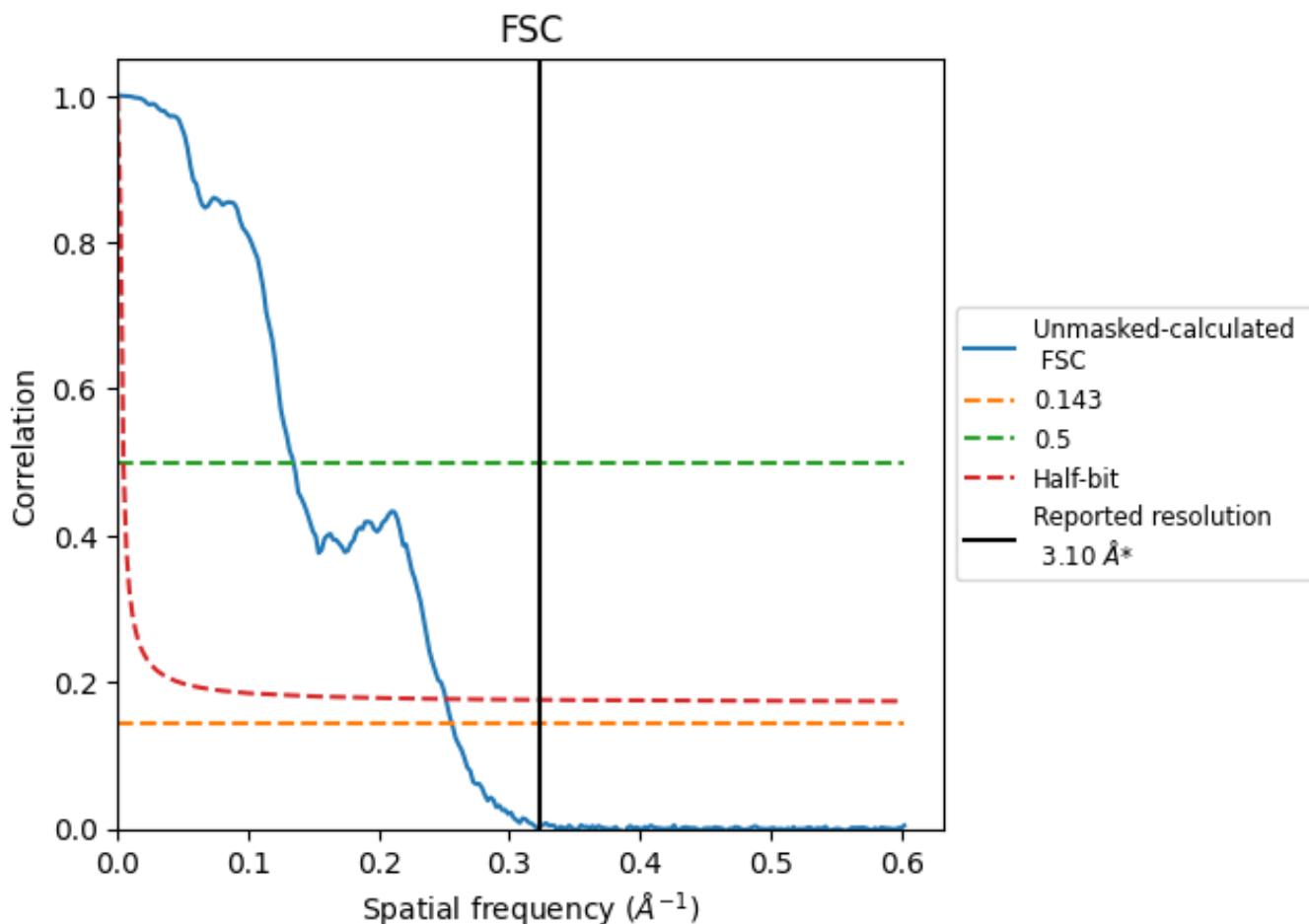
*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

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 0.323 Å^{-1}

8.2 Resolution estimates ⓘ
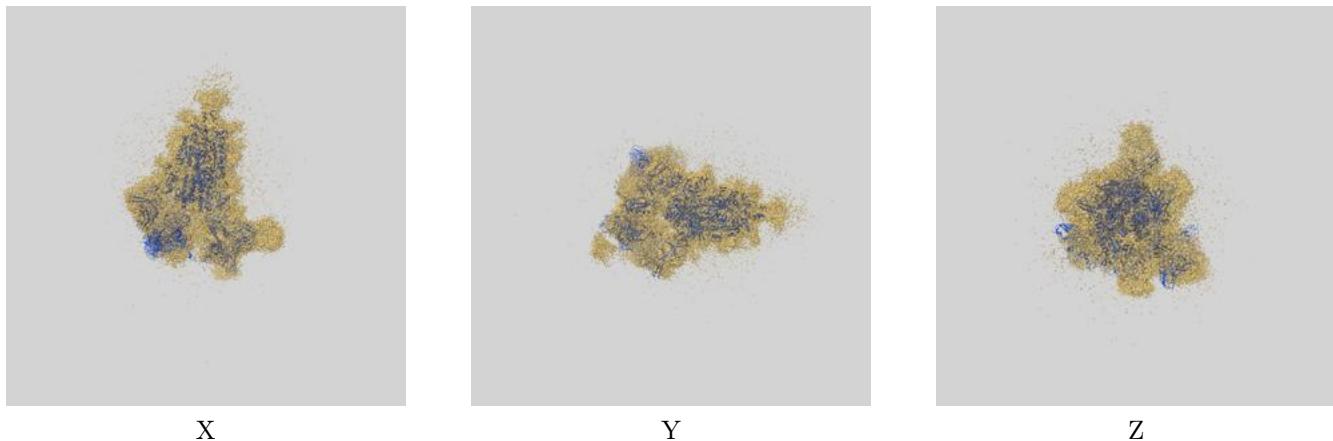
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.91	7.43	3.98

*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 3.91 differs from the reported value 3.1 by more than 10 %

9 Map-model fit ⓘ
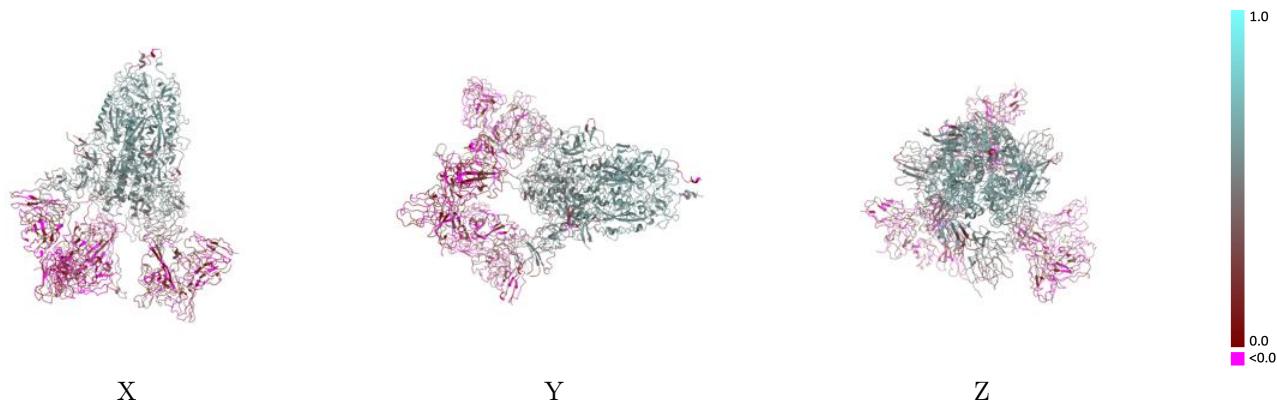
This section contains information regarding the fit between EMDB map EMD-37930 and PDB model 8WYJ. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay ⓘ

| X | Y | Z |
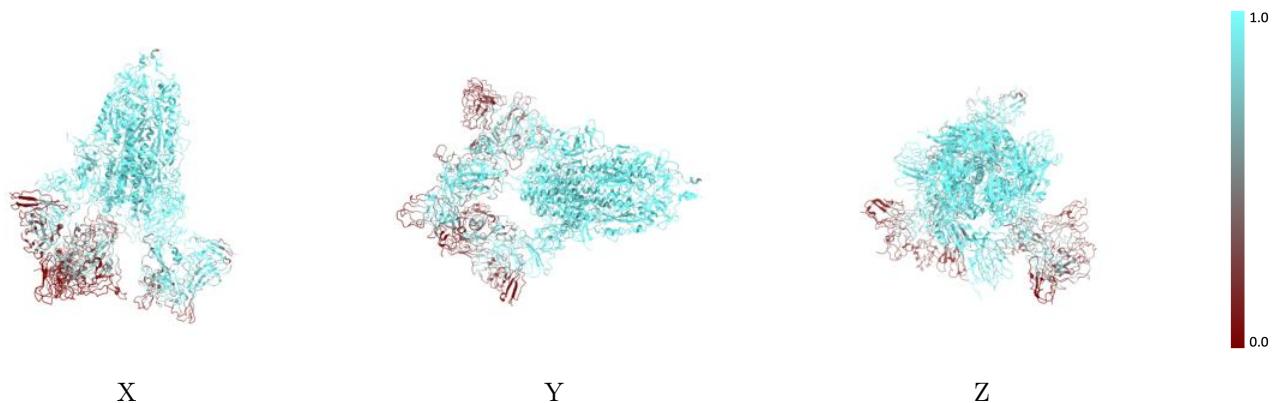
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model ⓘ

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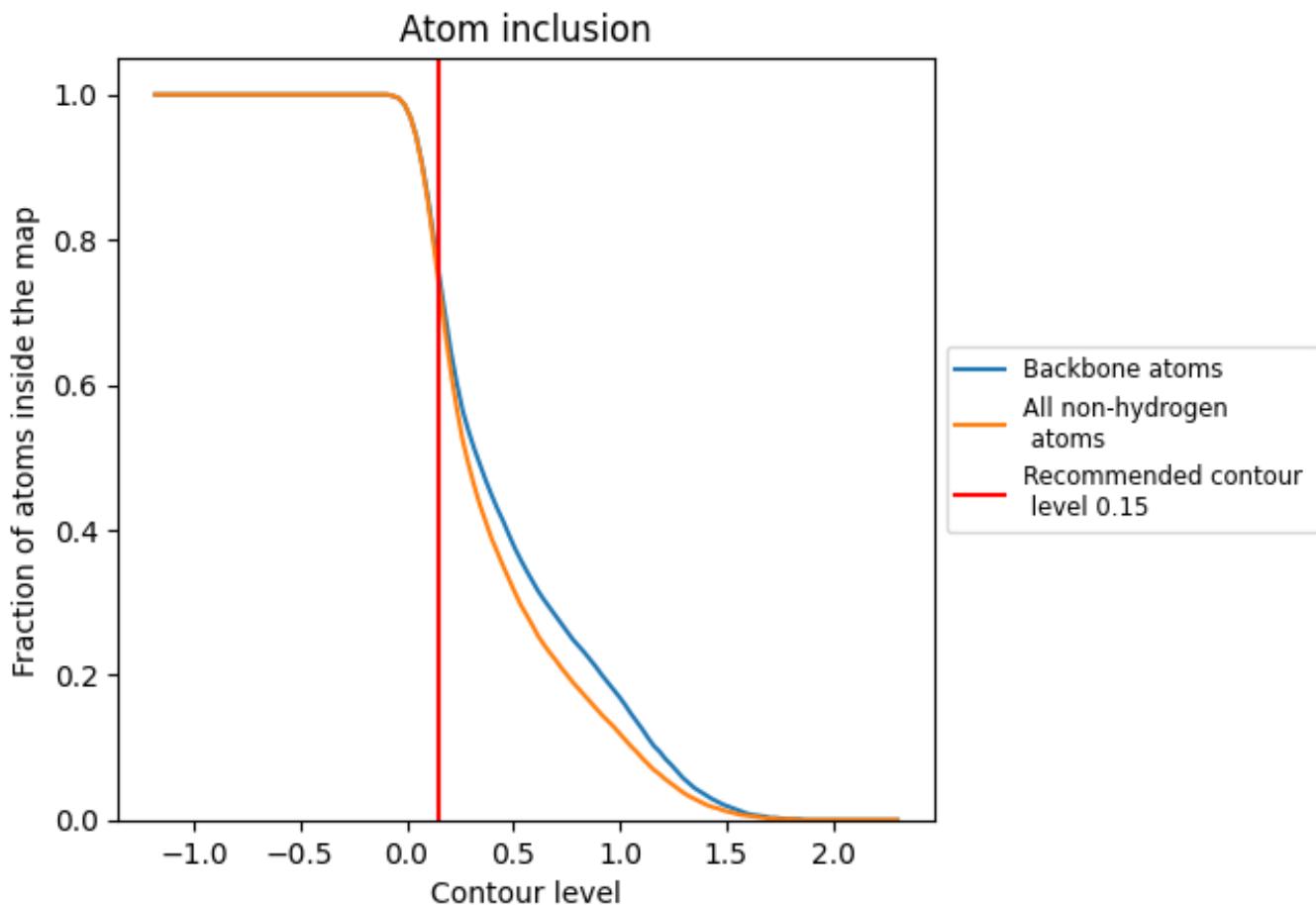
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

X   Y   Z

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 (0.15).
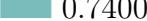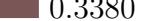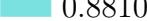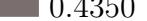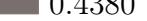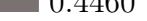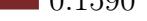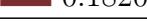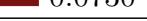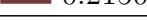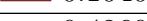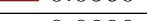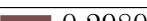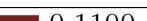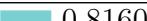
9.4 Atom inclusion ⓘ

At the recommended contour level, 76% of all backbone atoms, 74% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7400	0.3380
A	0.8810	0.4350
B	0.9130	0.4380
C	0.8600	0.4460
D	0.4440	0.1590
E	0.1820	0.0730
F	0.2150	0.0980
G	0.1040	0.0560
H	0.4260	0.0800
I	0.1550	0.0590
J	0.2980	0.1100
K	0.1570	0.0990
Q	0.8160	0.0940
R	0.8300	0.1120
S	0.4970	0.1000
T	0.5650	0.1180

1.0

0.0
<0.0