



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2026 – 12:28 AM UTC

PDB ID : 7K0C / pdb_00007k0c
EMDB ID : EMD-22591
Title : Structure of Secretory IgM Core
Authors : Kumar, N.; Arthur, C.P.; Ciferri, C.; Matsumoto, M.L.
Deposited on : 2020-09-04
Resolution : 3.30 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 ⓘ 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:

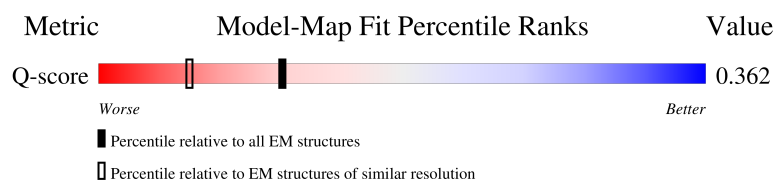
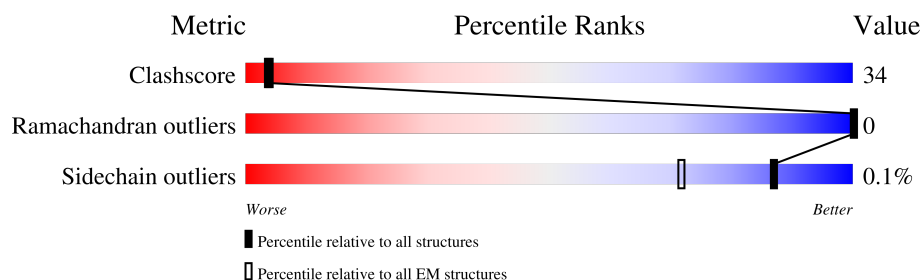
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
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 3.30 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	15087 (2.80 - 3.80)

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	C	591	
2	A	369	
2	B	369	
2	E	369	

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Mol	Chain	Length	Quality of chain
2	F	369	
2	G	369	
2	H	369	
2	I	369	
2	J	369	
2	K	369	
2	L	369	
3	D	137	
4	M	2	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 22540 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 Polymeric immunoglobulin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C	534	Total	C	N	O	S	0	0
			4109	2588	709	792	20		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	586	HIS	-	expression tag	UNP P01833
C	587	HIS	-	expression tag	UNP P01833
C	588	HIS	-	expression tag	UNP P01833
C	589	HIS	-	expression tag	UNP P01833
C	590	HIS	-	expression tag	UNP P01833
C	591	HIS	-	expression tag	UNP P01833

- Molecule 2 is a protein called Immunoglobulin heavy constant mu.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
2	B	227	Total	C	N	O	S	0	0
			1764	1111	299	346	8		
2	K	225	Total	C	N	O	S	0	0
			1748	1103	297	340	8		
2	L	224	Total	C	N	O	S	0	0
			1737	1097	293	339	8		
2	I	224	Total	C	N	O	S	0	0
			1743	1100	296	339	8		
2	J	221	Total	C	N	O	S	0	0
			1723	1087	292	336	8		
2	E	224	Total	C	N	O	S	0	0
			1742	1100	296	338	8		
2	H	230	Total	C	N	O	S	0	0
			1785	1124	301	351	9		
2	G	230	Total	C	N	O	S	0	0
			1786	1124	302	351	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	F	228	Total	C	N	O	S	0	0
			1773	1116	299	349	9		

There are 180 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	208	ASP	-	expression tag	UNP P01871
A	209	TYR	-	expression tag	UNP P01871
A	210	LYS	-	expression tag	UNP P01871
A	211	ASP	-	expression tag	UNP P01871
A	212	ASP	-	expression tag	UNP P01871
A	213	ASP	-	expression tag	UNP P01871
A	214	ASP	-	expression tag	UNP P01871
A	215	LYS	-	expression tag	UNP P01871
A	216	LEU	-	expression tag	UNP P01871
A	217	GLU	-	expression tag	UNP P01871
A	218	VAL	-	expression tag	UNP P01871
A	219	LEU	-	expression tag	UNP P01871
A	220	PHE	-	expression tag	UNP P01871
A	221	GLN	-	expression tag	UNP P01871
A	222	GLY	-	expression tag	UNP P01871
A	223	PRO	-	expression tag	UNP P01871
A	224	GLY	-	expression tag	UNP P01871
A	225	SER	-	expression tag	UNP P01871
B	208	ASP	-	expression tag	UNP P01871
B	209	TYR	-	expression tag	UNP P01871
B	210	LYS	-	expression tag	UNP P01871
B	211	ASP	-	expression tag	UNP P01871
B	212	ASP	-	expression tag	UNP P01871
B	213	ASP	-	expression tag	UNP P01871
B	214	ASP	-	expression tag	UNP P01871
B	215	LYS	-	expression tag	UNP P01871
B	216	LEU	-	expression tag	UNP P01871
B	217	GLU	-	expression tag	UNP P01871
B	218	VAL	-	expression tag	UNP P01871
B	219	LEU	-	expression tag	UNP P01871
B	220	PHE	-	expression tag	UNP P01871
B	221	GLN	-	expression tag	UNP P01871
B	222	GLY	-	expression tag	UNP P01871
B	223	PRO	-	expression tag	UNP P01871
B	224	GLY	-	expression tag	UNP P01871
B	225	SER	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
K	208	ASP	-	expression tag	UNP P01871
K	209	TYR	-	expression tag	UNP P01871
K	210	LYS	-	expression tag	UNP P01871
K	211	ASP	-	expression tag	UNP P01871
K	212	ASP	-	expression tag	UNP P01871
K	213	ASP	-	expression tag	UNP P01871
K	214	ASP	-	expression tag	UNP P01871
K	215	LYS	-	expression tag	UNP P01871
K	216	LEU	-	expression tag	UNP P01871
K	217	GLU	-	expression tag	UNP P01871
K	218	VAL	-	expression tag	UNP P01871
K	219	LEU	-	expression tag	UNP P01871
K	220	PHE	-	expression tag	UNP P01871
K	221	GLN	-	expression tag	UNP P01871
K	222	GLY	-	expression tag	UNP P01871
K	223	PRO	-	expression tag	UNP P01871
K	224	GLY	-	expression tag	UNP P01871
K	225	SER	-	expression tag	UNP P01871
L	208	ASP	-	expression tag	UNP P01871
L	209	TYR	-	expression tag	UNP P01871
L	210	LYS	-	expression tag	UNP P01871
L	211	ASP	-	expression tag	UNP P01871
L	212	ASP	-	expression tag	UNP P01871
L	213	ASP	-	expression tag	UNP P01871
L	214	ASP	-	expression tag	UNP P01871
L	215	LYS	-	expression tag	UNP P01871
L	216	LEU	-	expression tag	UNP P01871
L	217	GLU	-	expression tag	UNP P01871
L	218	VAL	-	expression tag	UNP P01871
L	219	LEU	-	expression tag	UNP P01871
L	220	PHE	-	expression tag	UNP P01871
L	221	GLN	-	expression tag	UNP P01871
L	222	GLY	-	expression tag	UNP P01871
L	223	PRO	-	expression tag	UNP P01871
L	224	GLY	-	expression tag	UNP P01871
L	225	SER	-	expression tag	UNP P01871
I	208	ASP	-	expression tag	UNP P01871
I	209	TYR	-	expression tag	UNP P01871
I	210	LYS	-	expression tag	UNP P01871
I	211	ASP	-	expression tag	UNP P01871
I	212	ASP	-	expression tag	UNP P01871
I	213	ASP	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
I	214	ASP	-	expression tag	UNP P01871
I	215	LYS	-	expression tag	UNP P01871
I	216	LEU	-	expression tag	UNP P01871
I	217	GLU	-	expression tag	UNP P01871
I	218	VAL	-	expression tag	UNP P01871
I	219	LEU	-	expression tag	UNP P01871
I	220	PHE	-	expression tag	UNP P01871
I	221	GLN	-	expression tag	UNP P01871
I	222	GLY	-	expression tag	UNP P01871
I	223	PRO	-	expression tag	UNP P01871
I	224	GLY	-	expression tag	UNP P01871
I	225	SER	-	expression tag	UNP P01871
J	208	ASP	-	expression tag	UNP P01871
J	209	TYR	-	expression tag	UNP P01871
J	210	LYS	-	expression tag	UNP P01871
J	211	ASP	-	expression tag	UNP P01871
J	212	ASP	-	expression tag	UNP P01871
J	213	ASP	-	expression tag	UNP P01871
J	214	ASP	-	expression tag	UNP P01871
J	215	LYS	-	expression tag	UNP P01871
J	216	LEU	-	expression tag	UNP P01871
J	217	GLU	-	expression tag	UNP P01871
J	218	VAL	-	expression tag	UNP P01871
J	219	LEU	-	expression tag	UNP P01871
J	220	PHE	-	expression tag	UNP P01871
J	221	GLN	-	expression tag	UNP P01871
J	222	GLY	-	expression tag	UNP P01871
J	223	PRO	-	expression tag	UNP P01871
J	224	GLY	-	expression tag	UNP P01871
J	225	SER	-	expression tag	UNP P01871
E	208	ASP	-	expression tag	UNP P01871
E	209	TYR	-	expression tag	UNP P01871
E	210	LYS	-	expression tag	UNP P01871
E	211	ASP	-	expression tag	UNP P01871
E	212	ASP	-	expression tag	UNP P01871
E	213	ASP	-	expression tag	UNP P01871
E	214	ASP	-	expression tag	UNP P01871
E	215	LYS	-	expression tag	UNP P01871
E	216	LEU	-	expression tag	UNP P01871
E	217	GLU	-	expression tag	UNP P01871
E	218	VAL	-	expression tag	UNP P01871
E	219	LEU	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
E	220	PHE	-	expression tag	UNP P01871
E	221	GLN	-	expression tag	UNP P01871
E	222	GLY	-	expression tag	UNP P01871
E	223	PRO	-	expression tag	UNP P01871
E	224	GLY	-	expression tag	UNP P01871
E	225	SER	-	expression tag	UNP P01871
H	208	ASP	-	expression tag	UNP P01871
H	209	TYR	-	expression tag	UNP P01871
H	210	LYS	-	expression tag	UNP P01871
H	211	ASP	-	expression tag	UNP P01871
H	212	ASP	-	expression tag	UNP P01871
H	213	ASP	-	expression tag	UNP P01871
H	214	ASP	-	expression tag	UNP P01871
H	215	LYS	-	expression tag	UNP P01871
H	216	LEU	-	expression tag	UNP P01871
H	217	GLU	-	expression tag	UNP P01871
H	218	VAL	-	expression tag	UNP P01871
H	219	LEU	-	expression tag	UNP P01871
H	220	PHE	-	expression tag	UNP P01871
H	221	GLN	-	expression tag	UNP P01871
H	222	GLY	-	expression tag	UNP P01871
H	223	PRO	-	expression tag	UNP P01871
H	224	GLY	-	expression tag	UNP P01871
H	225	SER	-	expression tag	UNP P01871
G	208	ASP	-	expression tag	UNP P01871
G	209	TYR	-	expression tag	UNP P01871
G	210	LYS	-	expression tag	UNP P01871
G	211	ASP	-	expression tag	UNP P01871
G	212	ASP	-	expression tag	UNP P01871
G	213	ASP	-	expression tag	UNP P01871
G	214	ASP	-	expression tag	UNP P01871
G	215	LYS	-	expression tag	UNP P01871
G	216	LEU	-	expression tag	UNP P01871
G	217	GLU	-	expression tag	UNP P01871
G	218	VAL	-	expression tag	UNP P01871
G	219	LEU	-	expression tag	UNP P01871
G	220	PHE	-	expression tag	UNP P01871
G	221	GLN	-	expression tag	UNP P01871
G	222	GLY	-	expression tag	UNP P01871
G	223	PRO	-	expression tag	UNP P01871
G	224	GLY	-	expression tag	UNP P01871
G	225	SER	-	expression tag	UNP P01871

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Chain	Residue	Modelled	Actual	Comment	Reference
F	208	ASP	-	expression tag	UNP P01871
F	209	TYR	-	expression tag	UNP P01871
F	210	LYS	-	expression tag	UNP P01871
F	211	ASP	-	expression tag	UNP P01871
F	212	ASP	-	expression tag	UNP P01871
F	213	ASP	-	expression tag	UNP P01871
F	214	ASP	-	expression tag	UNP P01871
F	215	LYS	-	expression tag	UNP P01871
F	216	LEU	-	expression tag	UNP P01871
F	217	GLU	-	expression tag	UNP P01871
F	218	VAL	-	expression tag	UNP P01871
F	219	LEU	-	expression tag	UNP P01871
F	220	PHE	-	expression tag	UNP P01871
F	221	GLN	-	expression tag	UNP P01871
F	222	GLY	-	expression tag	UNP P01871
F	223	PRO	-	expression tag	UNP P01871
F	224	GLY	-	expression tag	UNP P01871
F	225	SER	-	expression tag	UNP P01871

- Molecule 3 is a protein called Immunoglobulin J chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	104	Total	C	N	O	S	0	0
			838	521	148	162	7		

- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

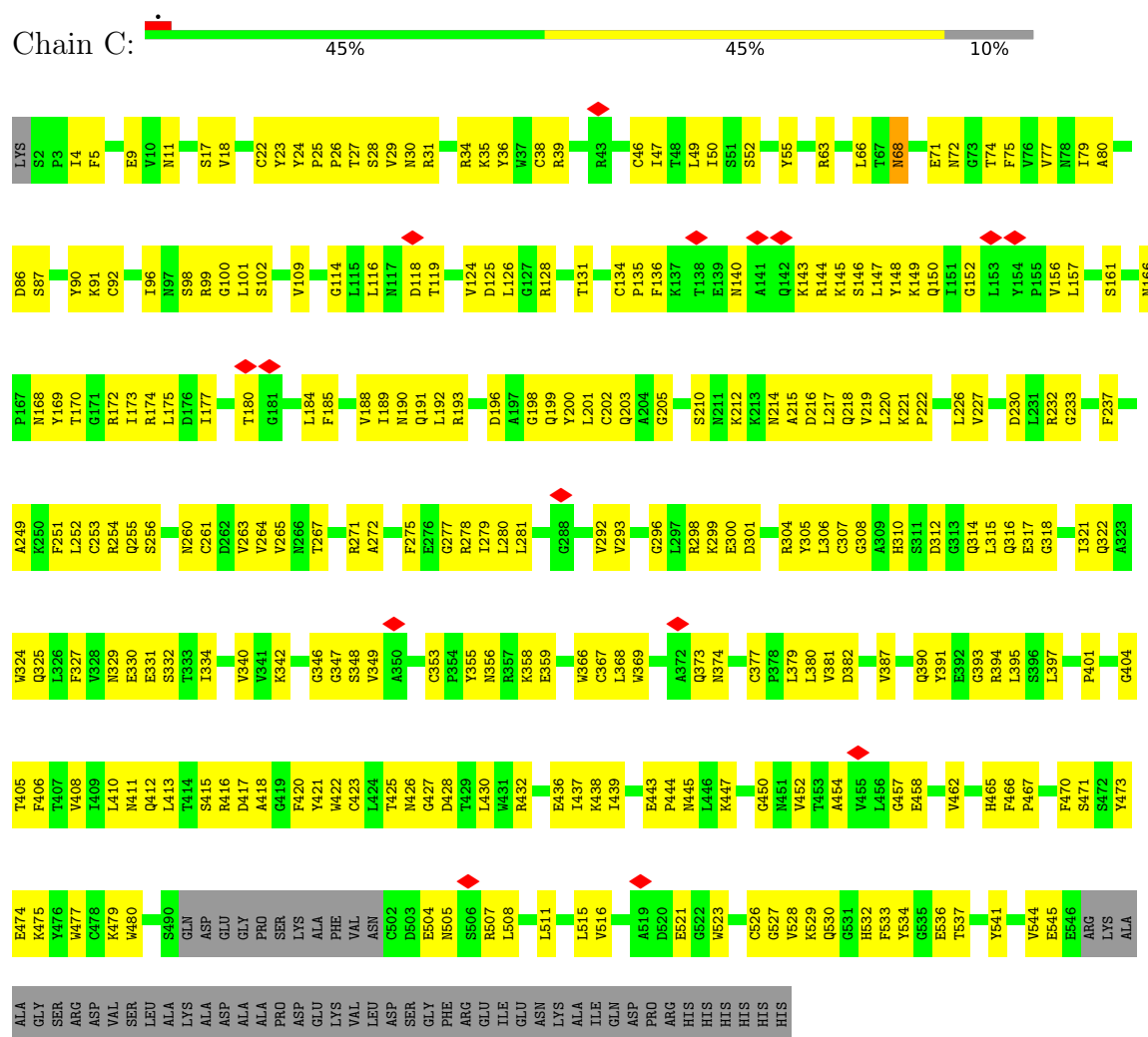


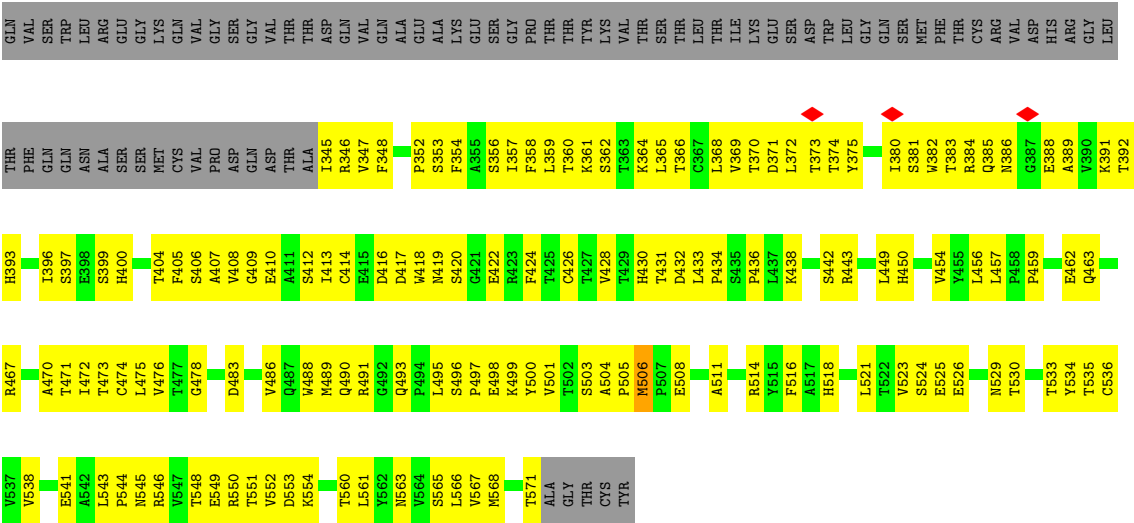
Mol	Chain	Residues	Atoms				AltConf	Trace
4	M	2	Total	C	N	O	0	0
			28	16	2	10		

3 Residue-property plots

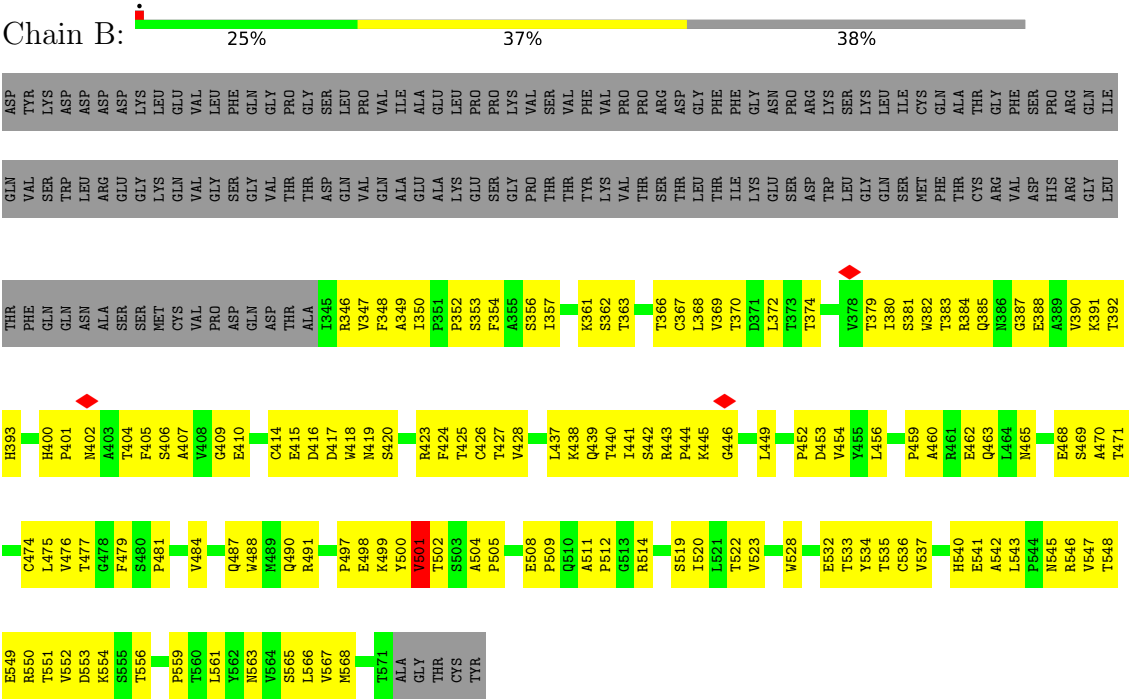
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Polymeric immunoglobulin receptor

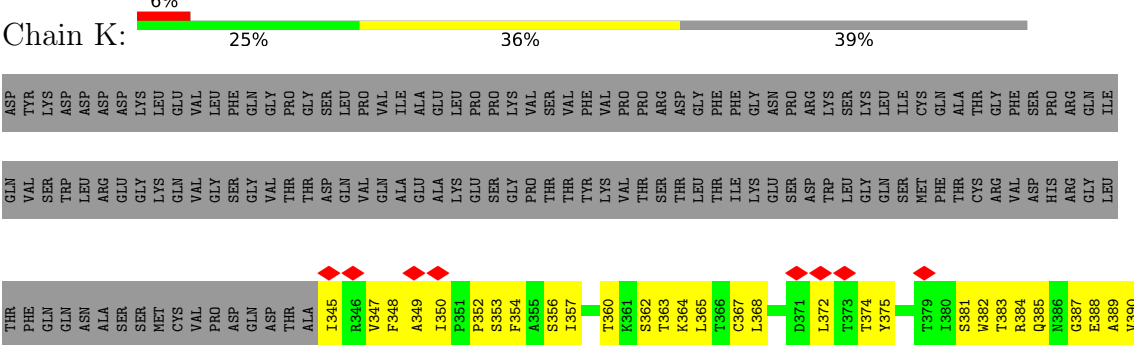


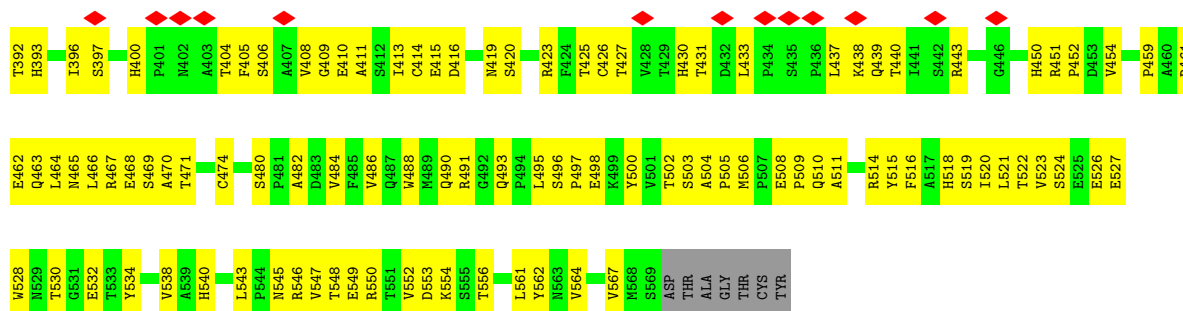


• Molecule 2: Immunoglobulin heavy constant mu

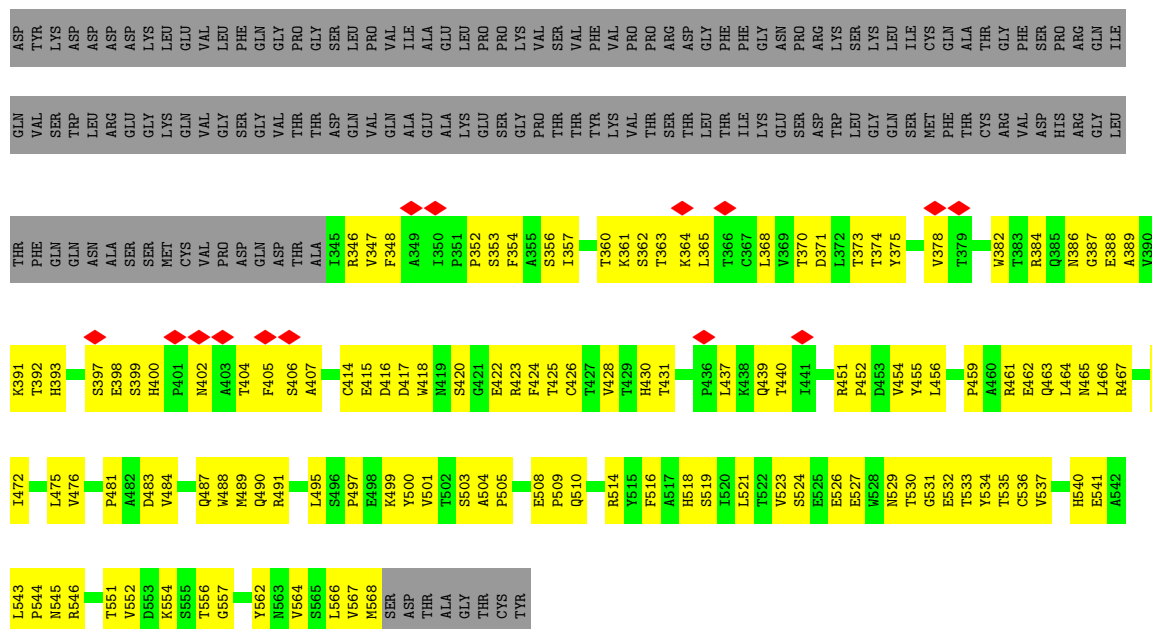
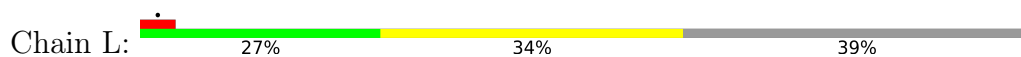


• Molecule 2: Immunoglobulin heavy constant mu

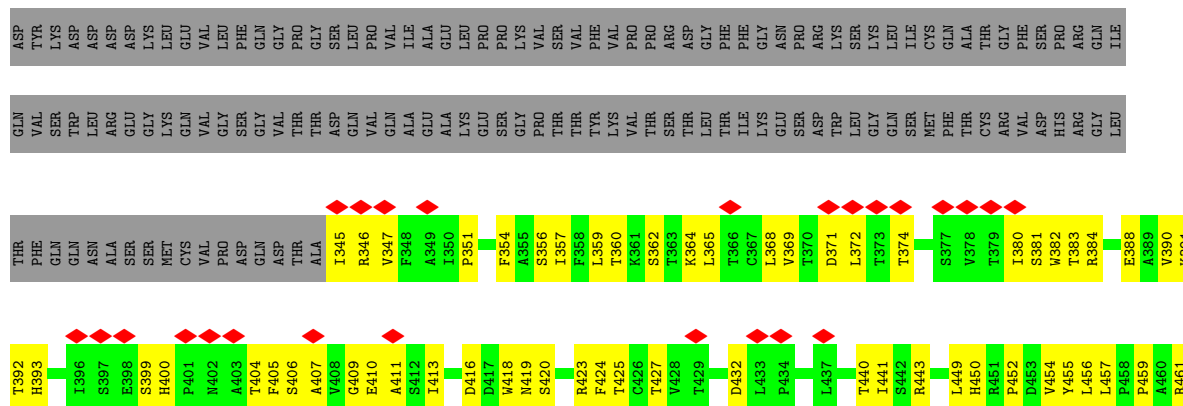
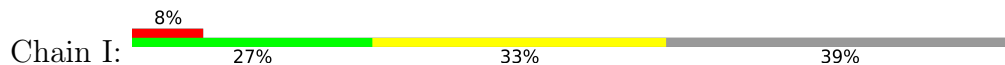


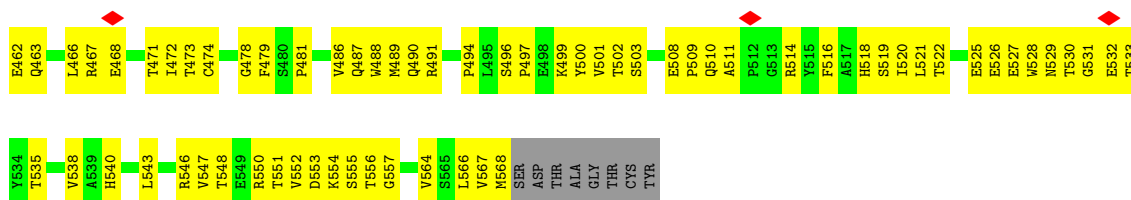


• Molecule 2: Immunoglobulin heavy constant mu

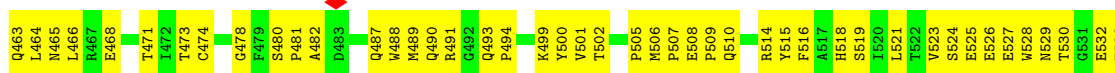
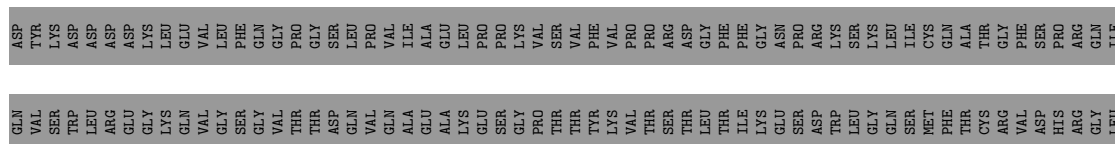
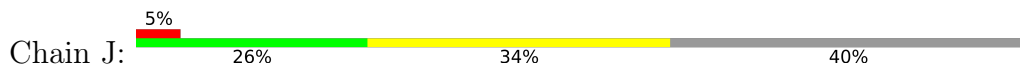


• Molecule 2: Immunoglobulin heavy constant mu

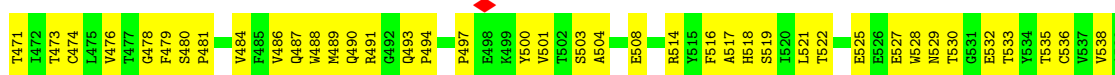
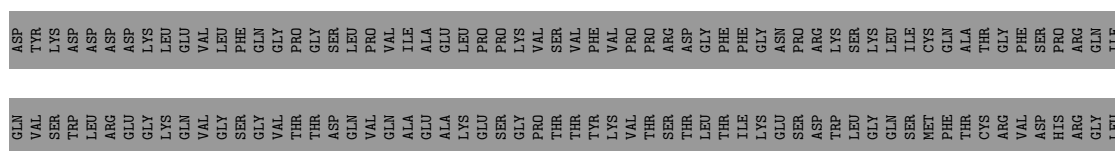
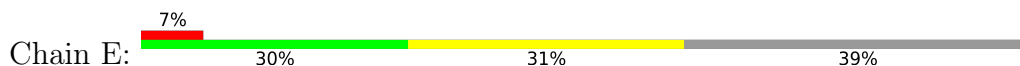




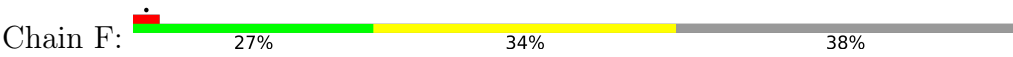
• Molecule 2: Immunoglobulin heavy constant mu



• Molecule 2: Immunoglobulin heavy constant mu







ASP	TTR	LYS	ASP	ASP	ASP	LYS	GLU	GLU	VAL	LEU	PHE	GLN	GLY	GLY	GLY	SER	LEU	PRO	VAL	ILE	ALA	GLU	LEU	PRO	PRO	LYS	VAL	VAL	PHE	VAL	VAL	PRO	ARG	ASP	GLY	PHE	GLY	ASN	PRO	ARG	LYS	LYS	LEU	ILE	CYS	GLN	ALA	THR	GLY	PHE	SER	PRO	ARG	GLN	ILE
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GLN	VAL	TRP	GLN	LEU	ARG	GLY	LYS	VAL	VAL	GLY	SER	GLY	VAL	THR	THR	ASP	GLY	ASP	GLN	VAL	VAL	ALA	ALA	LYS	GLU	SER	GLY	PRO	THR	THR	TYR	LYS	VAL	THR	THR	SER	THR	LEU	THR	ILE	LYS	GLU	ASN	SER	ASP	TRP	LEU	GLY	GLN	SER	MET	PHE	THR	CYS	THR	ALA	THR	ARG	VAL	ASP	HIS	ARG	GLY	LEU	ILE
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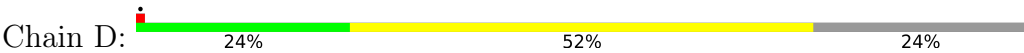
THR	PHE	GLN	GLN	ALA	SER	SER	CYS	CYS	PRO	ASP	GLN	ASP	THR	ALA	R345	R346	V347	F348	A349	I350	P351	P352	S353	F354	I357	F358	I359	T360	T363	R364	L365	T366	C367	L368	V369	T370	Y375	V378	T379	W382	T383	R384	Q385	N386	G387	A389	V390	H393	I396
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S397	E398	S399	H400	A403	T404	F405	S406	E410	P413	C414	E415	R423	F424	T425	C426	T429	H430	P436	L437	K438	Q439	T440	I441	S442	R443	P444	LYS	GLY	VAL	ALA	L449	H450	R451	P452	D453	V454	Y455	L456	R461	E462	Q463	R467	E468	S469	A470	F479	S480	P481	A482	D483
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

V484	F485	V486	Q487	W488	M489	Q490	G492	Q493	P494	L495	S496	P497	E498	K499	Y500	S503	A504	E508	R514	Y515	F516	A517	H518	L521	S524	E525	E526	E527	W528	N529	E532	T533	Y534	T535	C536	W537	V538	A539	H540	E542	L543	R546	V547	T548	E549	R550	T551	V552	D553	K554
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S555	T556	G557	K558	P559	T560	L561	Y562	N563	L566	V567	M568	S569	D570	T571	A572	G573	T574	C575	Y576
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● Molecule 3: Immunoglobulin J chain



GLN	GLU	ASP	E4	R5	L8	V9	D10	M11	K12	G13	C14	C15	I18	T19	S20	R21	T22	I23	R24	S25	S26	E27	D28	P29	N30	E31	D32	I33	V34	E35	R36	N37	I38	R39	L40	T41	V42	P43	L44	N45	N46	R47	E48	R49	I50	P53	T54	S55	P56	L57	R58	F61	V62	Y63	H64
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L65	C69	K70	LYS	ASP	PRO	THR	GLU	VAL	GLY	LEU	ASP	ASN	ILE	THR	ALA	GLN	GLN	ILE	CYS	ASP	GLU	ASP	SER	ALA	THR	E99	T100	T103	Y104	D105	R106	Y110	T111	A112	V113	V114	P115	Y118	G119	GLY	GLU	T122	K123	M124	L125	E126	T127	P131	D132
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A133	C134	Y135	P136	D137
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● Molecule 4: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1	MAG2
------	------

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	244123	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 ($e^-/\text{\AA}^2$)	1.02	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	42.554	Depositor
Minimum map value	-24.536	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	4.5	Depositor
Map size (Å)	480.00003, 480.00003, 480.00003	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2, 1.2, 1.2	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: NAG

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	C	0.34	0/4198	0.60	0/5708
2	A	0.49	1/1809 (0.1%)	0.68	4/2478 (0.2%)
2	B	0.43	0/1809	0.66	2/2478 (0.1%)
2	E	0.29	0/1787	0.50	0/2447
2	F	0.32	0/1818	0.53	0/2490
2	G	0.31	0/1831	0.59	2/2506 (0.1%)
2	H	0.30	0/1830	0.55	0/2507
2	I	0.27	0/1788	0.53	0/2449
2	J	0.29	0/1767	0.53	0/2420
2	K	0.34	0/1793	0.52	0/2455
2	L	0.29	0/1782	0.53	0/2442
3	D	0.48	0/850	0.73	0/1153
All	All	0.35	1/23062 (0.0%)	0.58	8/31533 (0.0%)

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
2	F	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	506	MET	C-N	11.29	1.48	1.33

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	506	MET	CA-C-N	11.27	131.39	119.89
2	A	506	MET	C-N-CA	11.27	131.39	119.89
2	B	501	VAL	CA-C-N	-6.26	114.16	122.99
2	B	501	VAL	C-N-CA	-6.26	114.16	122.99
2	G	536	CYS	CA-CB-SG	6.18	128.62	114.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	562	TYR	Peptide

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	C	4109	0	3992	232	0
2	A	1764	0	1725	138	0
2	B	1764	0	1724	126	0
2	E	1742	0	1708	117	0
2	F	1773	0	1721	141	0
2	G	1786	0	1737	154	0
2	H	1785	0	1735	124	0
2	I	1743	0	1708	118	0
2	J	1723	0	1682	125	0
2	K	1748	0	1713	127	0
2	L	1737	0	1697	134	0
3	D	838	0	833	77	0
4	M	28	0	25	1	0
All	All	22540	0	22000	1495	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 34.

The worst 5 of 1495 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)
2:K:562:TYR:OH	2:H:568:MET:SD	2.20	1.00
2:I:564:VAL:HG21	2:J:564:VAL:HG21	1.42	1.00
2:A:374:THR:HG23	2:A:405:PHE:HB3	1.49	0.93
2:L:500:TYR:HA	2:L:521:LEU:HD21	1.46	0.93
1:C:391:TYR:HE1	1:C:394:ARG:HH11	1.16	0.93

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	C	530/591 (90%)	482 (91%)	48 (9%)	0	100	100
2	A	225/369 (61%)	199 (88%)	26 (12%)	0	100	100
2	B	225/369 (61%)	182 (81%)	43 (19%)	0	100	100
2	E	222/369 (60%)	189 (85%)	33 (15%)	0	100	100
2	F	224/369 (61%)	181 (81%)	43 (19%)	0	100	100
2	G	226/369 (61%)	192 (85%)	34 (15%)	0	100	100
2	H	226/369 (61%)	187 (83%)	39 (17%)	0	100	100
2	I	222/369 (60%)	187 (84%)	35 (16%)	0	100	100
2	J	217/369 (59%)	188 (87%)	29 (13%)	0	100	100
2	K	223/369 (60%)	185 (83%)	38 (17%)	0	100	100
2	L	222/369 (60%)	188 (85%)	34 (15%)	0	100	100
3	D	98/137 (72%)	69 (70%)	29 (30%)	0	100	100
All	All	2860/4418 (65%)	2429 (85%)	431 (15%)	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	C	450/501 (90%)	448 (100%)	2 (0%)	84	84
2	A	203/326 (62%)	203 (100%)	0	100	100
2	B	203/326 (62%)	202 (100%)	1 (0%)	81	83
2	E	200/326 (61%)	200 (100%)	0	100	100
2	F	204/326 (63%)	204 (100%)	0	100	100
2	G	205/326 (63%)	205 (100%)	0	100	100
2	H	205/326 (63%)	205 (100%)	0	100	100
2	I	200/326 (61%)	200 (100%)	0	100	100
2	J	198/326 (61%)	198 (100%)	0	100	100
2	K	201/326 (62%)	201 (100%)	0	100	100
2	L	199/326 (61%)	199 (100%)	0	100	100
3	D	99/129 (77%)	99 (100%)	0	100	100
All	All	2567/3890 (66%)	2564 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	68	ASN
1	C	426	ASN
2	B	501	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	463	GLN
2	G	487	GLN
2	F	487	GLN
2	I	465	ASN
2	I	400	HIS

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 ⓘ

2 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	M	1	3,4	14,14,15	0.77	1 (7%)	17,19,21	0.61	0
4	NAG	M	2	4	14,14,15	0.19	0	17,19,21	0.38	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	M	1	3,4	-	3/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	1	NAG	O5-C1	-2.81	1.39	1.43

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

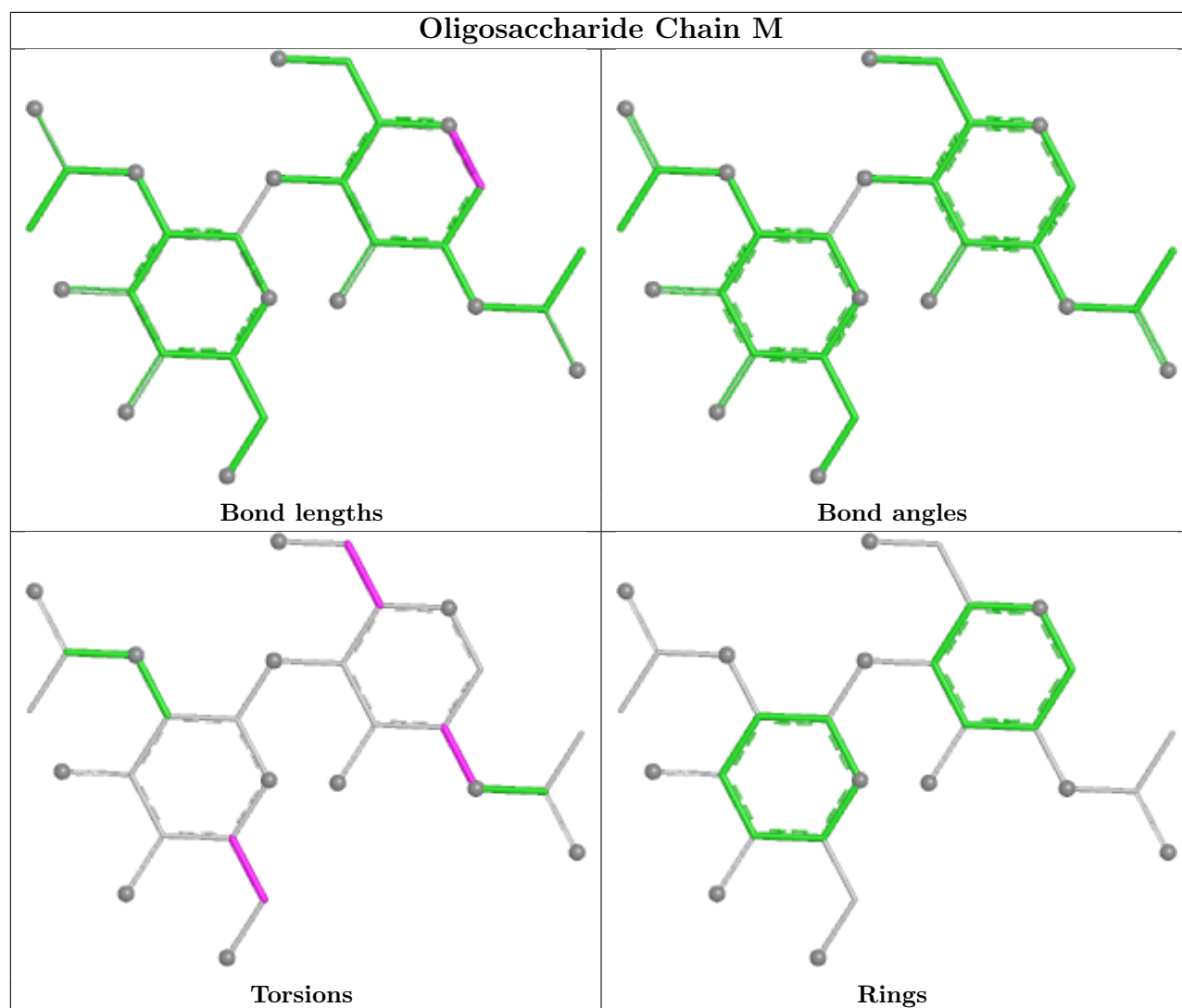
Mol	Chain	Res	Type	Atoms
4	M	1	NAG	O5-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	M	2	NAG	O5-C5-C6-O6
4	M	1	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	M	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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.

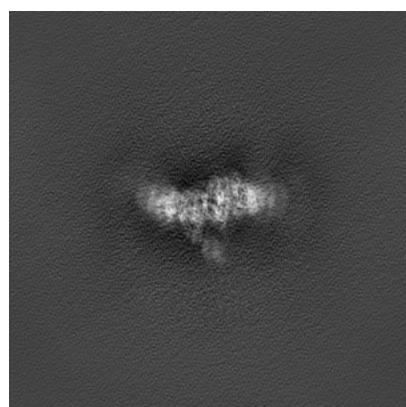
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22591. These allow visual inspection of the internal detail of the map and identification of artifacts.

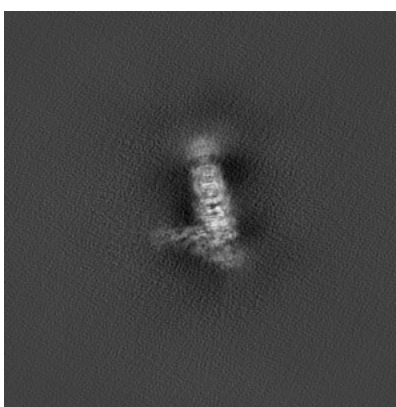
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

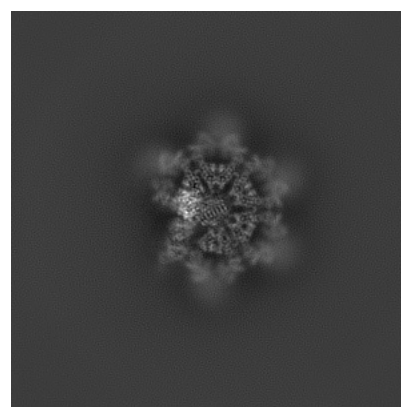
6.1.1 Primary map



X



Y

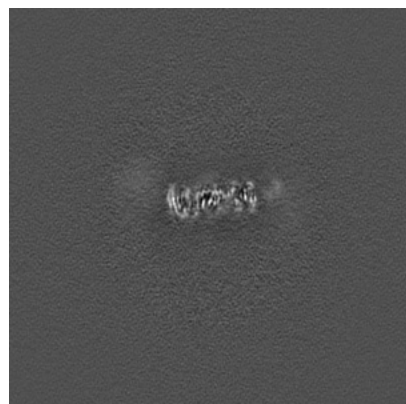


Z

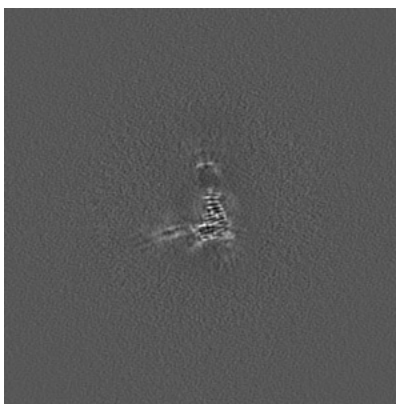
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

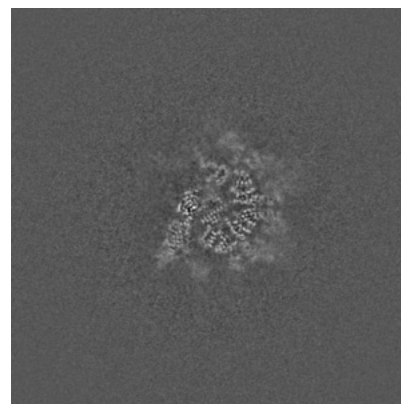
6.2.1 Primary map



X Index: 200



Y Index: 200

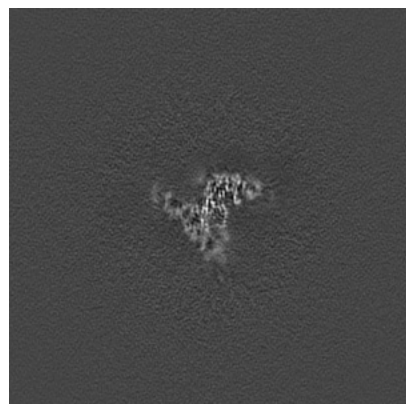


Z Index: 200

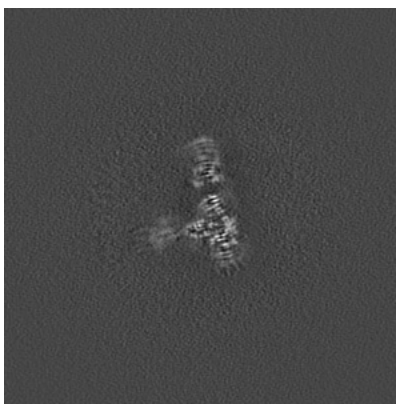
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

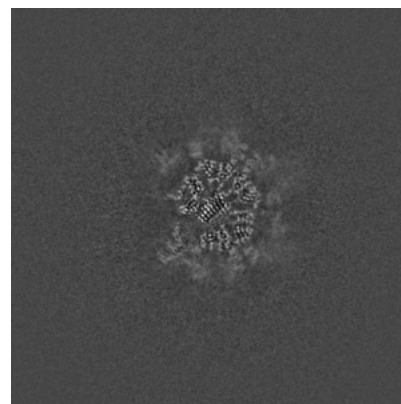
6.3.1 Primary map



X Index: 175



Y Index: 209

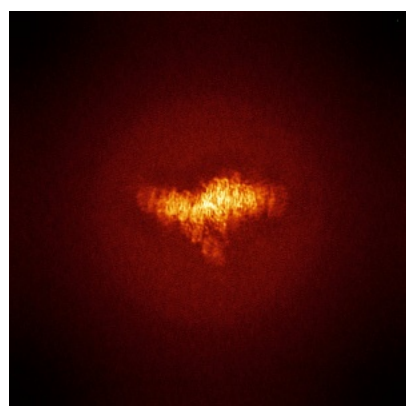


Z Index: 207

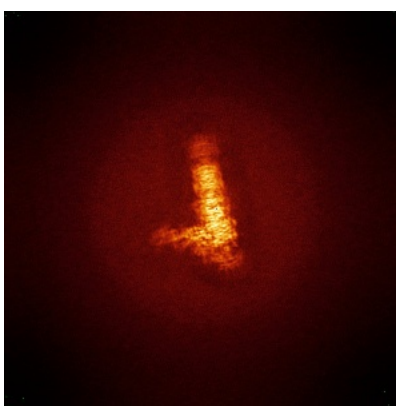
The images above show the largest variance slices of the map in three orthogonal directions.

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

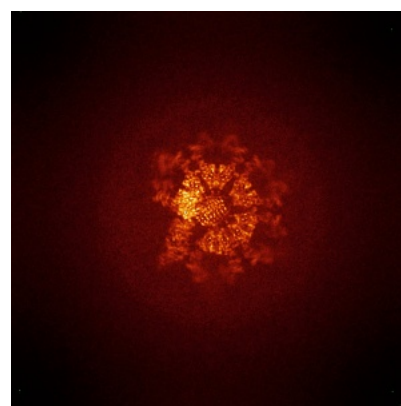
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 4.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

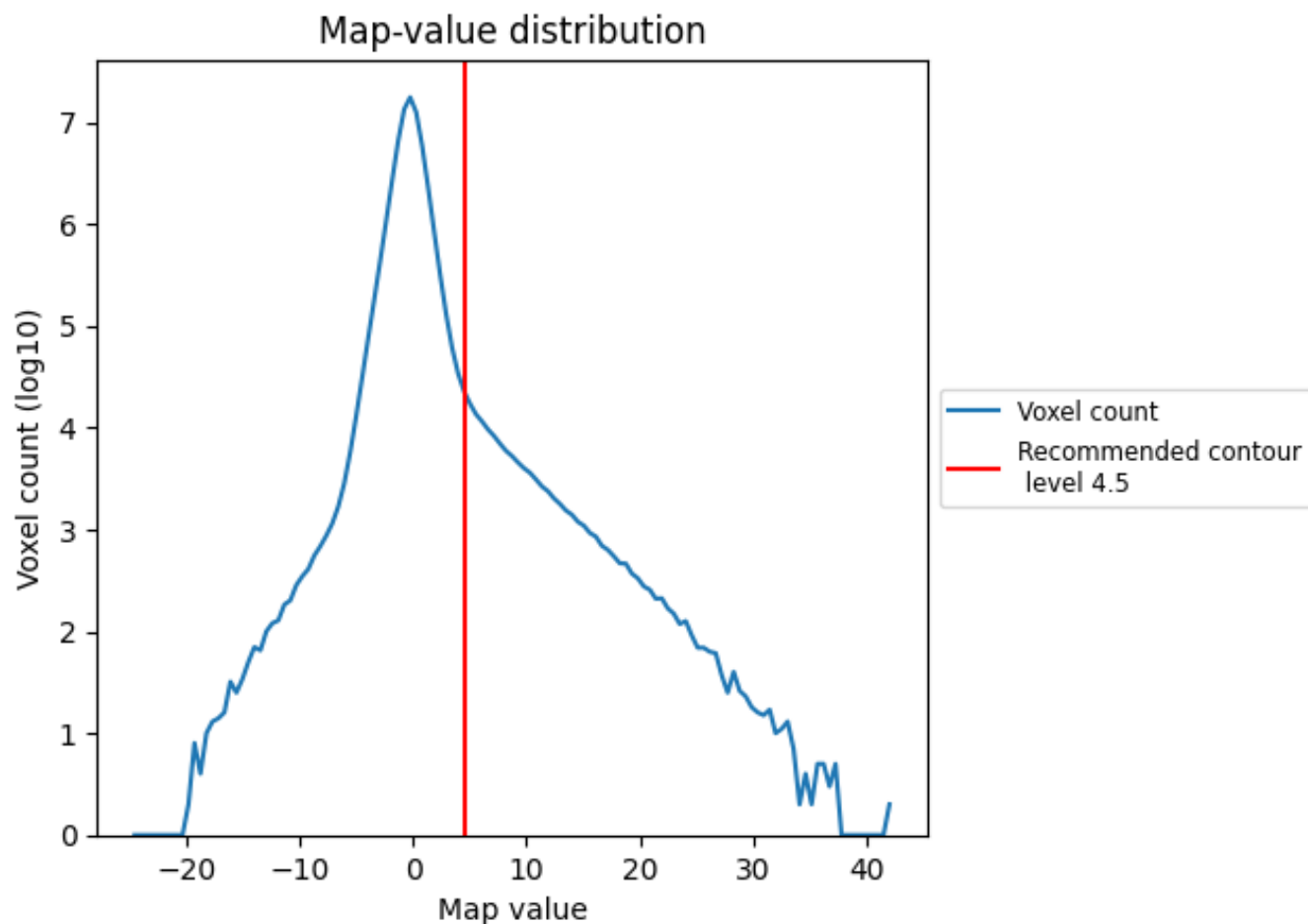
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

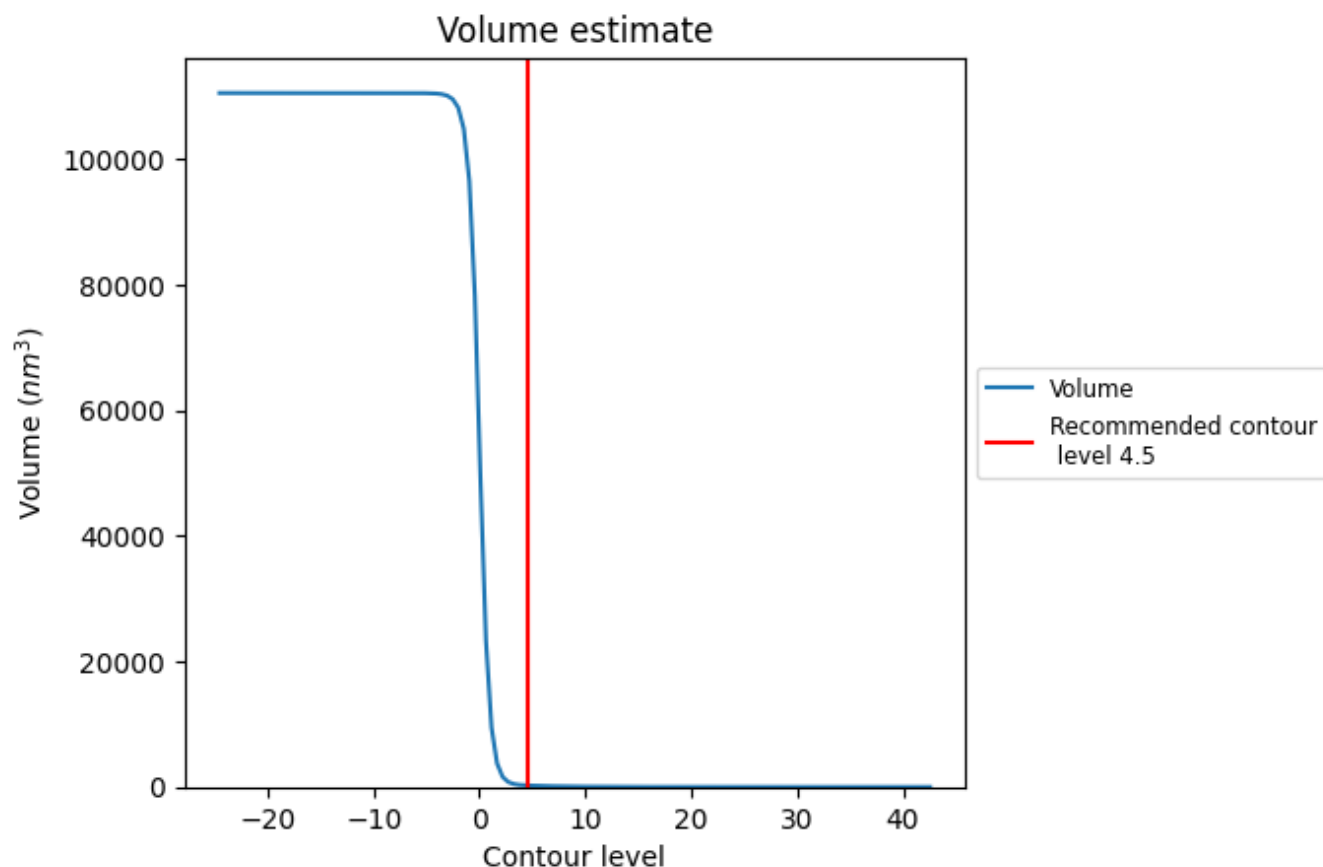
This section contains the results of statistical analysis of the map.

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.

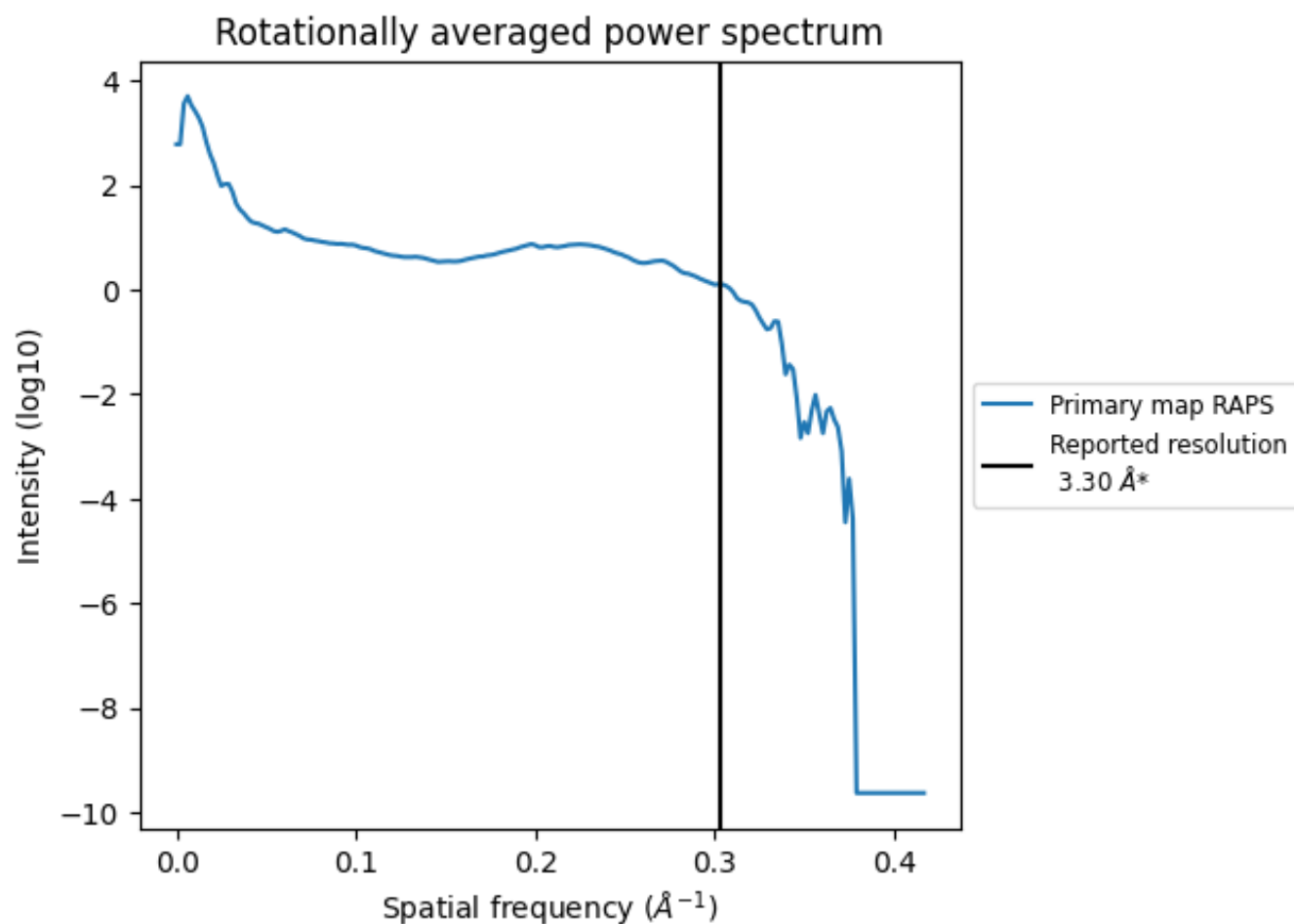
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 241 nm^3 ; this corresponds to an approximate mass of 218 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 0.303 Å⁻¹

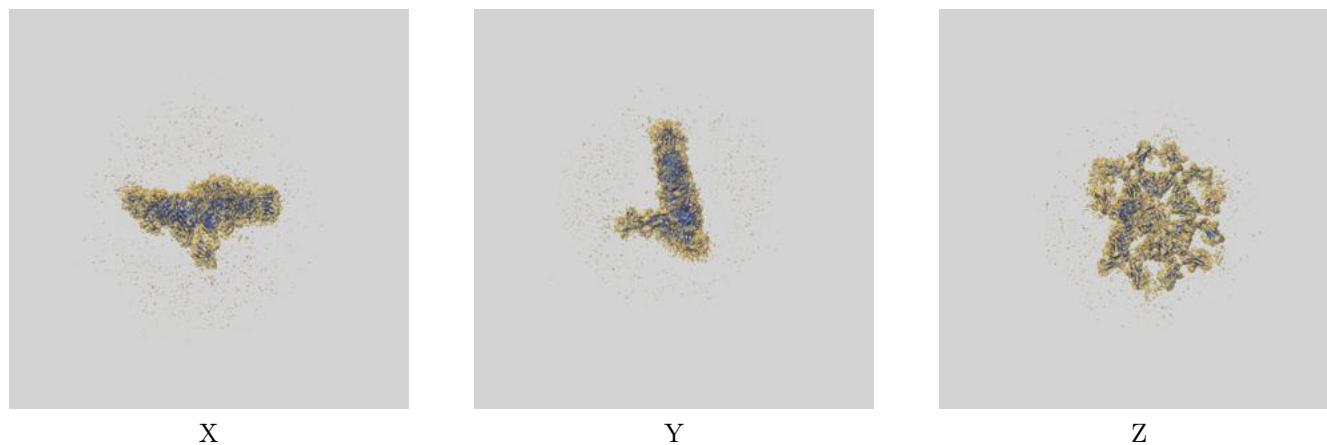
8 Fourier-Shell correlation ⓘ

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

9 Map-model fit [i](#)

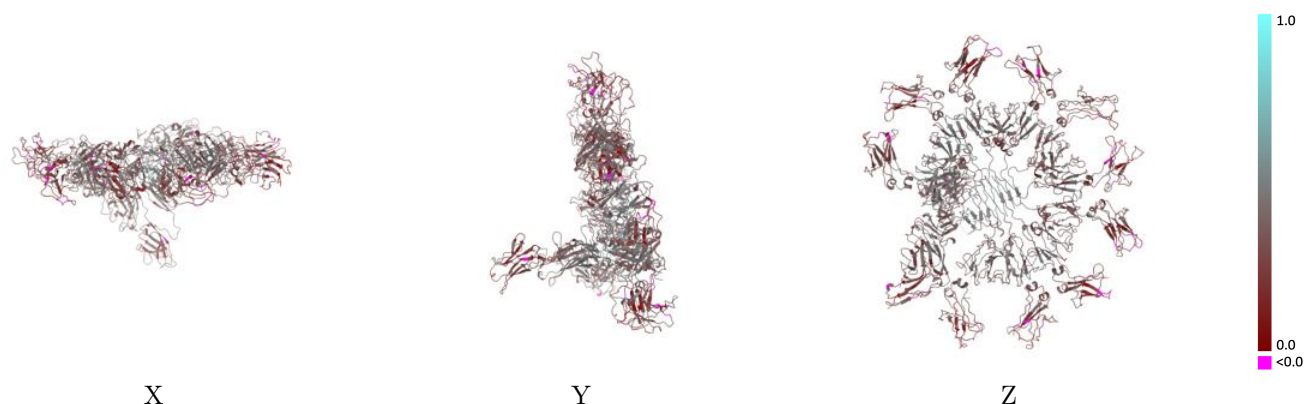
This section contains information regarding the fit between EMDB map EMD-22591 and PDB model 7K0C. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 4.5 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](#)



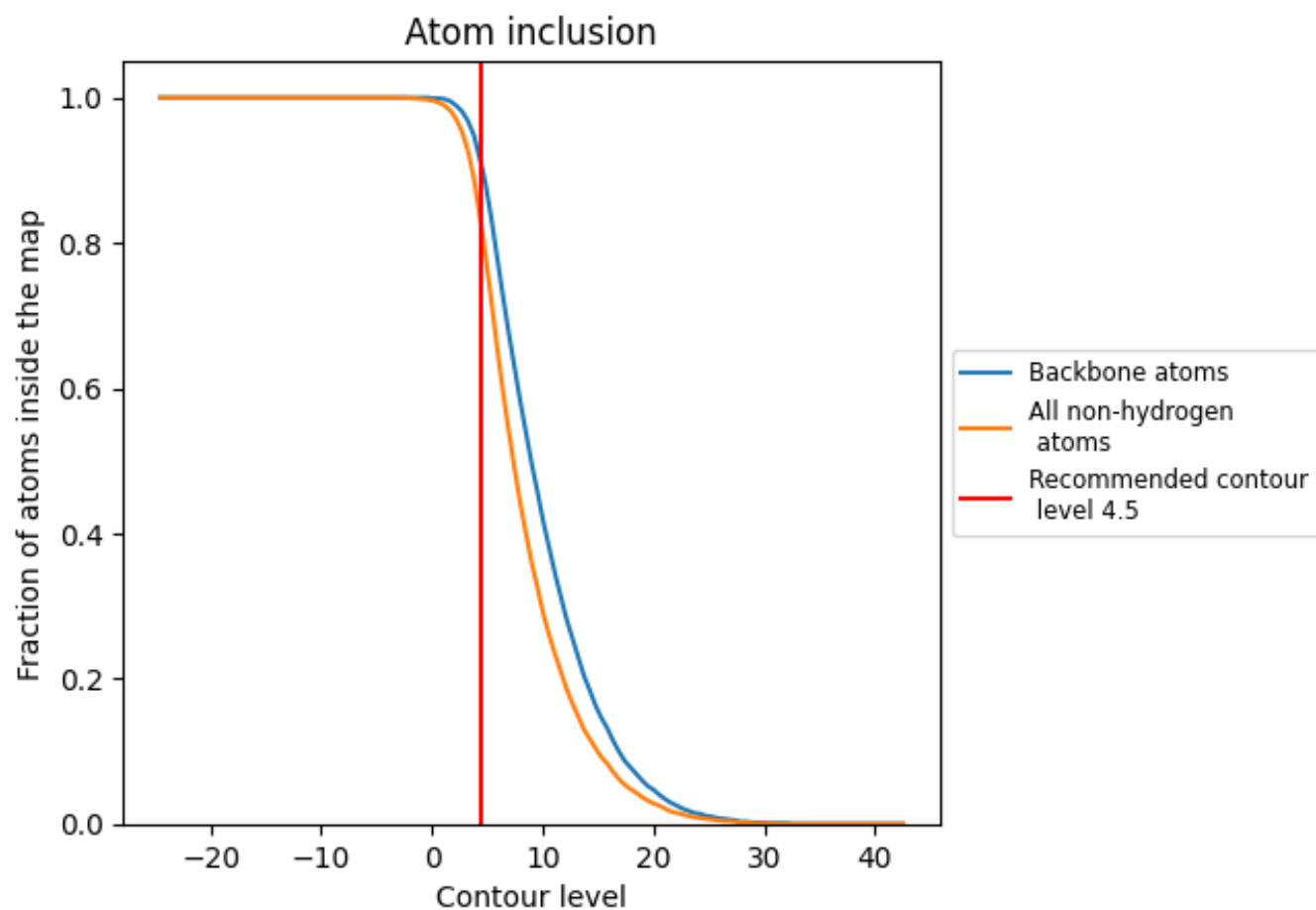
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 82% 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 (4.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8190	0.3620
A	0.8990	0.3980
B	0.8830	0.3850
C	0.8460	0.3620
D	0.9080	0.4390
E	0.7580	0.3440
F	0.8110	0.3540
G	0.8010	0.3610
H	0.8090	0.3460
I	0.7540	0.3460
J	0.7820	0.3330
K	0.7910	0.3660
L	0.7960	0.3430
M	0.9290	0.4010

