



wwPDB EM Validation Summary Report ⓘ

Oct 27, 2024 – 11:32 AM EDT

PDB ID : 7TL0
EMDB ID : EMD-25982
Title : Cryo-EM structure of hMPV preF bound by Fabs MPE8 and SAN32-2
Authors : Rush, S.A.; Hsieh, C.-L.; McLellan, J.S.
Deposited on : 2022-01-17
Resolution : 3.06 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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
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

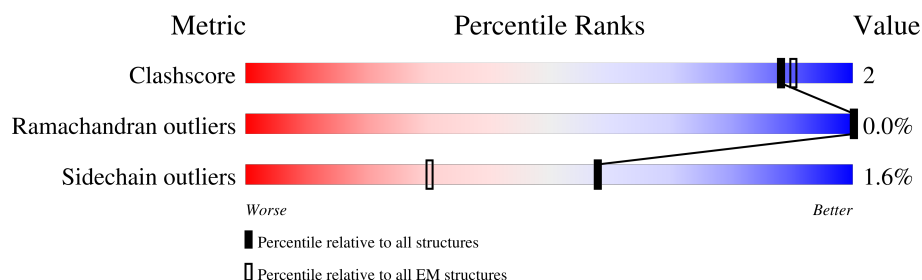
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.06 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.










Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	A	551	
1	B	551	
1	C	551	
2	D	224	
2	F	224	
2	H	224	
3	E	214	
3	G	214	

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Mol	Chain	Length	Quality of chain
3	I	214	
4	J	228	
4	L	228	
4	N	228	
5	K	216	
5	M	216	
5	O	216	
6	P	2	
6	Q	2	
6	R	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 40491 atoms, of which 20031 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 Fusion glycoprotein F0.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	433	Total	C	H	N	O	S	0	0
			6577	2058	3291	564	635	29		
1	B	433	Total	C	H	N	O	S	0	0
			6577	2058	3291	564	635	29		
1	C	433	Total	C	H	N	O	S	0	0
			6577	2058	3291	564	635	29		

There are 225 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	100	ARG	GLN	engineered mutation	UNP H6X1Z0
A	101	ARG	SER	engineered mutation	UNP H6X1Z0
A	110	CYS	LEU	engineered mutation	UNP H6X1Z0
A	127	CYS	THR	engineered mutation	UNP H6X1Z0
A	140	CYS	ALA	engineered mutation	UNP H6X1Z0
A	147	CYS	ALA	engineered mutation	UNP H6X1Z0
A	153	CYS	ASN	engineered mutation	UNP H6X1Z0
A	185	PRO	ALA	engineered mutation	UNP H6X1Z0
A	219	LYS	LEU	engineered mutation	UNP H6X1Z0
A	231	ILE	VAL	engineered mutation	UNP H6X1Z0
A	322	CYS	ASN	engineered mutation	UNP H6X1Z0
A	365	CYS	THR	engineered mutation	UNP H6X1Z0
A	453	GLN	GLU	engineered mutation	UNP H6X1Z0
A	463	CYS	VAL	engineered mutation	UNP H6X1Z0
A	491	GLY	-	expression tag	UNP H6X1Z0
A	492	GLY	-	expression tag	UNP H6X1Z0
A	493	GLY	-	expression tag	UNP H6X1Z0
A	494	SER	-	expression tag	UNP H6X1Z0
A	495	GLY	-	expression tag	UNP H6X1Z0
A	496	TYR	-	expression tag	UNP H6X1Z0
A	497	ILE	-	expression tag	UNP H6X1Z0
A	498	PRO	-	expression tag	UNP H6X1Z0
A	499	GLU	-	expression tag	UNP H6X1Z0
A	500	ALA	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	501	PRO	-	expression tag	UNP H6X1Z0
A	502	ARG	-	expression tag	UNP H6X1Z0
A	503	ASP	-	expression tag	UNP H6X1Z0
A	504	GLY	-	expression tag	UNP H6X1Z0
A	505	GLN	-	expression tag	UNP H6X1Z0
A	506	ALA	-	expression tag	UNP H6X1Z0
A	507	TYR	-	expression tag	UNP H6X1Z0
A	508	VAL	-	expression tag	UNP H6X1Z0
A	509	ARG	-	expression tag	UNP H6X1Z0
A	510	LYS	-	expression tag	UNP H6X1Z0
A	511	ASP	-	expression tag	UNP H6X1Z0
A	512	GLY	-	expression tag	UNP H6X1Z0
A	513	GLU	-	expression tag	UNP H6X1Z0
A	514	TRP	-	expression tag	UNP H6X1Z0
A	515	VAL	-	expression tag	UNP H6X1Z0
A	516	LEU	-	expression tag	UNP H6X1Z0
A	517	LEU	-	expression tag	UNP H6X1Z0
A	518	SER	-	expression tag	UNP H6X1Z0
A	519	THR	-	expression tag	UNP H6X1Z0
A	520	PHE	-	expression tag	UNP H6X1Z0
A	521	LEU	-	expression tag	UNP H6X1Z0
A	522	GLY	-	expression tag	UNP H6X1Z0
A	523	ARG	-	expression tag	UNP H6X1Z0
A	524	SER	-	expression tag	UNP H6X1Z0
A	525	LEU	-	expression tag	UNP H6X1Z0
A	526	GLU	-	expression tag	UNP H6X1Z0
A	527	VAL	-	expression tag	UNP H6X1Z0
A	528	LEU	-	expression tag	UNP H6X1Z0
A	529	PHE	-	expression tag	UNP H6X1Z0
A	530	GLN	-	expression tag	UNP H6X1Z0
A	531	GLY	-	expression tag	UNP H6X1Z0
A	532	PRO	-	expression tag	UNP H6X1Z0
A	533	GLY	-	expression tag	UNP H6X1Z0
A	534	HIS	-	expression tag	UNP H6X1Z0
A	535	HIS	-	expression tag	UNP H6X1Z0
A	536	HIS	-	expression tag	UNP H6X1Z0
A	537	HIS	-	expression tag	UNP H6X1Z0
A	538	HIS	-	expression tag	UNP H6X1Z0
A	539	HIS	-	expression tag	UNP H6X1Z0
A	540	HIS	-	expression tag	UNP H6X1Z0
A	541	HIS	-	expression tag	UNP H6X1Z0
A	542	SER	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	543	ALA	-	expression tag	UNP H6X1Z0
A	544	TRP	-	expression tag	UNP H6X1Z0
A	545	SER	-	expression tag	UNP H6X1Z0
A	546	HIS	-	expression tag	UNP H6X1Z0
A	547	PRO	-	expression tag	UNP H6X1Z0
A	548	GLN	-	expression tag	UNP H6X1Z0
A	549	PHE	-	expression tag	UNP H6X1Z0
A	550	GLU	-	expression tag	UNP H6X1Z0
A	551	LYS	-	expression tag	UNP H6X1Z0
B	100	ARG	GLN	engineered mutation	UNP H6X1Z0
B	101	ARG	SER	engineered mutation	UNP H6X1Z0
B	110	CYS	LEU	engineered mutation	UNP H6X1Z0
B	127	CYS	THR	engineered mutation	UNP H6X1Z0
B	140	CYS	ALA	engineered mutation	UNP H6X1Z0
B	147	CYS	ALA	engineered mutation	UNP H6X1Z0
B	153	CYS	ASN	engineered mutation	UNP H6X1Z0
B	185	PRO	ALA	engineered mutation	UNP H6X1Z0
B	219	LYS	LEU	engineered mutation	UNP H6X1Z0
B	231	ILE	VAL	engineered mutation	UNP H6X1Z0
B	322	CYS	ASN	engineered mutation	UNP H6X1Z0
B	365	CYS	THR	engineered mutation	UNP H6X1Z0
B	453	GLN	GLU	engineered mutation	UNP H6X1Z0
B	463	CYS	VAL	engineered mutation	UNP H6X1Z0
B	491	GLY	-	expression tag	UNP H6X1Z0
B	492	GLY	-	expression tag	UNP H6X1Z0
B	493	GLY	-	expression tag	UNP H6X1Z0
B	494	SER	-	expression tag	UNP H6X1Z0
B	495	GLY	-	expression tag	UNP H6X1Z0
B	496	TYR	-	expression tag	UNP H6X1Z0
B	497	ILE	-	expression tag	UNP H6X1Z0
B	498	PRO	-	expression tag	UNP H6X1Z0
B	499	GLU	-	expression tag	UNP H6X1Z0
B	500	ALA	-	expression tag	UNP H6X1Z0
B	501	PRO	-	expression tag	UNP H6X1Z0
B	502	ARG	-	expression tag	UNP H6X1Z0
B	503	ASP	-	expression tag	UNP H6X1Z0
B	504	GLY	-	expression tag	UNP H6X1Z0
B	505	GLN	-	expression tag	UNP H6X1Z0
B	506	ALA	-	expression tag	UNP H6X1Z0
B	507	TYR	-	expression tag	UNP H6X1Z0
B	508	VAL	-	expression tag	UNP H6X1Z0
B	509	ARG	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	510	LYS	-	expression tag	UNP H6X1Z0
B	511	ASP	-	expression tag	UNP H6X1Z0
B	512	GLY	-	expression tag	UNP H6X1Z0
B	513	GLU	-	expression tag	UNP H6X1Z0
B	514	TRP	-	expression tag	UNP H6X1Z0
B	515	VAL	-	expression tag	UNP H6X1Z0
B	516	LEU	-	expression tag	UNP H6X1Z0
B	517	LEU	-	expression tag	UNP H6X1Z0
B	518	SER	-	expression tag	UNP H6X1Z0
B	519	THR	-	expression tag	UNP H6X1Z0
B	520	PHE	-	expression tag	UNP H6X1Z0
B	521	LEU	-	expression tag	UNP H6X1Z0
B	522	GLY	-	expression tag	UNP H6X1Z0
B	523	ARG	-	expression tag	UNP H6X1Z0
B	524	SER	-	expression tag	UNP H6X1Z0
B	525	LEU	-	expression tag	UNP H6X1Z0
B	526	GLU	-	expression tag	UNP H6X1Z0
B	527	VAL	-	expression tag	UNP H6X1Z0
B	528	LEU	-	expression tag	UNP H6X1Z0
B	529	PHE	-	expression tag	UNP H6X1Z0
B	530	GLN	-	expression tag	UNP H6X1Z0
B	531	GLY	-	expression tag	UNP H6X1Z0
B	532	PRO	-	expression tag	UNP H6X1Z0
B	533	GLY	-	expression tag	UNP H6X1Z0
B	534	HIS	-	expression tag	UNP H6X1Z0
B	535	HIS	-	expression tag	UNP H6X1Z0
B	536	HIS	-	expression tag	UNP H6X1Z0
B	537	HIS	-	expression tag	UNP H6X1Z0
B	538	HIS	-	expression tag	UNP H6X1Z0
B	539	HIS	-	expression tag	UNP H6X1Z0
B	540	HIS	-	expression tag	UNP H6X1Z0
B	541	HIS	-	expression tag	UNP H6X1Z0
B	542	SER	-	expression tag	UNP H6X1Z0
B	543	ALA	-	expression tag	UNP H6X1Z0
B	544	TRP	-	expression tag	UNP H6X1Z0
B	545	SER	-	expression tag	UNP H6X1Z0
B	546	HIS	-	expression tag	UNP H6X1Z0
B	547	PRO	-	expression tag	UNP H6X1Z0
B	548	GLN	-	expression tag	UNP H6X1Z0
B	549	PHE	-	expression tag	UNP H6X1Z0
B	550	GLU	-	expression tag	UNP H6X1Z0
B	551	LYS	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	100	ARG	GLN	engineered mutation	UNP H6X1Z0
C	101	ARG	SER	engineered mutation	UNP H6X1Z0
C	110	CYS	LEU	engineered mutation	UNP H6X1Z0
C	127	CYS	THR	engineered mutation	UNP H6X1Z0
C	140	CYS	ALA	engineered mutation	UNP H6X1Z0
C	147	CYS	ALA	engineered mutation	UNP H6X1Z0
C	153	CYS	ASN	engineered mutation	UNP H6X1Z0
C	185	PRO	ALA	engineered mutation	UNP H6X1Z0
C	219	LYS	LEU	engineered mutation	UNP H6X1Z0
C	231	ILE	VAL	engineered mutation	UNP H6X1Z0
C	322	CYS	ASN	engineered mutation	UNP H6X1Z0
C	365	CYS	THR	engineered mutation	UNP H6X1Z0
C	453	GLN	GLU	engineered mutation	UNP H6X1Z0
C	463	CYS	VAL	engineered mutation	UNP H6X1Z0
C	491	GLY	-	expression tag	UNP H6X1Z0
C	492	GLY	-	expression tag	UNP H6X1Z0
C	493	GLY	-	expression tag	UNP H6X1Z0
C	494	SER	-	expression tag	UNP H6X1Z0
C	495	GLY	-	expression tag	UNP H6X1Z0
C	496	TYR	-	expression tag	UNP H6X1Z0
C	497	ILE	-	expression tag	UNP H6X1Z0
C	498	PRO	-	expression tag	UNP H6X1Z0
C	499	GLU	-	expression tag	UNP H6X1Z0
C	500	ALA	-	expression tag	UNP H6X1Z0
C	501	PRO	-	expression tag	UNP H6X1Z0
C	502	ARG	-	expression tag	UNP H6X1Z0
C	503	ASP	-	expression tag	UNP H6X1Z0
C	504	GLY	-	expression tag	UNP H6X1Z0
C	505	GLN	-	expression tag	UNP H6X1Z0
C	506	ALA	-	expression tag	UNP H6X1Z0
C	507	TYR	-	expression tag	UNP H6X1Z0
C	508	VAL	-	expression tag	UNP H6X1Z0
C	509	ARG	-	expression tag	UNP H6X1Z0
C	510	LYS	-	expression tag	UNP H6X1Z0
C	511	ASP	-	expression tag	UNP H6X1Z0
C	512	GLY	-	expression tag	UNP H6X1Z0
C	513	GLU	-	expression tag	UNP H6X1Z0
C	514	TRP	-	expression tag	UNP H6X1Z0
C	515	VAL	-	expression tag	UNP H6X1Z0
C	516	LEU	-	expression tag	UNP H6X1Z0
C	517	LEU	-	expression tag	UNP H6X1Z0
C	518	SER	-	expression tag	UNP H6X1Z0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	519	THR	-	expression tag	UNP H6X1Z0
C	520	PHE	-	expression tag	UNP H6X1Z0
C	521	LEU	-	expression tag	UNP H6X1Z0
C	522	GLY	-	expression tag	UNP H6X1Z0
C	523	ARG	-	expression tag	UNP H6X1Z0
C	524	SER	-	expression tag	UNP H6X1Z0
C	525	LEU	-	expression tag	UNP H6X1Z0
C	526	GLU	-	expression tag	UNP H6X1Z0
C	527	VAL	-	expression tag	UNP H6X1Z0
C	528	LEU	-	expression tag	UNP H6X1Z0
C	529	PHE	-	expression tag	UNP H6X1Z0
C	530	GLN	-	expression tag	UNP H6X1Z0
C	531	GLY	-	expression tag	UNP H6X1Z0
C	532	PRO	-	expression tag	UNP H6X1Z0
C	533	GLY	-	expression tag	UNP H6X1Z0
C	534	HIS	-	expression tag	UNP H6X1Z0
C	535	HIS	-	expression tag	UNP H6X1Z0
C	536	HIS	-	expression tag	UNP H6X1Z0
C	537	HIS	-	expression tag	UNP H6X1Z0
C	538	HIS	-	expression tag	UNP H6X1Z0
C	539	HIS	-	expression tag	UNP H6X1Z0
C	540	HIS	-	expression tag	UNP H6X1Z0
C	541	HIS	-	expression tag	UNP H6X1Z0
C	542	SER	-	expression tag	UNP H6X1Z0
C	543	ALA	-	expression tag	UNP H6X1Z0
C	544	TRP	-	expression tag	UNP H6X1Z0
C	545	SER	-	expression tag	UNP H6X1Z0
C	546	HIS	-	expression tag	UNP H6X1Z0
C	547	PRO	-	expression tag	UNP H6X1Z0
C	548	GLN	-	expression tag	UNP H6X1Z0
C	549	PHE	-	expression tag	UNP H6X1Z0
C	550	GLU	-	expression tag	UNP H6X1Z0
C	551	LYS	-	expression tag	UNP H6X1Z0

- Molecule 2 is a protein called SAN32-2 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	D	120	Total	C	H	N	O	S	1	0
			1857	604	912	154	183	4		
2	F	120	Total	C	H	N	O	S	1	0
			1857	604	912	154	183	4		
2	H	120	Total	C	H	N	O	S	1	0
			1857	604	912	154	183	4		

- Molecule 3 is a protein called SAN32-2 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	E	105	Total	C	H	N	O	S	0	0
			1578	510	766	133	166	3		
3	G	105	Total	C	H	N	O	S	0	0
			1578	510	766	133	166	3		
3	I	105	Total	C	H	N	O	S	0	0
			1578	510	766	133	166	3		

- Molecule 4 is a protein called MPE8 Fab heavy chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	J	124	Total	C	H	N	O	S	0	0
			1838	587	903	159	185	4		
4	L	124	Total	C	H	N	O	S	0	0
			1838	587	903	159	185	4		
4	N	124	Total	C	H	N	O	S	0	0
			1838	587	903	159	185	4		

- Molecule 5 is a protein called MPE8 Fab light chain.

Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	107	Total	C	H	N	O	S	0	0
			1536	486	750	135	163	2		
5	M	107	Total	C	H	N	O	S	0	0
			1536	486	750	135	163	2		
5	O	107	Total	C	H	N	O	S	0	0
			1536	486	750	135	163	2		

- Molecule 6 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



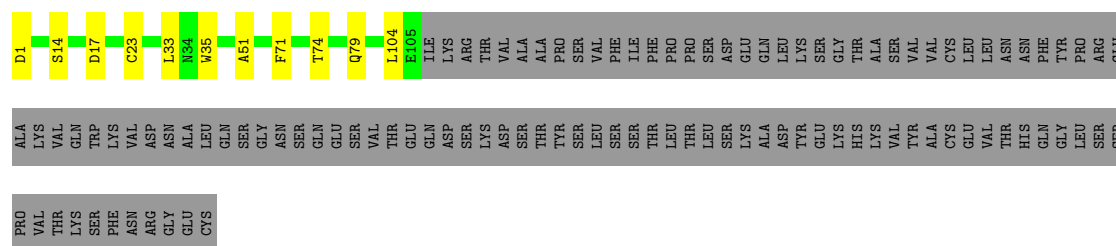
Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	Q	2	Total	C	H	N	O	0	0
			55	16	27	2	10		
6	R	2	Total	C	H	N	O	0	0
			55	16	27	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



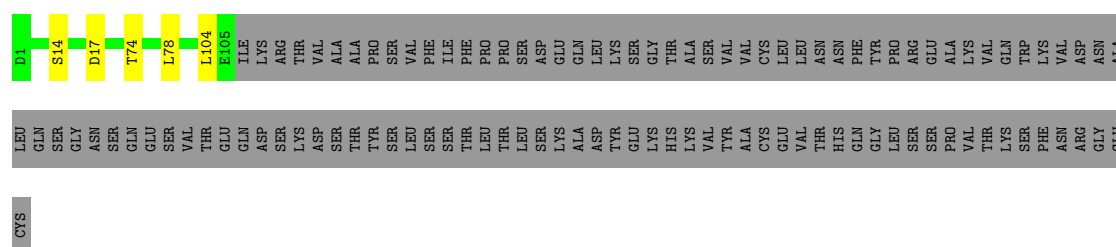
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	C	1	Total	C	H	N	O	0
			28	8	14	1	5	

Chain G:  44% 5% 51%



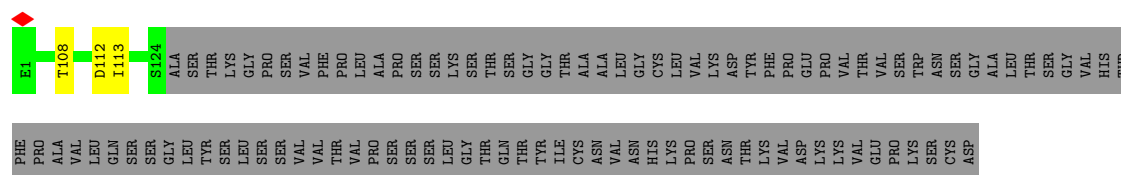
- Molecule 3: SAN32-2 Fab light chain

Chain I:  47% 1% 51%



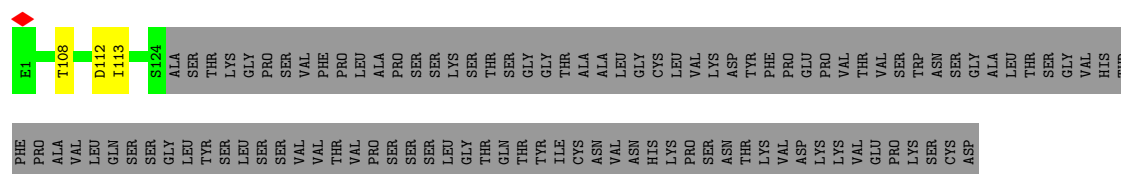
- Molecule 4: MPE8 Fab heavy chain

Chain J:  53% 1% 46%



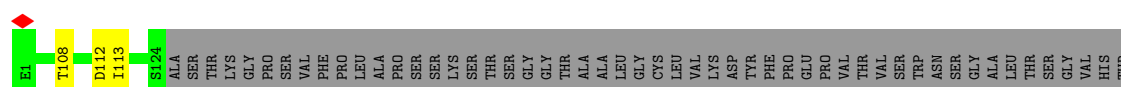
- Molecule 4: MPE8 Fab heavy chain

Chain L:  53% 1% 46%



- Molecule 4: MPE8 Fab heavy chain

Chain N:  53% 1% 46%



PHE PRO ALA VAL LEU GLN SER SER GLY LEU TYR SER GLN LEU SER SER VAL VAL THR VAL PRO SER SER SER SER LEU GLY THR GLN THR TYR ILE CYS ASN ASN VAL ASN HIS LYS SER PRO SER ASN LYS ASP LYS VAL GLY VAL PRO LYS SER CYS ASP

• Molecule 5: MPE8 Fab light chain



GLN SER V3 R56 D62 V109 LEU GLN SER GLN PRO LYS ALA VAL PRO VAL THR LEU PHE SER PRO LEU SER SER GLN THR TYR ILE CYS ASN LYS THR VAL CYS LEU SER ASP PHE TYR PRO GLY ALA VAL THR VAL ALA TRP LYS ALA ASP SER PRO VAL LYS

ALA GLY VAL THR THR PRO SER LYS GLN ASN ASN LYS TYR VAL ALA SER THR TYR LEU LEU PRO GLN TRP LYS HIS SER LYS THR SER CYS GLN VAL THR SER THR VAL ALA THR PRO GLU CYS SER

• Molecule 5: MPE8 Fab light chain



GLN SER V3 R56 D62 E85 K106 V109 LEU GLN PRO GLN LYS ALA VAL PRO VAL THR LEU PHE PRO SER SER GLN GLU GLU TRP LYS THR ALA THR VAL CYS LEU SER ILE THR HIS GLU ASP PHE TYR PRO GLY VAL ALA VAL THR VAL ALA TRP LYS ALA ASP SER

SER PRO VAL LYS ALA GLY VAL THR THR PRO SER LYS GLN SER ASN LYS TYR ALA VAL SER SER THR TYR LEU SER LEU THR PRO GLN GLU TRP LYS THR VAL CYS GLN THR THR HIS VAL GLU THR VAL VAL THR PRO THR LYS GLU CYS SER

• Molecule 5: MPE8 Fab light chain



GLN SER V3 D52 N55 R56 D62 E85 K106 V109 LEU GLN PRO GLN LYS ALA VAL PRO VAL THR LEU PHE PRO SER SER GLN GLU GLU TRP LYS THR ALA THR VAL CYS LEU SER ILE THR HIS GLU ASP PHE TYR PRO GLY ALA VAL THR VAL ALA TRP LYS

ALA ASP SER SER PRO VAL LYS GLY VAL GLU THR THR PRO SER LYS GLN SER ASN LYS TYR ALA VAL SER SER THR TYR LEU SER LEU THR PRO GLN GLU TRP LYS THR VAL CYS GLN THR THR HIS VAL GLU THR VAL VAL THR PRO THR LYS GLU CYS THR

GLU CYS SER

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1 NAG2

• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



NAG1 NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	134989	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 ($e^-/\text{\AA}^2$)	70	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	29000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	44.181	Depositor
Minimum map value	-10.731	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.015	Depositor
Recommended contour level	6	Depositor
Map size (Å)	349.92, 349.92, 349.92	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.366875, 1.366875, 1.366875	Depositor

5 Model quality

5.1 Standard geometry

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	A	0.43	0/3334	0.54	0/4514
1	B	0.42	0/3334	0.55	0/4514
1	C	0.43	0/3334	0.55	0/4514
2	D	0.54	0/971	0.52	0/1317
2	F	0.55	0/971	0.51	0/1317
2	H	0.55	0/971	0.53	0/1317
3	E	0.52	0/831	0.58	0/1129
3	G	0.51	0/831	0.55	0/1129
3	I	0.52	0/831	0.57	0/1129
4	J	0.44	0/955	0.55	0/1292
4	L	0.44	0/955	0.55	0/1292
4	N	0.44	0/955	0.54	0/1292
5	K	0.45	0/803	0.56	0/1096
5	M	0.45	0/803	0.57	0/1096
5	O	0.46	0/803	0.58	0/1096
All	All	0.46	0/20682	0.55	0/28044

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	A	3286	3291	3289	16	0
1	B	3286	3291	3289	17	0
1	C	3286	3291	3289	4	0
2	D	945	912	903	10	0
2	F	945	912	903	6	0
2	H	945	912	903	4	0
3	E	812	766	766	5	0
3	G	812	766	766	3	0
3	I	812	766	766	3	0
4	J	935	903	903	1	0
4	L	935	903	903	1	0
4	N	935	903	903	1	0
5	K	786	750	749	1	0
5	M	786	750	749	2	0
5	O	786	750	749	3	0
6	P	28	27	25	0	0
6	Q	28	27	25	0	0
6	R	28	27	25	0	0
7	A	28	28	26	2	0
7	B	28	28	26	2	0
7	C	28	28	26	0	0
All	All	20460	20031	19983	71	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 2.

The worst 5 of 71 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:B:356:THR:O	7:B:602:NAG:O6	1.86	0.93
1:A:295:LYS:O	1:A:298:ASN:ND2	2.23	0.71
7:A:602:NAG:O7	7:A:602:NAG:O3	2.12	0.66
1:A:105:LEU:HD21	1:B:370:ILE:HD13	1.77	0.66
1:A:327:GLU:OE2	1:A:329:ARG:NH2	2.29	0.64

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	A	429/551 (78%)	414 (96%)	15 (4%)	0	100	100
1	B	429/551 (78%)	407 (95%)	22 (5%)	0	100	100
1	C	429/551 (78%)	414 (96%)	15 (4%)	0	100	100
2	D	118/224 (53%)	111 (94%)	7 (6%)	0	100	100
2	F	118/224 (53%)	110 (93%)	8 (7%)	0	100	100
2	H	118/224 (53%)	110 (93%)	8 (7%)	0	100	100
3	E	103/214 (48%)	95 (92%)	8 (8%)	0	100	100
3	G	103/214 (48%)	96 (93%)	6 (6%)	1 (1%)	13	38
3	I	103/214 (48%)	97 (94%)	6 (6%)	0	100	100
4	J	122/228 (54%)	119 (98%)	3 (2%)	0	100	100
4	L	122/228 (54%)	119 (98%)	3 (2%)	0	100	100
4	N	122/228 (54%)	118 (97%)	4 (3%)	0	100	100
5	K	105/216 (49%)	97 (92%)	8 (8%)	0	100	100
5	M	105/216 (49%)	98 (93%)	7 (7%)	0	100	100
5	O	105/216 (49%)	97 (92%)	8 (8%)	0	100	100
All	All	2631/4299 (61%)	2502 (95%)	128 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	51	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	368/468 (79%)	360 (98%)	8 (2%)	47	68
1	B	368/468 (79%)	361 (98%)	7 (2%)	52	72
1	C	368/468 (79%)	361 (98%)	7 (2%)	52	72
2	D	104/194 (54%)	102 (98%)	2 (2%)	52	72
2	F	104/194 (54%)	103 (99%)	1 (1%)	73	85
2	H	104/194 (54%)	103 (99%)	1 (1%)	73	85
3	E	90/188 (48%)	88 (98%)	2 (2%)	47	68
3	G	90/188 (48%)	86 (96%)	4 (4%)	24	51
3	I	90/188 (48%)	89 (99%)	1 (1%)	70	83
4	J	100/190 (53%)	99 (99%)	1 (1%)	73	85
4	L	100/190 (53%)	99 (99%)	1 (1%)	73	85
4	N	100/190 (53%)	99 (99%)	1 (1%)	73	85
5	K	87/181 (48%)	87 (100%)	0	100	100
5	M	87/181 (48%)	87 (100%)	0	100	100
5	O	87/181 (48%)	87 (100%)	0	100	100
All	All	2247/3663 (61%)	2211 (98%)	36 (2%)	58	76

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	74	THR
4	N	108	THR
3	G	79	GLN
3	I	74	THR
1	B	345	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 16 such sidechains are listed below:

Mol	Chain	Res	Type
5	M	39	GLN
5	K	55	ASN
3	G	27	GLN
5	K	39	GLN
3	G	24	GLN

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 ⓘ

6 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$
6	NAG	P	1	6,1	14,14,15	0.24	0	17,19,21	0.48	0
6	NAG	P	2	6	14,14,15	0.19	0	17,19,21	0.73	1 (5%)
6	NAG	Q	1	6,1	14,14,15	0.24	0	17,19,21	0.57	0
6	NAG	Q	2	6	14,14,15	0.54	0	17,19,21	0.58	0
6	NAG	R	1	6,1	14,14,15	0.33	0	17,19,21	0.48	0
6	NAG	R	2	6	14,14,15	0.21	0	17,19,21	0.65	1 (5%)

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

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	P	2	NAG	C1-O5-C5	2.51	115.55	112.19
6	R	2	NAG	C1-O5-C5	2.16	115.08	112.19

There are no chirality outliers.

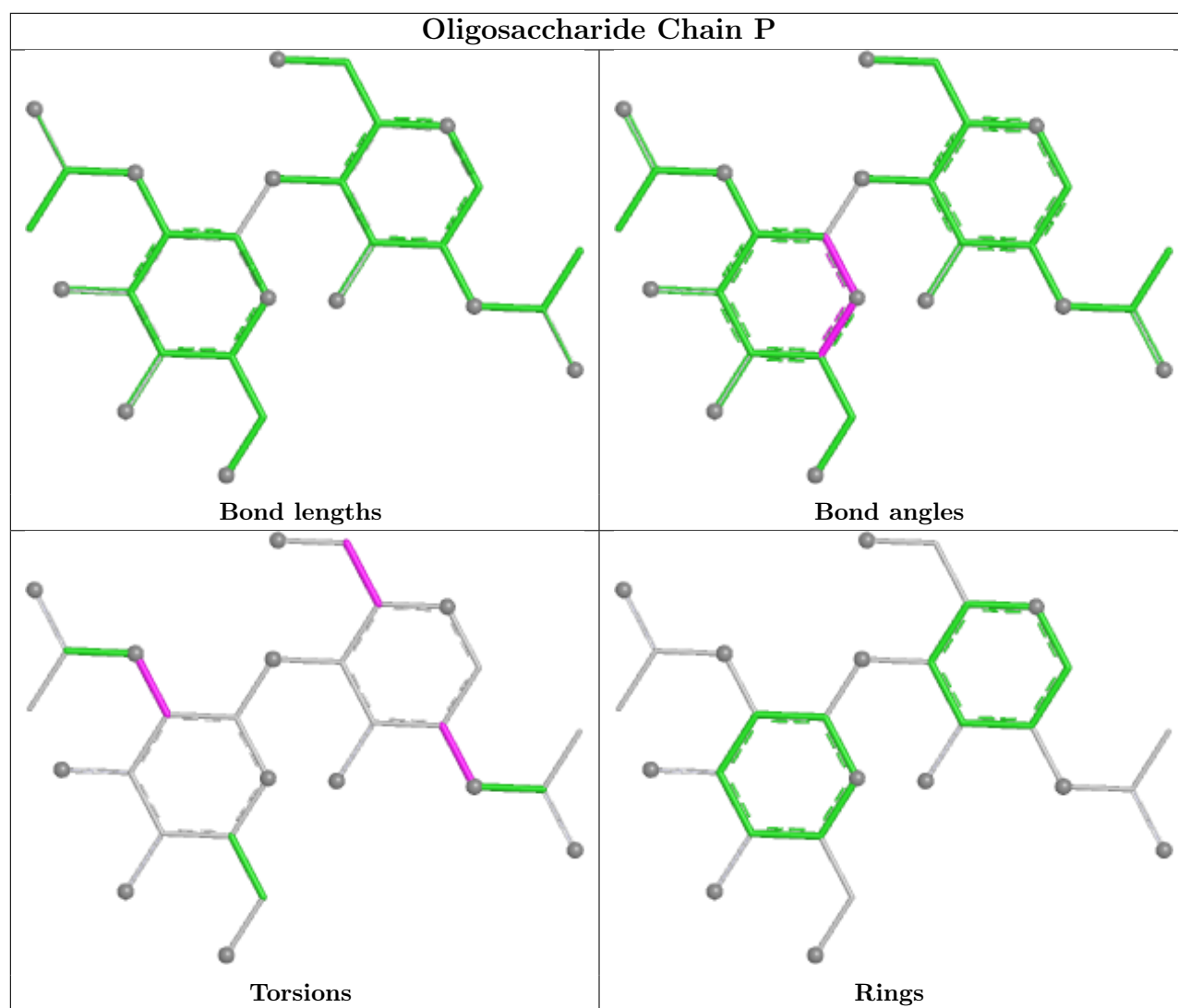
5 of 15 torsion outliers are listed below:

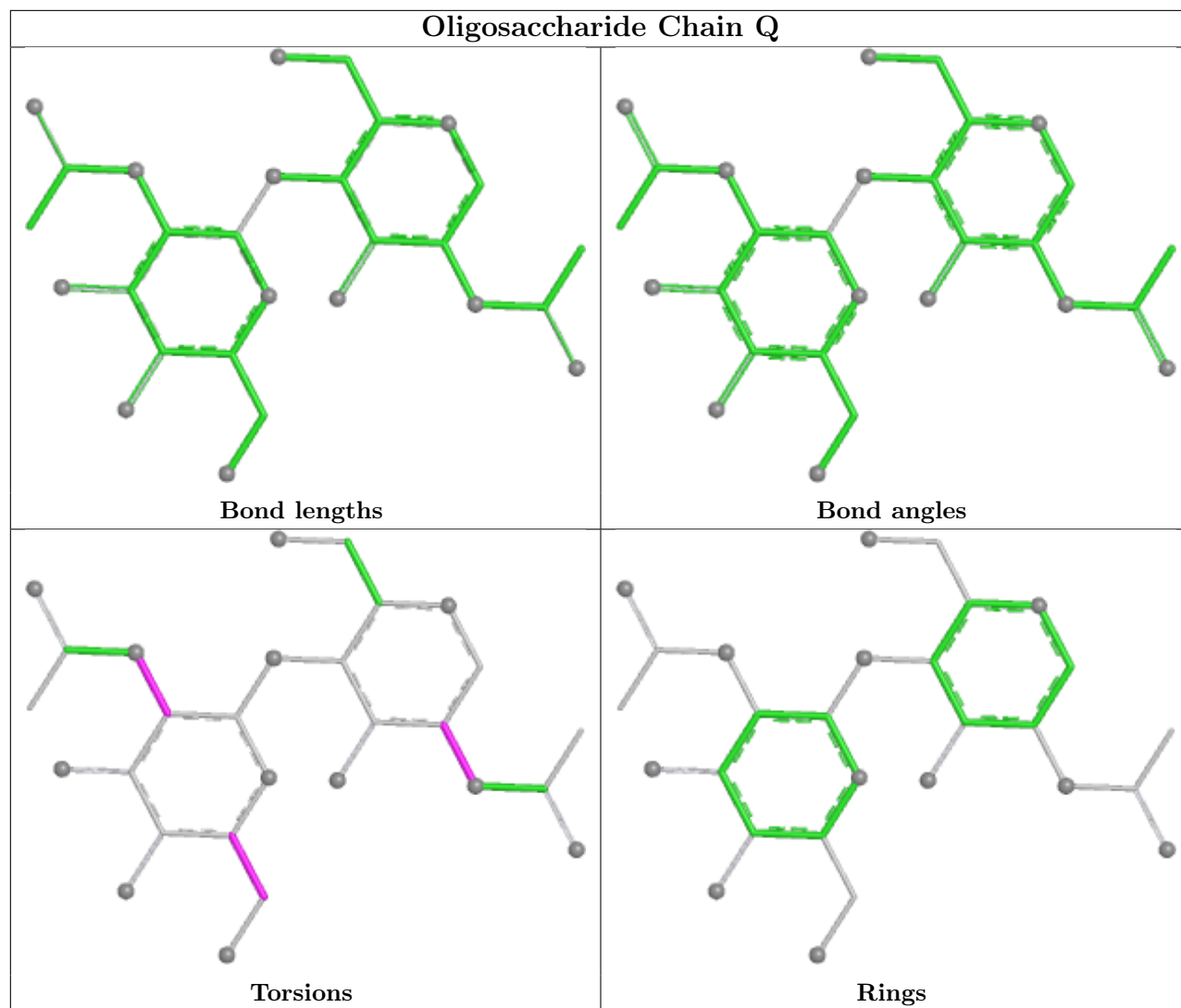
Mol	Chain	Res	Type	Atoms
6	P	1	NAG	O5-C5-C6-O6
6	P	1	NAG	C4-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
6	P	1	NAG	C1-C2-N2-C7
6	P	2	NAG	C1-C2-N2-C7

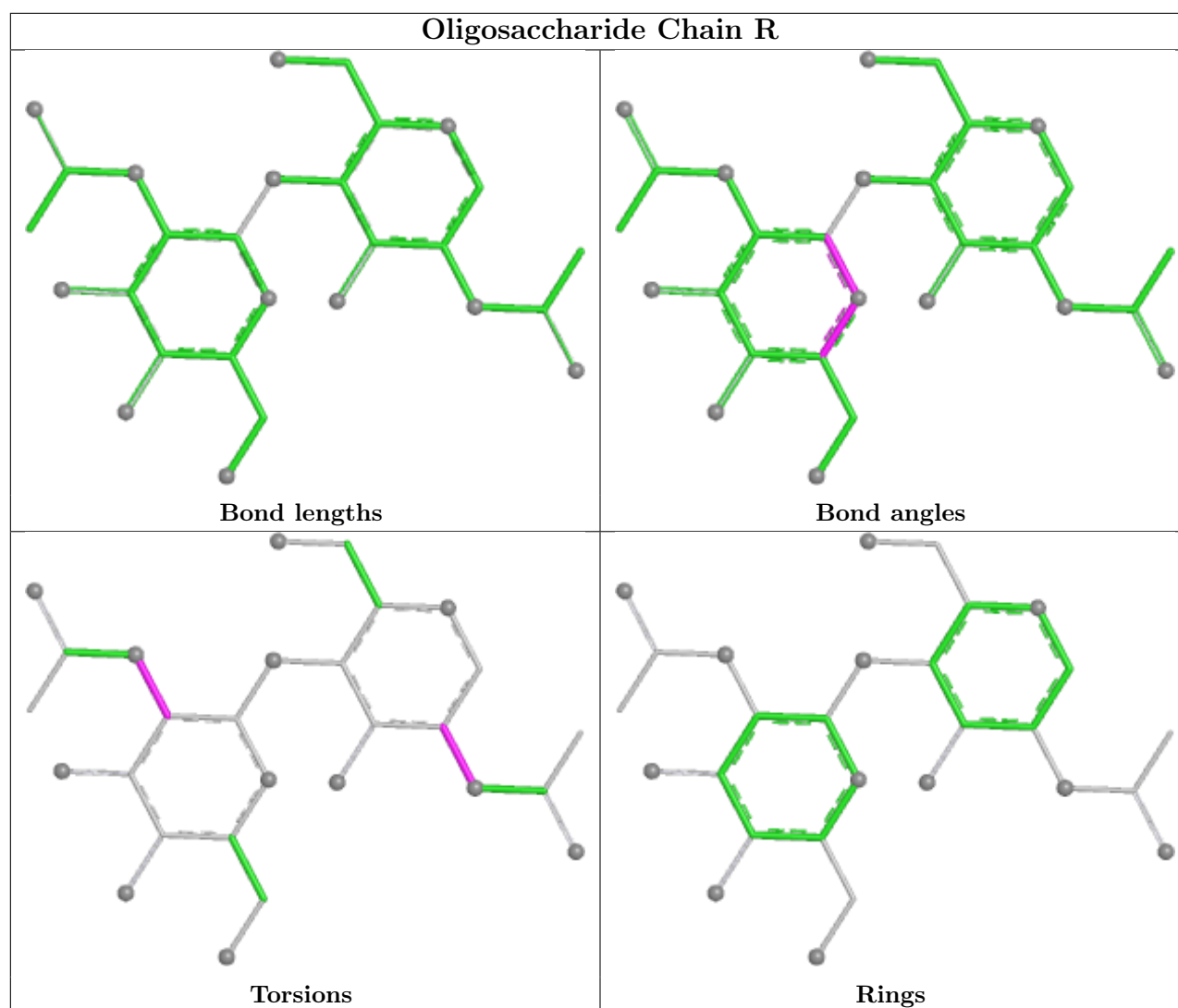
There are no ring outliers.

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 oligosaccharide.







5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	NAG	C	601	1	14,14,15	0.72	1 (7%)	17,19,21	1.31	1 (5%)
7	NAG	B	602	1	14,14,15	0.98	1 (7%)	17,19,21	0.72	0
7	NAG	C	602	1	14,14,15	0.33	0	17,19,21	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	A	601	1	14,14,15	0.46	0	17,19,21	0.70	1 (5%)
7	NAG	A	602	1	14,14,15	0.36	0	17,19,21	0.92	1 (5%)
7	NAG	B	601	1	14,14,15	0.35	0	17,19,21	0.67	1 (5%)

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	NAG	C	601	1	-	0/6/23/26	0/1/1/1
7	NAG	B	602	1	-	0/6/23/26	0/1/1/1
7	NAG	C	602	1	-	4/6/23/26	0/1/1/1
7	NAG	A	601	1	-	1/6/23/26	0/1/1/1
7	NAG	A	602	1	-	4/6/23/26	0/1/1/1
7	NAG	B	601	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	602	NAG	C1-C2	3.33	1.56	1.52
7	C	601	NAG	O5-C1	2.17	1.47	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	601	NAG	C1-O5-C5	5.28	119.26	112.19
7	A	602	NAG	C1-O5-C5	3.58	116.98	112.19
7	A	601	NAG	C1-O5-C5	2.48	115.52	112.19
7	B	601	NAG	C1-O5-C5	2.42	115.42	112.19

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	601	NAG	O5-C5-C6-O6
7	A	602	NAG	O5-C5-C6-O6
7	C	602	NAG	O5-C5-C6-O6
7	A	602	NAG	C4-C5-C6-O6
7	A	602	NAG	C1-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	602	NAG	2	0
7	A	602	NAG	2	0

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.

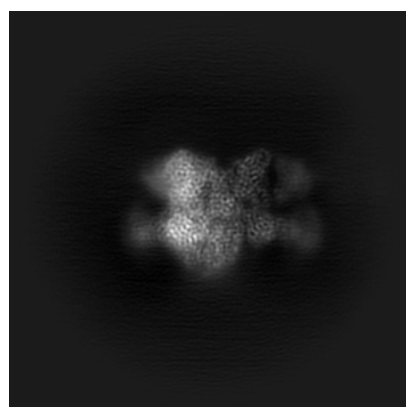
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-25982. These allow visual inspection of the internal detail of the map and identification of artifacts.

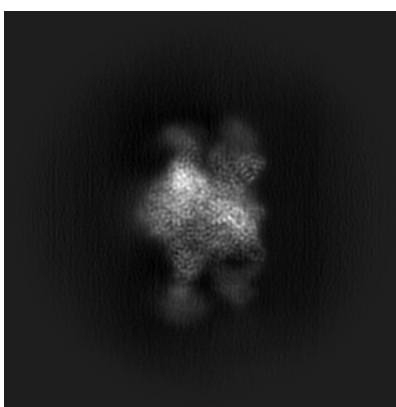
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

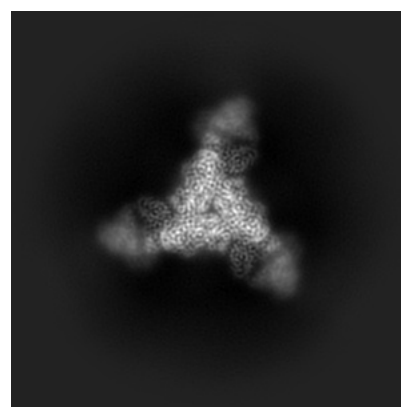
6.1.1 Primary map



X



Y

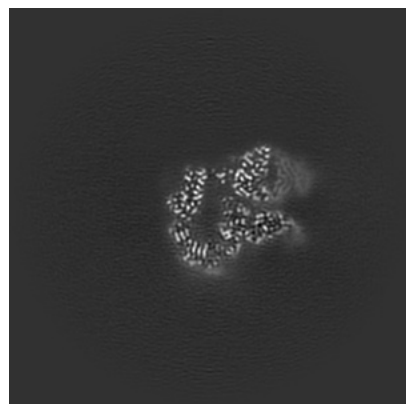


Z

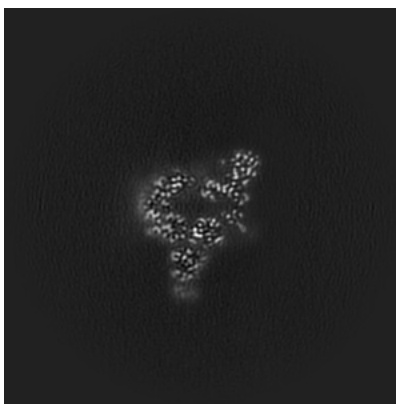
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

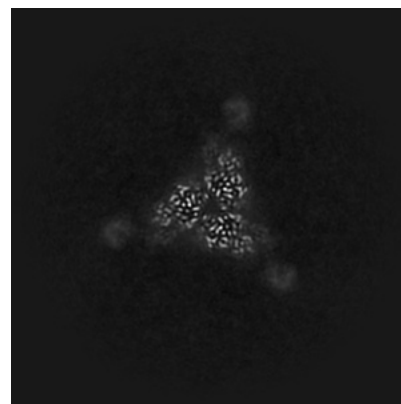
6.2.1 Primary map



X Index: 128



Y Index: 128

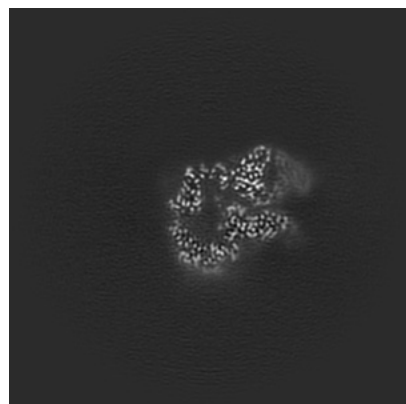


Z Index: 128

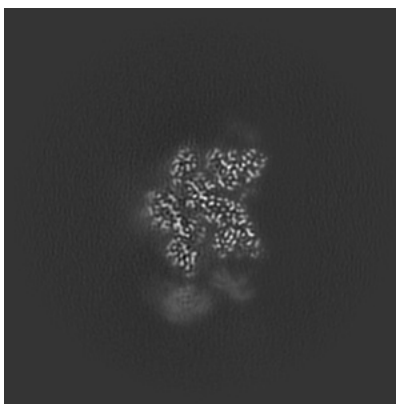
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

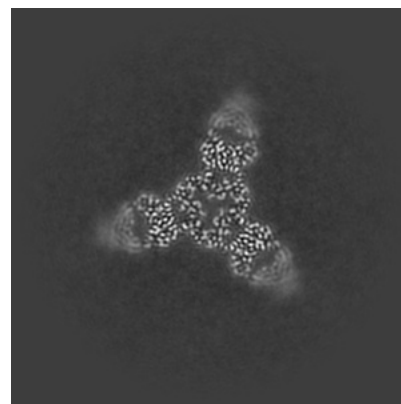
6.3.1 Primary map



X Index: 126



Y Index: 115

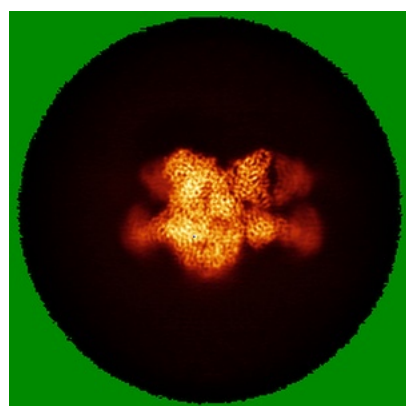


Z Index: 114

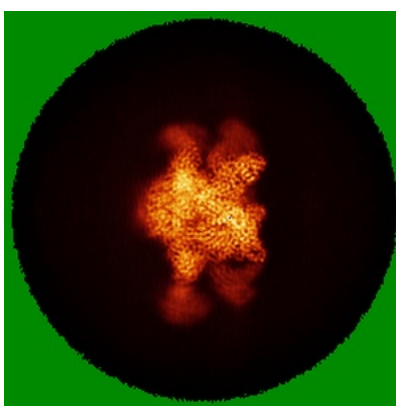
The images above show the largest variance slices of the map in three orthogonal directions.

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

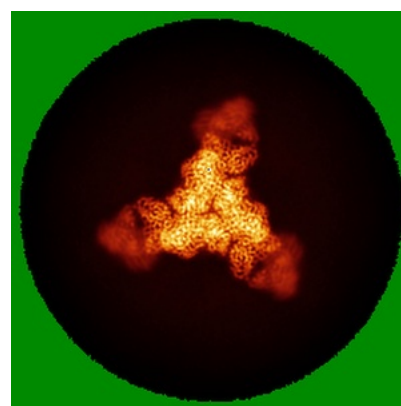
6.4.1 Primary map



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 6.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

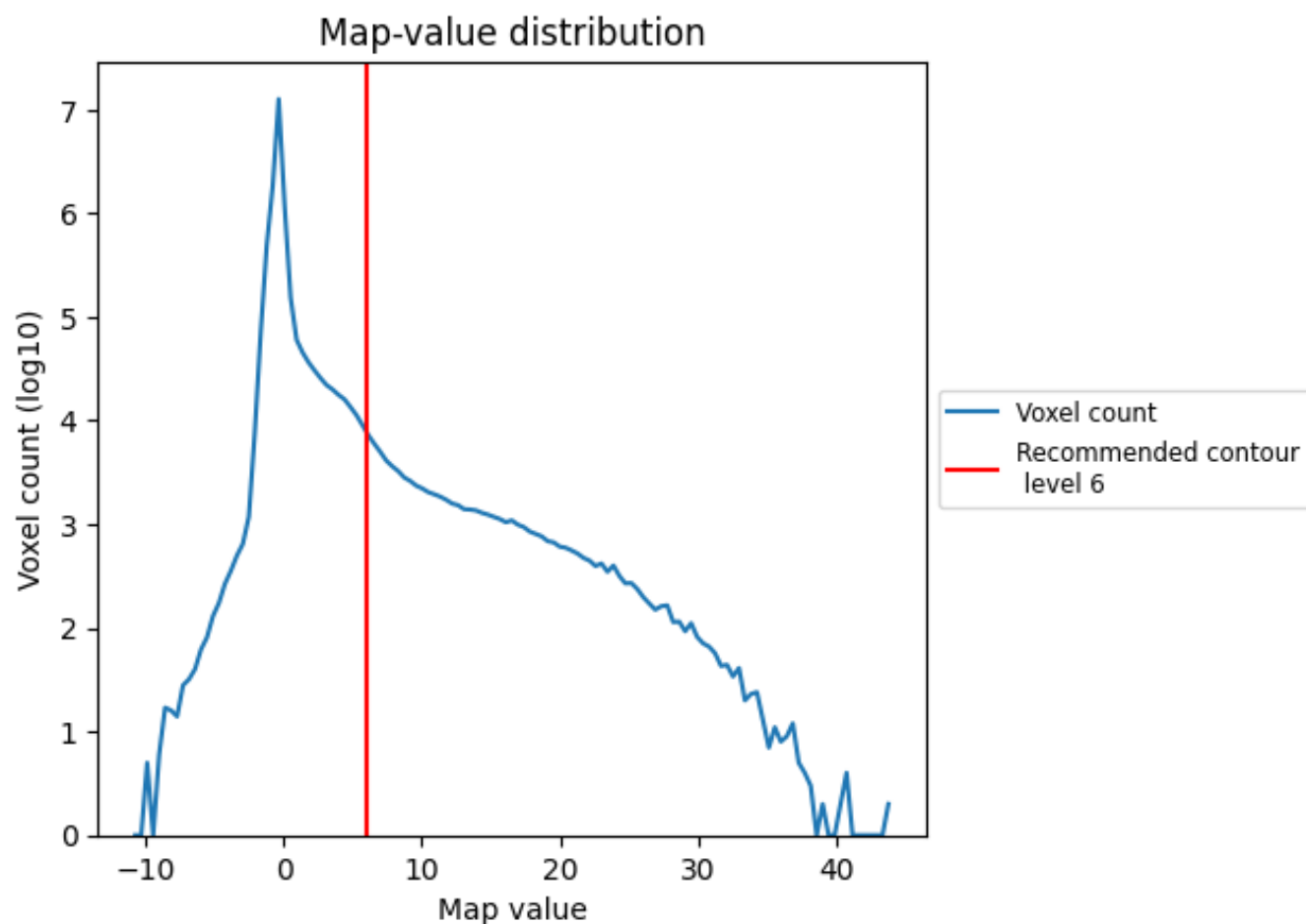
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

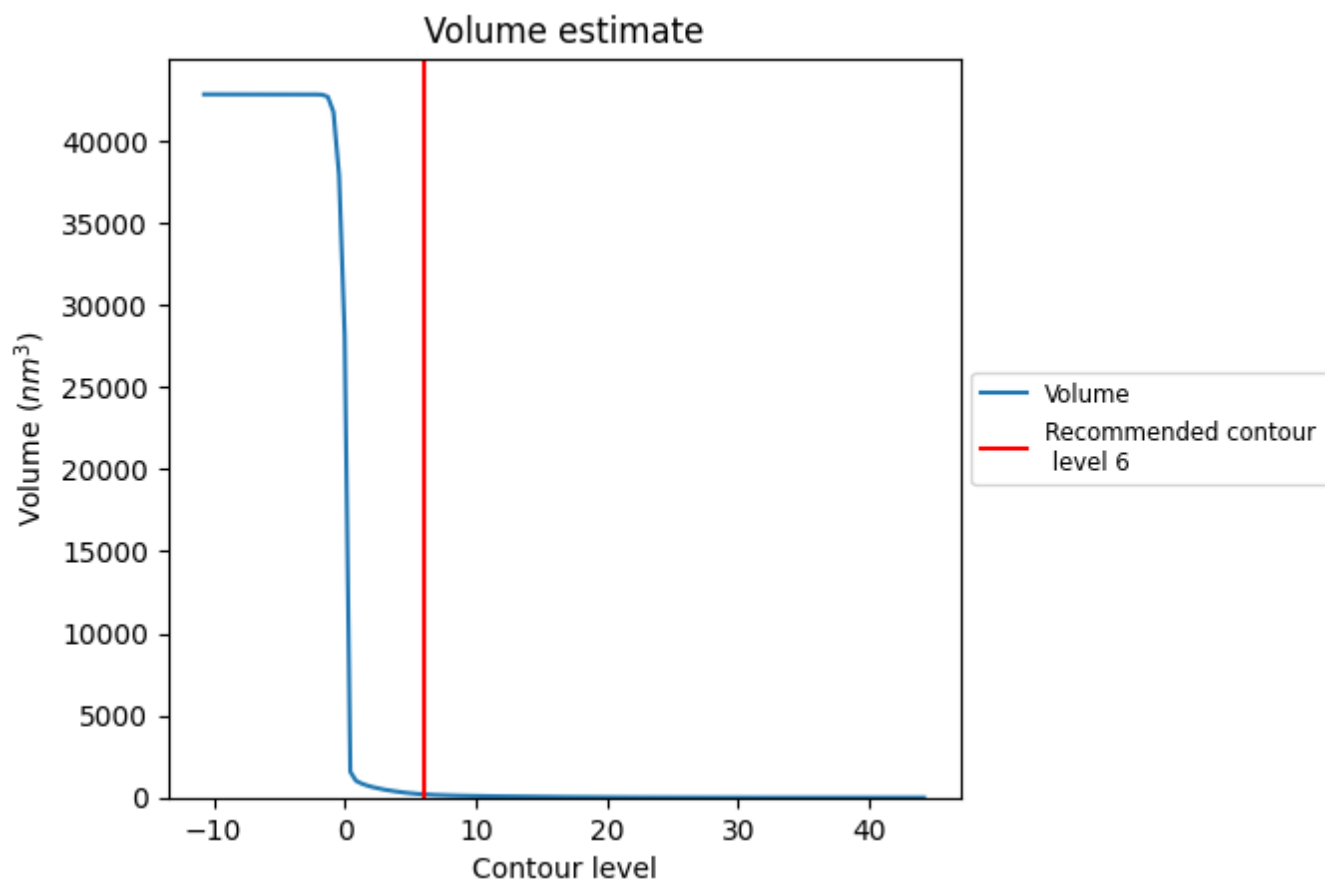
This section contains the results of statistical analysis of the map.

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.

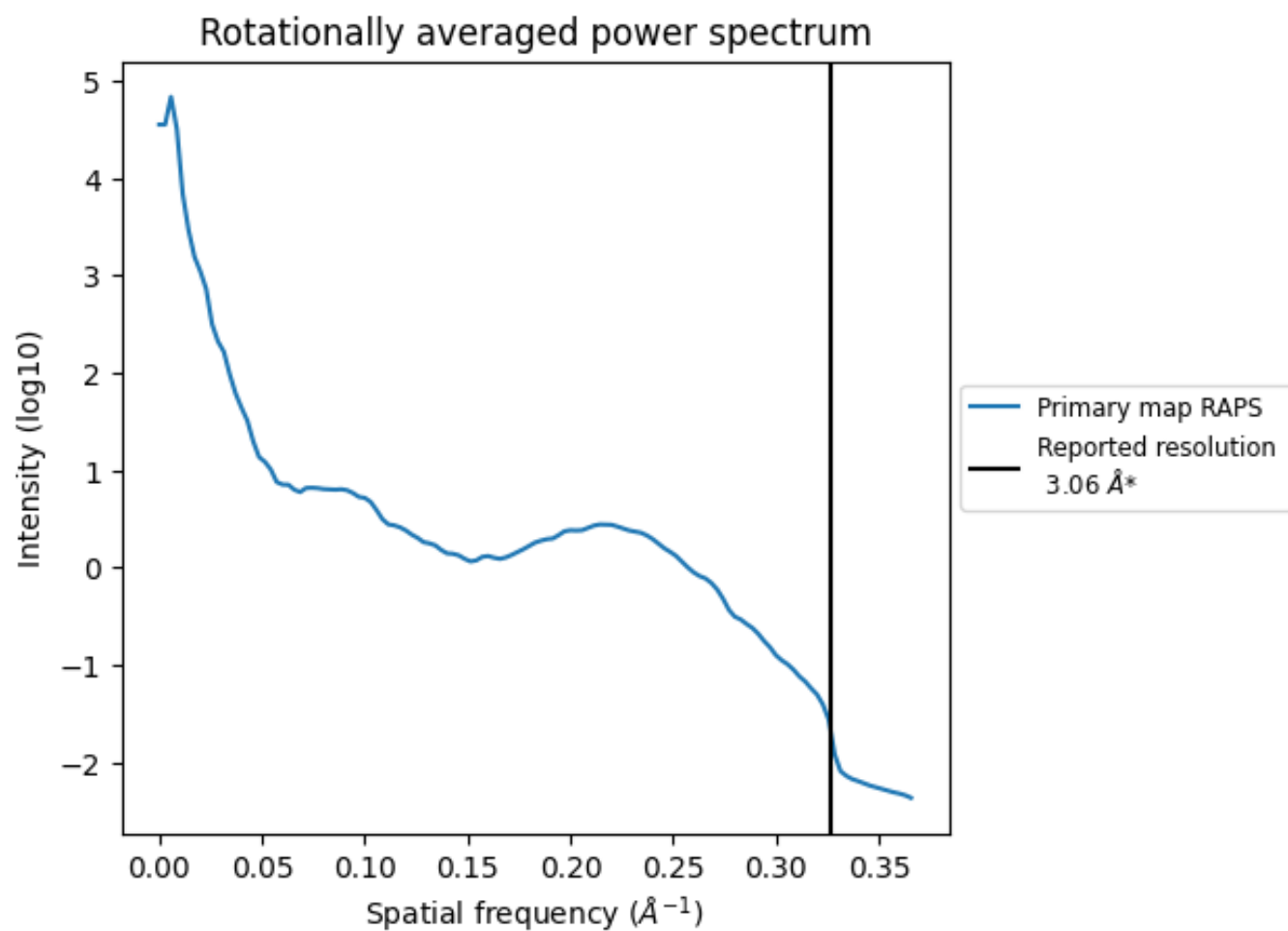
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 0.327 Å⁻¹

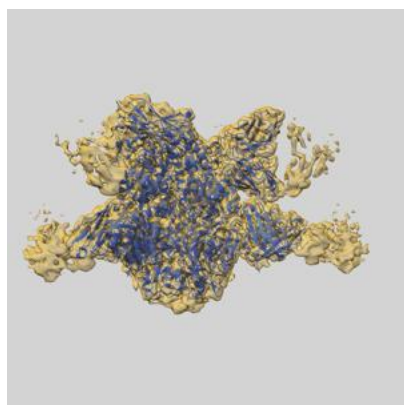
8 Fourier-Shell correlation

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

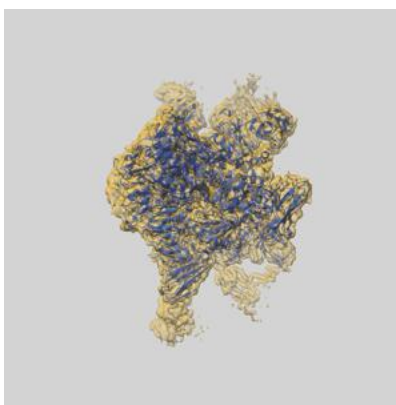
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-25982 and PDB model 7TL0. Per-residue inclusion information can be found in section [3](#) on page [12](#).

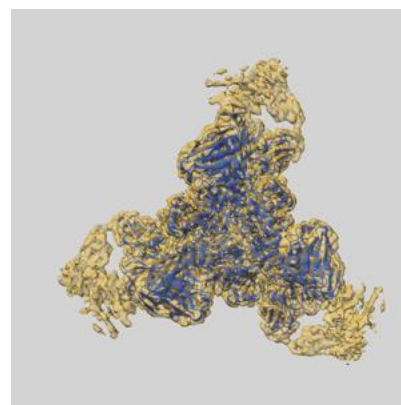
9.1 Map-model overlay [i](#)



X



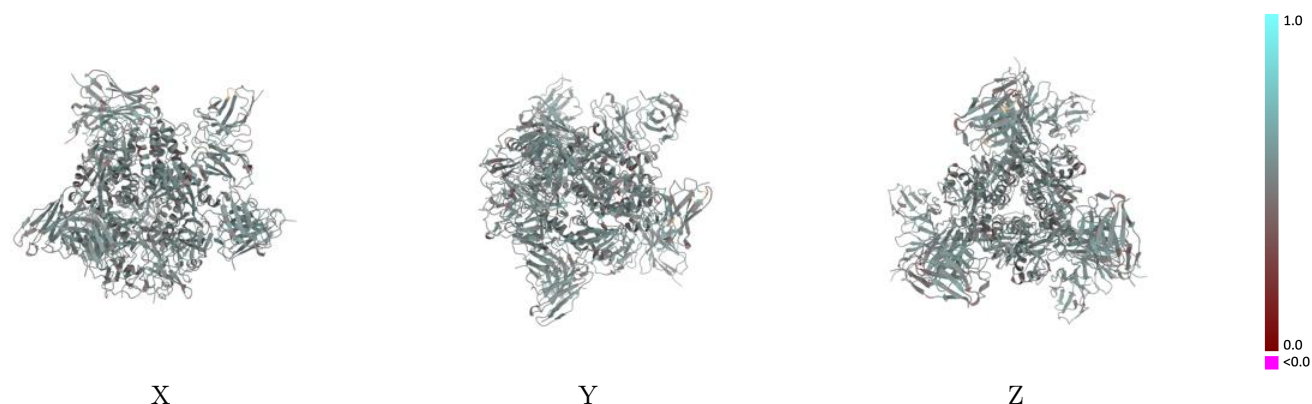
Y



Z

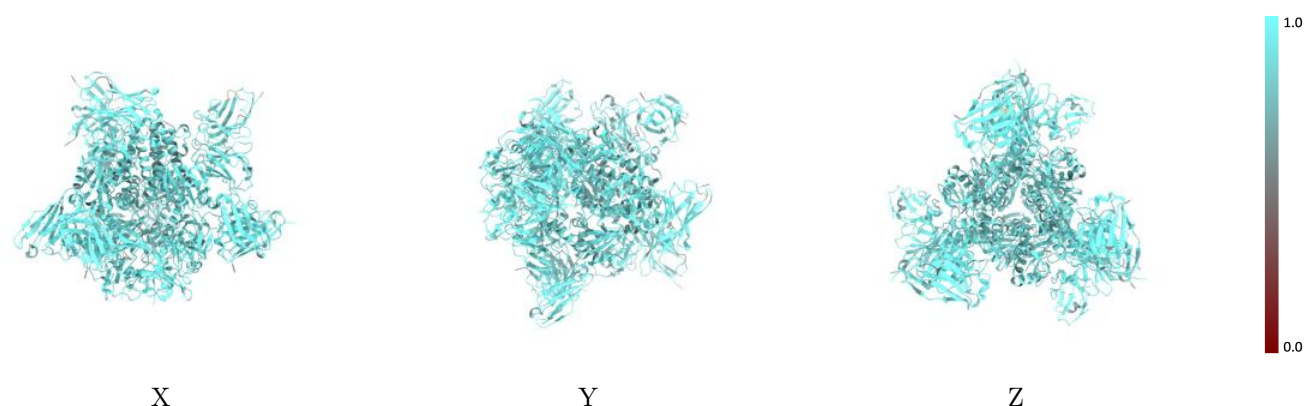
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



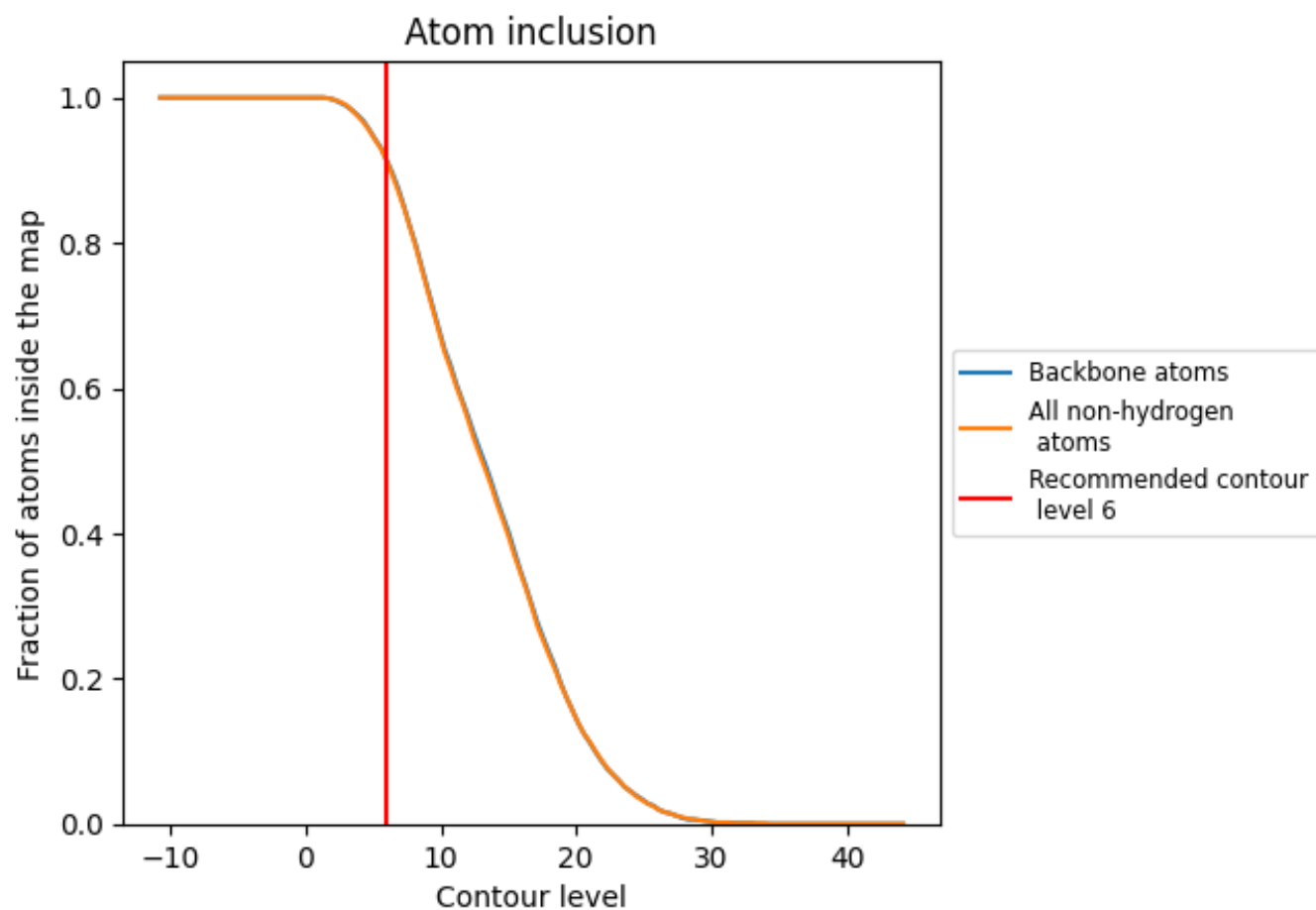
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (6).

9.4 Atom inclusion ⓘ



At the recommended contour level, 91% of all backbone atoms, 91% 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 (6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9130	<div><div></div></div> 0.5210
A	<div><div></div></div> 0.9090	<div><div></div></div> 0.5190
B	<div><div></div></div> 0.9110	<div><div></div></div> 0.5170
C	<div><div></div></div> 0.9110	<div><div></div></div> 0.5180
D	<div><div></div></div> 0.9260	<div><div></div></div> 0.5200
E	<div><div></div></div> 0.9310	<div><div></div></div> 0.5210
F	<div><div></div></div> 0.9190	<div><div></div></div> 0.5240
G	<div><div></div></div> 0.9270	<div><div></div></div> 0.5220
H	<div><div></div></div> 0.9140	<div><div></div></div> 0.5190
I	<div><div></div></div> 0.9240	<div><div></div></div> 0.5230
J	<div><div></div></div> 0.9210	<div><div></div></div> 0.5310
K	<div><div></div></div> 0.9230	<div><div></div></div> 0.5260
L	<div><div></div></div> 0.9330	<div><div></div></div> 0.5300
M	<div><div></div></div> 0.9220	<div><div></div></div> 0.5300
N	<div><div></div></div> 0.9230	<div><div></div></div> 0.5280
O	<div><div></div></div> 0.9300	<div><div></div></div> 0.5250
P	<div><div></div></div> 0.7500	<div><div></div></div> 0.4710
Q	<div><div></div></div> 0.7500	<div><div></div></div> 0.4670
R	<div><div></div></div> 0.7860	<div><div></div></div> 0.4540

1.0

0.0

<0.0