



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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 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

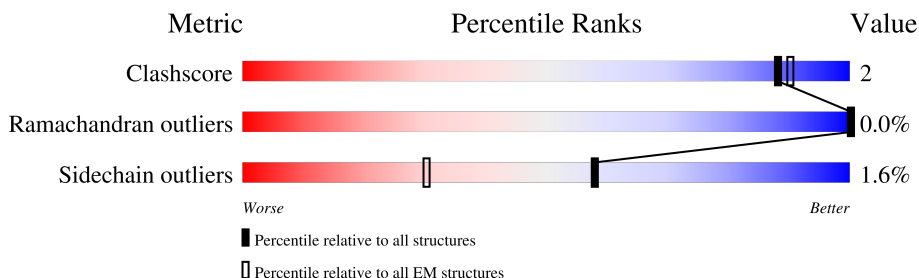
# 1 Overall quality at a glance

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

Mol	Chain	Length	Quality of chain
1	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.

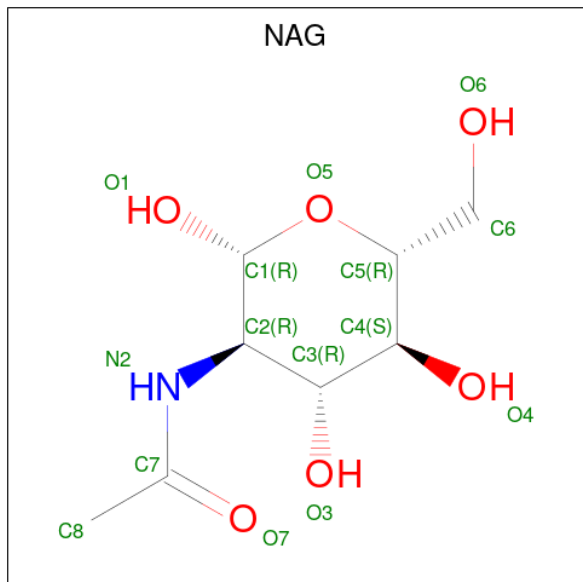
Mol	Chain	Residues	Atoms						AltConf	Trace
5	K	107	Total	C	H	N	O	S	0	0
			1536	486	750	135	163	2		
5	M	107	Total	C	H	N	O	S	0	0
			1536	486	750	135	163	2		
5	O	107	Total	C	H	N	O	S	0	0
			1536	486	750	135	163	2		

- 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		

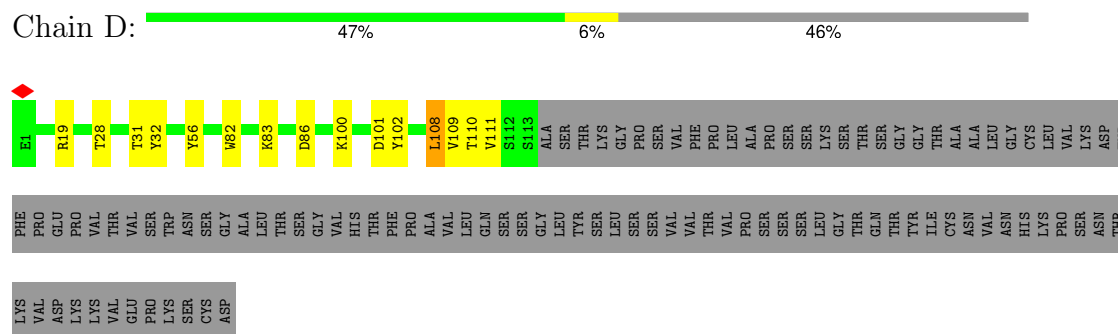
- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



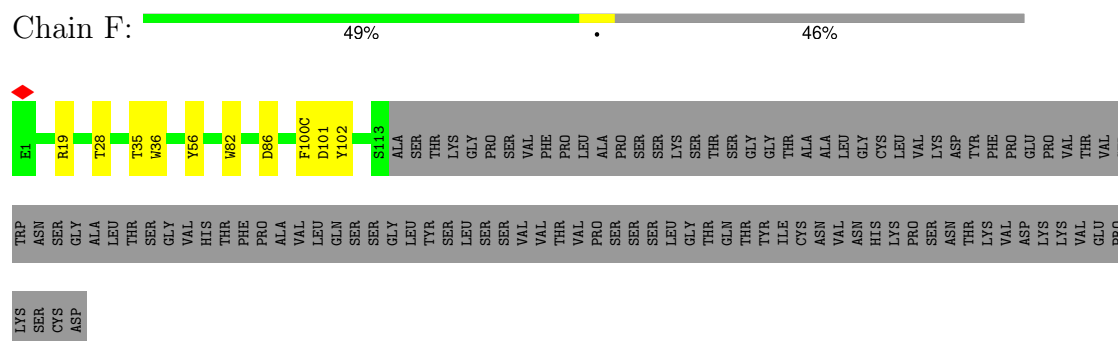
Mol	Chain	Residues	Atoms					AltConf
7	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	A	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	B	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	C	1	Total	C	H	N	O	0
			28	8	14	1	5	
7	C	1	Total	C	H	N	O	0
			28	8	14	1	5	



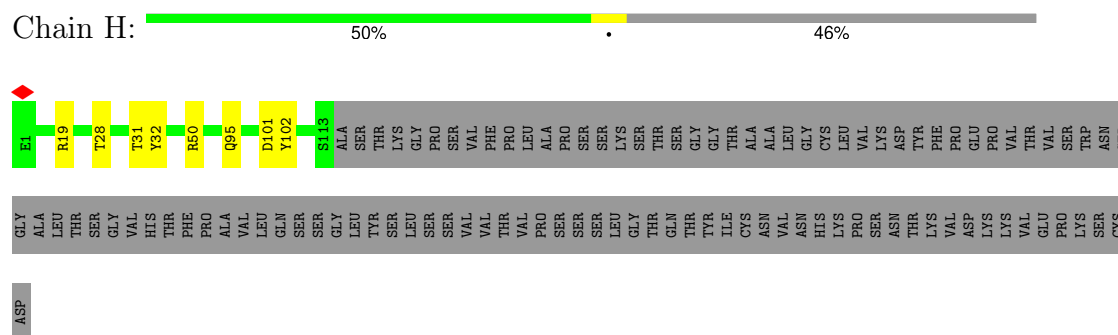
- Molecule 2: SAN32-2 Fab heavy chain



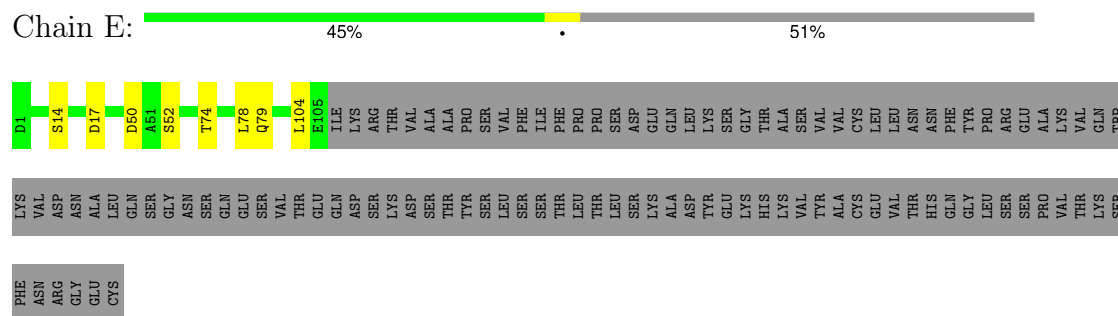
- Molecule 2: SAN32-2 Fab heavy chain



- Molecule 2: SAN32-2 Fab heavy chain



- Molecule 3: SAN32-2 Fab light chain



- Molecule 3: SAN32-2 Fab light chain

PRO	ALA	D1
VAL	LYS	S14
THR	VAL	
LYS	GLN	D17
SER	TRP	
PHE	LYS	C23
ASN	VAL	
ARG	ASP	L33
GLY	ASN	N34
GLU	ALA	N35
CYS	LEU	
	GLN	A51
	SER	
	GLY	F71
	ASN	
	SER	
	GLN	T74
	GLU	
	SER	Q79
	VAL	
	THR	L104
	GLU	E105
	GLN	I1E
	ASP	LYS
	SER	ARG
	LYS	THR
	ASP	VAL
	SER	ALA
	THR	ALA
	TYR	PRO
	SER	SER
	LEU	VAL
	SER	PHE
	SER	ILE
	THR	PHE
	LEU	PRO
	THR	PRO
	LEU	SER
	SER	ASP
	SER	GLU
	LYS	GLN
	ALA	LEU
	ASP	LYS
	TYR	LYS
	GLU	GLY
	LYS	THR
	HIS	ALA
	VAL	SER
	TYR	VAL
	ALA	VAL
	CYS	CYS
	GLU	LEU
	VAL	LEU
	THR	ASN
	HIS	ASN
	GLN	PHE
	GLY	TYR
	LEU	PRO
	SER	ARG
	SER	GLN

CYS	D1	S14	D17	T74	L78	L104	E105	ILE	LYS	ARG	THR	VAL	ALA	ALA	PRO	PRO	SER	VAL	PHE	ILE	PHE	PRO	PRO	SER	ASP	GLU	GLN	LEU	LYS	SER	GLY	THR	ALA	SER	VAL	VAL	CYS	CYS	LEU	LEU	ASN	ASN	PHE	TYR	PRO	ARG	GLU	ALA	LYS	VAL	GLN	TRP	LYS	ASN	VAL	ASP	ASN	ALA	
	LEU	GLN	SER	GLY	ASN	SER	GLN	GLN	ASP	SER	LYS	ASP	SER	THR	THR	SER	LEU	LEU	SER	SER	THR	LEU	THR	LEU	SER	SER	LYS	ALA	ASP	TYR	GLU	LYS	HIS	VAL	VAL	ALA	ALA	CYS	GLU	VAL	THR	THR	HIS	GLN	GLY	LEU	SER	SER	PRO	VAL	THR	LYS	SER	PHE	LYS	ASN	ARG	GLY	GLU

PHE	PRO	ALA	VAL	LEU	GLN	SER	SER	GLY	LEU	TYR	SER	LEU	SER	SER	VAL	VAL	THR	VAL	THR	PRO	PRO	SER	SER	LEU	GLY	THR	TYR	THR	ILE	CYS	ASN	ASN	VAL	ASN	HIS	LYS	PRO	PRO	SER	SER	GLU	GLY	VAL	THR	VAL	SER	TRP	ASN	SER	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS
E1	T108	D112	I113	S124	ALA	SER	THR	GLY	PRO	PHE	VAL	SER	SER	VAL	VAL	THR	THR	GLN	SER	GLY	THR	THR	THR	GLY	THR	ALA	ALA	LEU	GLY	CYS	LEU	VAL	VAL	LYS	ASP	TYR	PHE	PRO	GLU	PRO	VAL	VAL	THR	VAL	SER	TRP	ASN	SER	GLY	ALA	LEU	THR	SER	GLY	VAL	HIS	

PHE	PRO	ALA	VAL	LEU	GLN	SER	SER	GLY	LEU	TYR	SER	LEU	SER	SER	VAL	VAL	THR	VAL	THR	PRO	SER	SER	LEU	GLY	THR	TYR	ILE	CYS	ASN	ASN	ASN	VAL	ASP	GLU	LEU	LYS	PRO	SER	SER	THR	THR	ASN	ASP	LYS	PHE	VAL	ASP	LYS	LYS	VAL	VAL	GLU	VAL	SER	LYS	THR	TRP	ASN	GLY	SER	THR	LEU	ALA	GLY	SER	VAL	HIS
E1	T108	D112	I113	S124	ALA	SER	THR	GLY	PRO	PHE	VAL	SER	SER	VAL	THR	PRO	ALA	PRO	SER	SER	SER	LYS	SER	THR	THR	GLY	THR	ALA	ALA	LEU	GLY	CYS	LEU	VAL	LYS	ASP	THR	PHE	PRO	GLU	PRO	VAL	VAL	THR	VAL	SER	THR	TRP	ASN	GLY	SER	THR	THR	LEU	ALA	GLY	VAL	HIS									

E1
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• Molecule 5: MPE8 Fab light chain

Chain K: 49% 50%

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

• Molecule 5: MPE8 Fab light chain

Chain M: 48% 50%

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

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

• Molecule 5: MPE8 Fab light chain

Chain O: 47% 50%

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

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

GLU  
CYS  
SER

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

Chain P: 50% 50%

NAG1  
NAG2

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

Chain Q: 100%

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.

All (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
1:B:388:VAL:HG12	1:B:421:ASP:OD2	1.99	0.62
3:E:14:SER:N	3:E:17:ASP:OD2	2.30	0.62
1:A:353:ASN:O	1:A:356:THR:N	2.34	0.61
1:A:181:LYS:HE3	2:D:56:TYR:OH	2.01	0.60
1:B:181:LYS:HE3	2:F:56:TYR:OH	2.00	0.60
2:D:101:ASP:OD1	2:D:102:TYR:N	2.34	0.60
3:I:14:SER:N	3:I:17:ASP:OD2	2.33	0.59
5:K:56:ARG:NH2	5:K:62:ASP:OD1	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:14:SER:N	3:G:17:ASP:OD2	2.34	0.58
1:A:105:LEU:HD21	1:B:370:ILE:CD1	2.36	0.55
2:H:101:ASP:OD1	2:H:102:TYR:N	2.39	0.55
4:L:112:ASP:OD1	4:L:113:ILE:N	2.38	0.55
2:F:101:ASP:OD1	2:F:102:TYR:N	2.37	0.54
5:O:56:ARG:NH2	5:O:62:ASP:OD1	2.41	0.54
4:J:112:ASP:OD1	4:J:113:ILE:N	2.42	0.53
4:N:112:ASP:OD1	4:N:113:ILE:N	2.42	0.53
1:A:342:ASN:ND2	1:B:421:ASP:OD2	2.43	0.51
1:B:420:ILE:O	1:B:421:ASP:HB2	2.12	0.50
1:B:62:ASP:OD1	1:B:63:GLY:N	2.44	0.50
2:F:82:TRP:NE1	2:F:86:ASP:OD2	2.45	0.49
5:M:56:ARG:NH2	5:M:62:ASP:OD1	2.45	0.49
1:A:62:ASP:OD1	1:A:63:GLY:N	2.46	0.49
2:D:82:TRP:NE1	2:D:86:ASP:OD2	2.46	0.49
1:B:50:LEU:HB3	1:B:267:VAL:HG13	1.94	0.48
2:F:28:THR:HG23	2:F:28:THR:O	2.13	0.48
2:H:28:THR:O	2:H:28:THR:HG23	2.12	0.48
1:B:352:ILE:HB	7:B:602:NAG:H81	1.97	0.47
2:D:28:THR:O	2:D:28:THR:HG23	2.14	0.47
1:C:37:SER:HB3	1:C:283:CYS:SG	2.54	0.46
1:A:184:ILE:HG23	1:A:185:PRO:HD2	1.98	0.46
1:C:50:LEU:HB3	1:C:267:VAL:HG13	1.96	0.46
5:M:85:GLU:OE2	5:M:106:LYS:NZ	2.46	0.46
1:B:353:ASN:ND2	1:B:356:THR:OG1	2.46	0.46
2:D:100:LYS:NZ	3:E:50:ASP:OD2	2.43	0.45
1:B:37:SER:HB3	1:B:283:CYS:SG	2.56	0.45
2:D:83:LYS:O	2:D:111:VAL:HG11	2.16	0.45
1:B:302:LEU:HD12	1:B:464:PHE:HE2	1.81	0.45
3:I:104:LEU:C	3:I:104:LEU:HD23	2.37	0.45
1:C:62:ASP:OD1	1:C:63:GLY:N	2.49	0.45
1:A:352:ILE:HD13	7:A:602:NAG:H82	1.98	0.45
1:B:405:LYS:HE2	1:B:405:LYS:HA	2.00	0.44
2:H:50:ARG:NH1	2:H:95:GLN:OE1	2.43	0.44
5:O:52:ASP:HB2	5:O:55:ASN:HD22	1.82	0.44
2:D:108:LEU:HD23	2:D:109:VAL:N	2.33	0.43
1:A:128:ILE:O	1:A:134:VAL:HG23	2.19	0.43
1:A:79:ARG:NH2	3:E:52:SER:OG	2.52	0.43
2:D:31:THR:HG23	2:D:32:TYR:CD2	2.53	0.43
3:E:104:LEU:C	3:E:104:LEU:HD23	2.39	0.43
5:O:85:GLU:OE2	5:O:106:LYS:NZ	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:THR:HG23	2:H:32:TYR:CD2	2.54	0.43
2:F:35:THR:HG1	2:F:100(C):PHE:HE1	1.65	0.42
2:F:35:THR:HG22	2:F:36:TRP:N	2.34	0.42
3:G:23:CYS:HB2	3:G:35:TRP:CH2	2.54	0.42
3:E:78:LEU:HD11	3:E:104:LEU:HD21	2.02	0.41
1:B:50:LEU:HB3	1:B:267:VAL:CG1	2.50	0.41
2:D:108:LEU:HD22	2:D:110:THR:HG23	2.02	0.41
1:B:327:GLU:OE2	1:B:329:ARG:NH2	2.50	0.41
1:A:333:VAL:HG13	1:A:333:VAL:O	2.21	0.41
3:G:33:LEU:HD22	3:G:71:PHE:CG	2.56	0.41
1:A:50:LEU:HB3	1:A:267:VAL:CG1	2.50	0.41
1:A:298:ASN:HD22	1:A:298:ASN:C	2.25	0.40
1:B:128:ILE:O	1:B:134:VAL:HG23	2.21	0.40
3:I:78:LEU:HD11	3:I:104:LEU:HD21	2.01	0.40
2:D:31:THR:HG23	2:D:32:TYR:CE2	2.56	0.40
1:C:419:THR:HA	1:C:423:THR:O	2.21	0.40
1:A:419:THR:HA	1:A:423:THR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	55	VAL
1	A	147	CYS
1	A	229	ARG
1	A	266	SER
1	A	298	ASN
1	A	389	SER
1	A	447	ASP
1	B	41	THR
1	B	147	CYS
1	B	224	ASP
1	B	266	SER
1	B	345	GLU
1	B	389	SER
1	B	419	THR
1	C	41	THR
1	C	147	CYS
1	C	156	ARG
1	C	266	SER
1	C	345	GLU
1	C	353	ASN
1	C	389	SER
2	D	19[A]	ARG
2	D	108	LEU
3	E	74	THR
3	E	79	GLN
2	F	19[A]	ARG
3	G	1	ASP
3	G	74	THR
3	G	79	GLN

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Mol	Chain	Res	Type
3	G	104	LEU
2	H	19[A]	ARG
3	I	74	THR
4	J	108	THR
4	L	108	THR
4	N	108	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
1	A	342	ASN
1	A	462	GLN
1	C	462	GLN
3	E	24	GLN
3	E	27	GLN
2	F	66	HIS
3	G	24	GLN
3	G	27	GLN
3	I	24	GLN
3	I	27	GLN
3	I	79	GLN
5	K	39	GLN
5	K	55	ASN
5	M	39	GLN
5	O	55	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

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(°)	Ideal(°)
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.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	P	1	NAG	O5-C5-C6-O6

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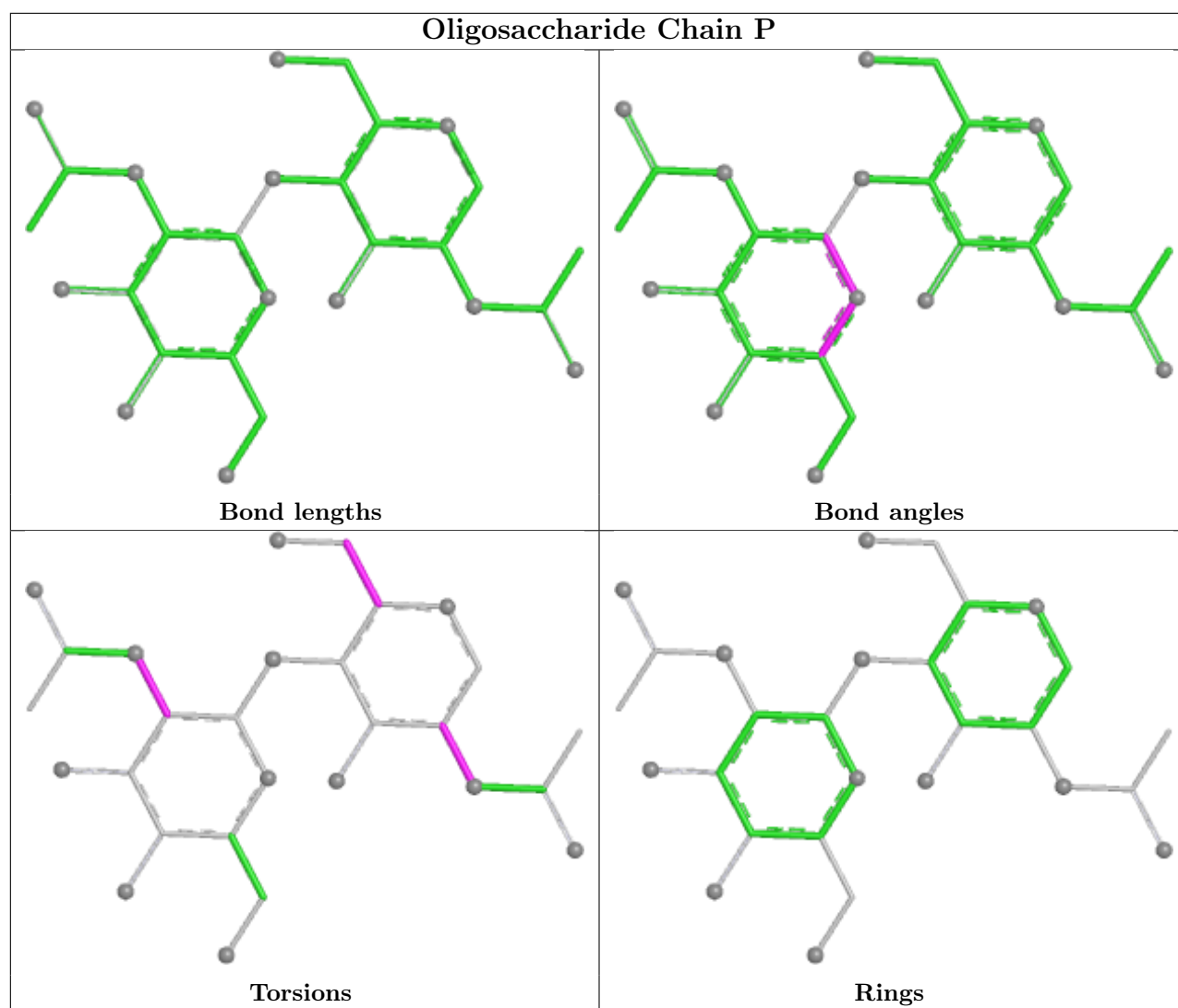
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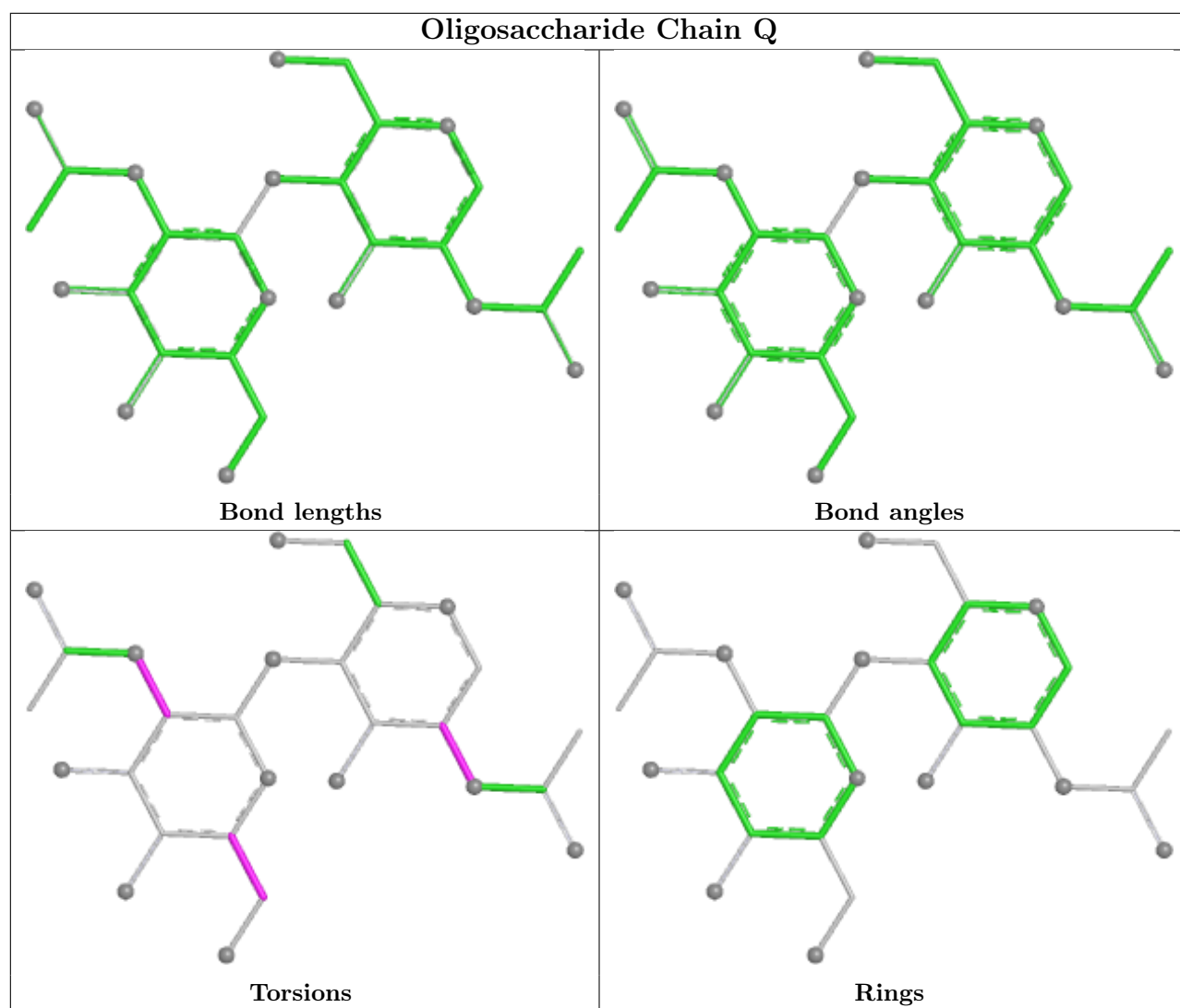
Mol	Chain	Res	Type	Atoms
6	P	1	NAG	C4-C5-C6-O6
6	Q	2	NAG	O5-C5-C6-O6
6	P	1	NAG	C1-C2-N2-C7
6	P	2	NAG	C1-C2-N2-C7
6	Q	1	NAG	C1-C2-N2-C7
6	Q	2	NAG	C1-C2-N2-C7
6	R	1	NAG	C1-C2-N2-C7
6	R	2	NAG	C1-C2-N2-C7
6	P	1	NAG	C3-C2-N2-C7
6	P	2	NAG	C3-C2-N2-C7
6	Q	2	NAG	C3-C2-N2-C7
6	R	2	NAG	C3-C2-N2-C7
6	Q	1	NAG	C3-C2-N2-C7
6	R	1	NAG	C3-C2-N2-C7

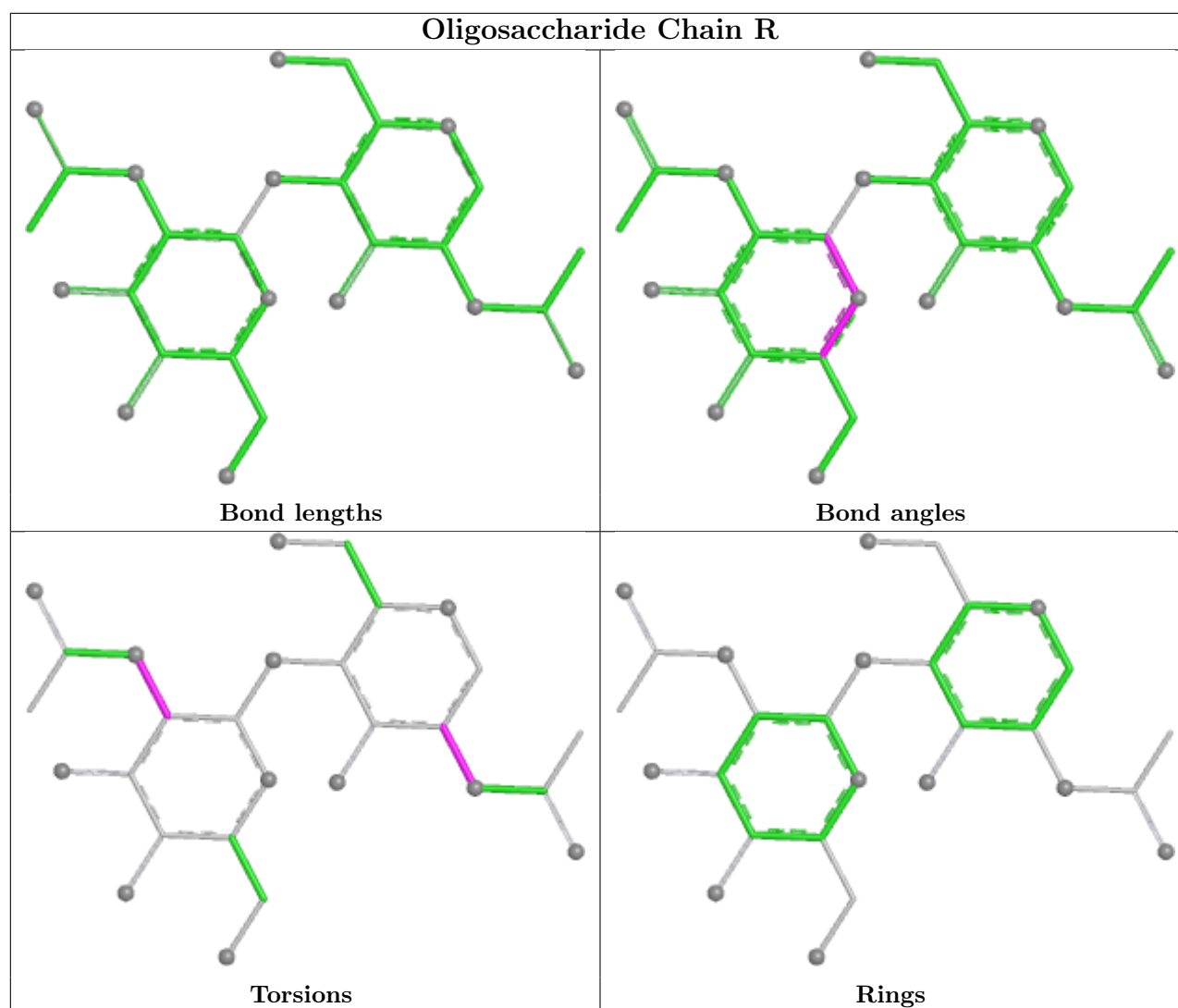
There are no ring outliers.

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.

All (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

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Mol	Chain	Res	Type	Atoms
7	C	602	NAG	C1-C2-N2-C7
7	C	602	NAG	C4-C5-C6-O6
7	B	601	NAG	C4-C5-C6-O6
7	A	602	NAG	C3-C2-N2-C7
7	C	602	NAG	C3-C2-N2-C7
7	A	601	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.

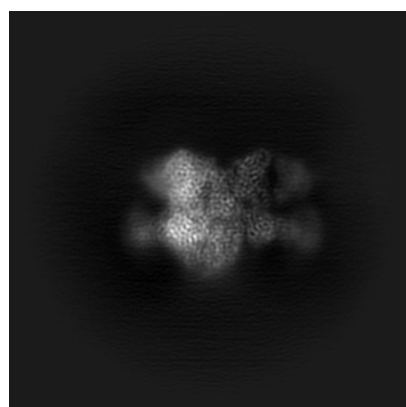
## 6 Map visualisation [i](#)

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.

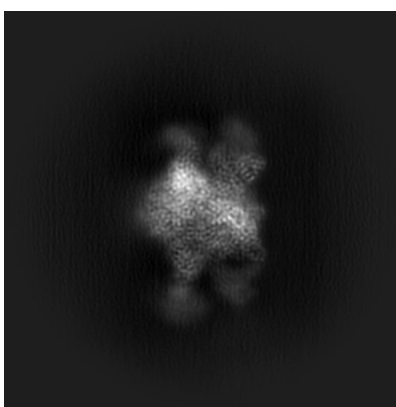
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

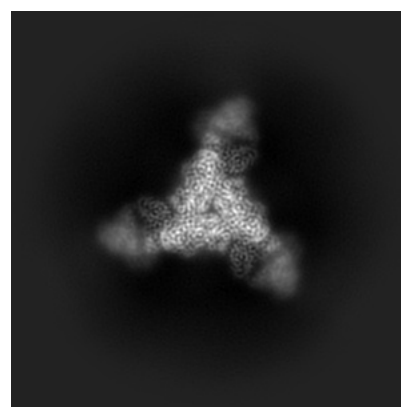
#### 6.1.1 Primary map



X



Y

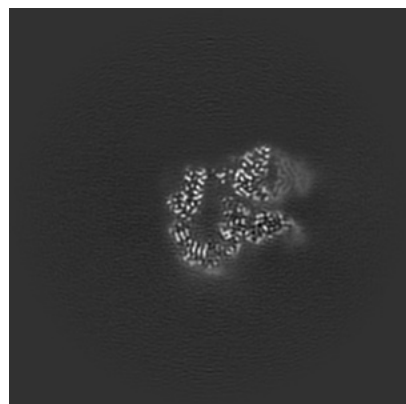


Z

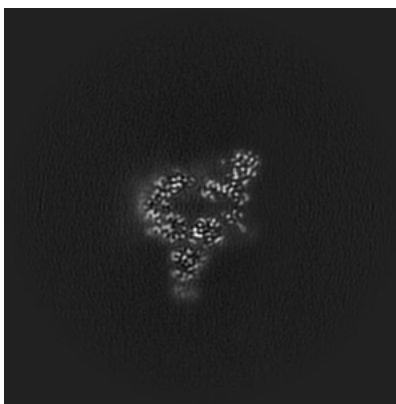
The images above show the map projected in three orthogonal directions.

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

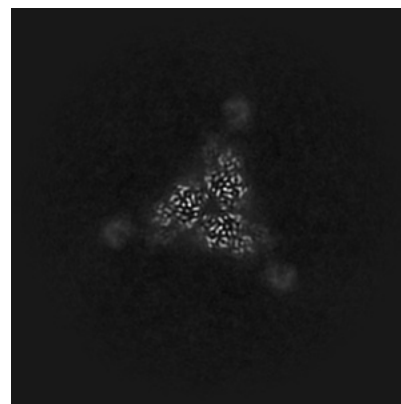
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

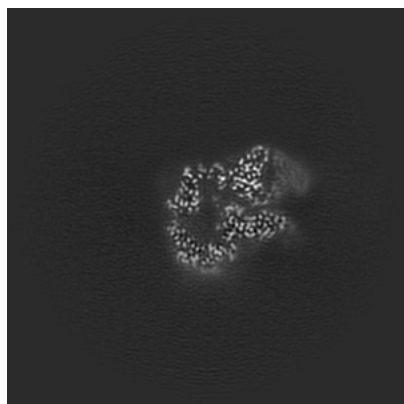


Z Index: 128

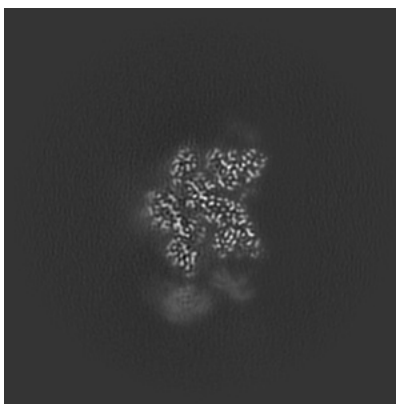
The images above show central slices of the map in three orthogonal directions.

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

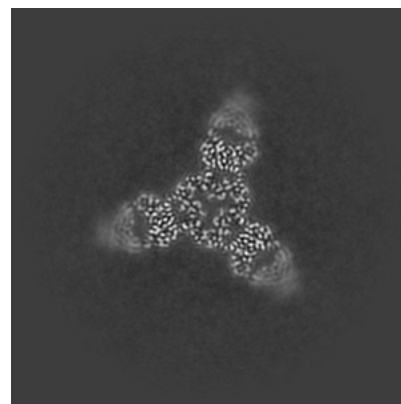
### 6.3.1 Primary map



X Index: 126



Y Index: 115

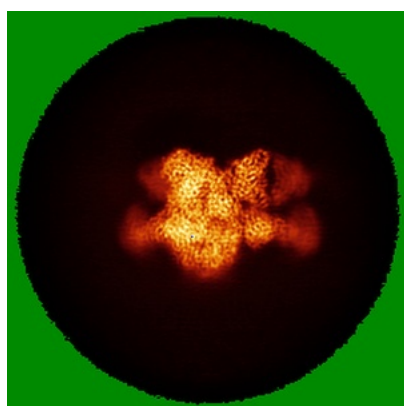


Z Index: 114

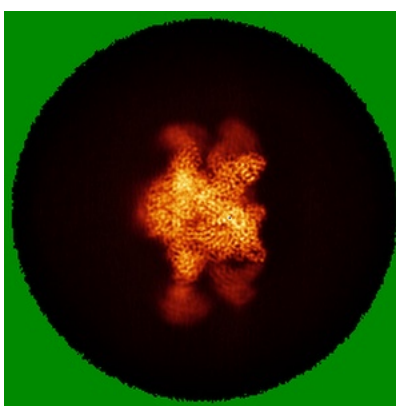
The images above show the largest variance slices of the map in three orthogonal directions.

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

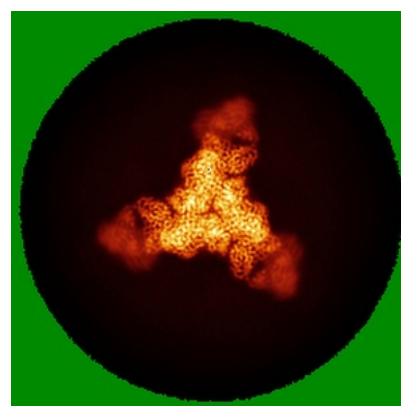
### 6.4.1 Primary map



X



Y

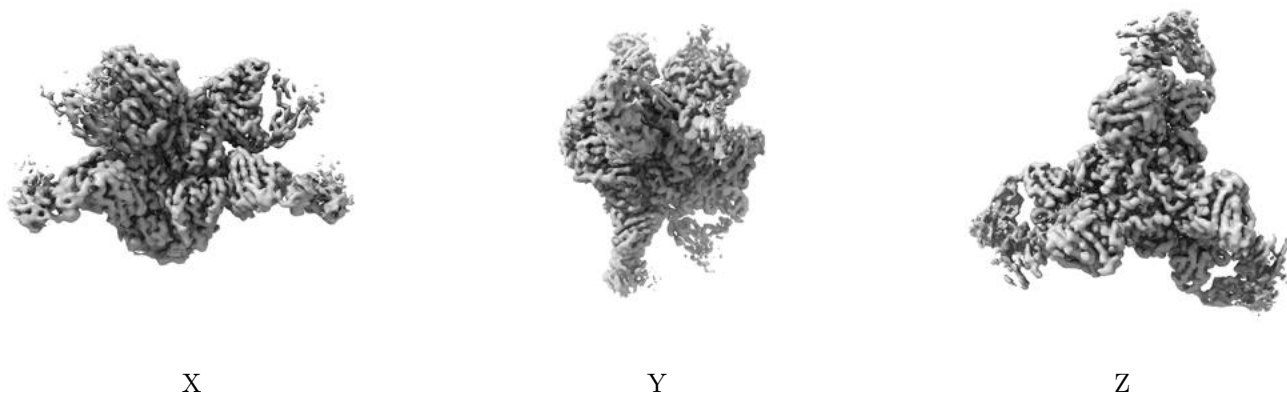


Z

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.

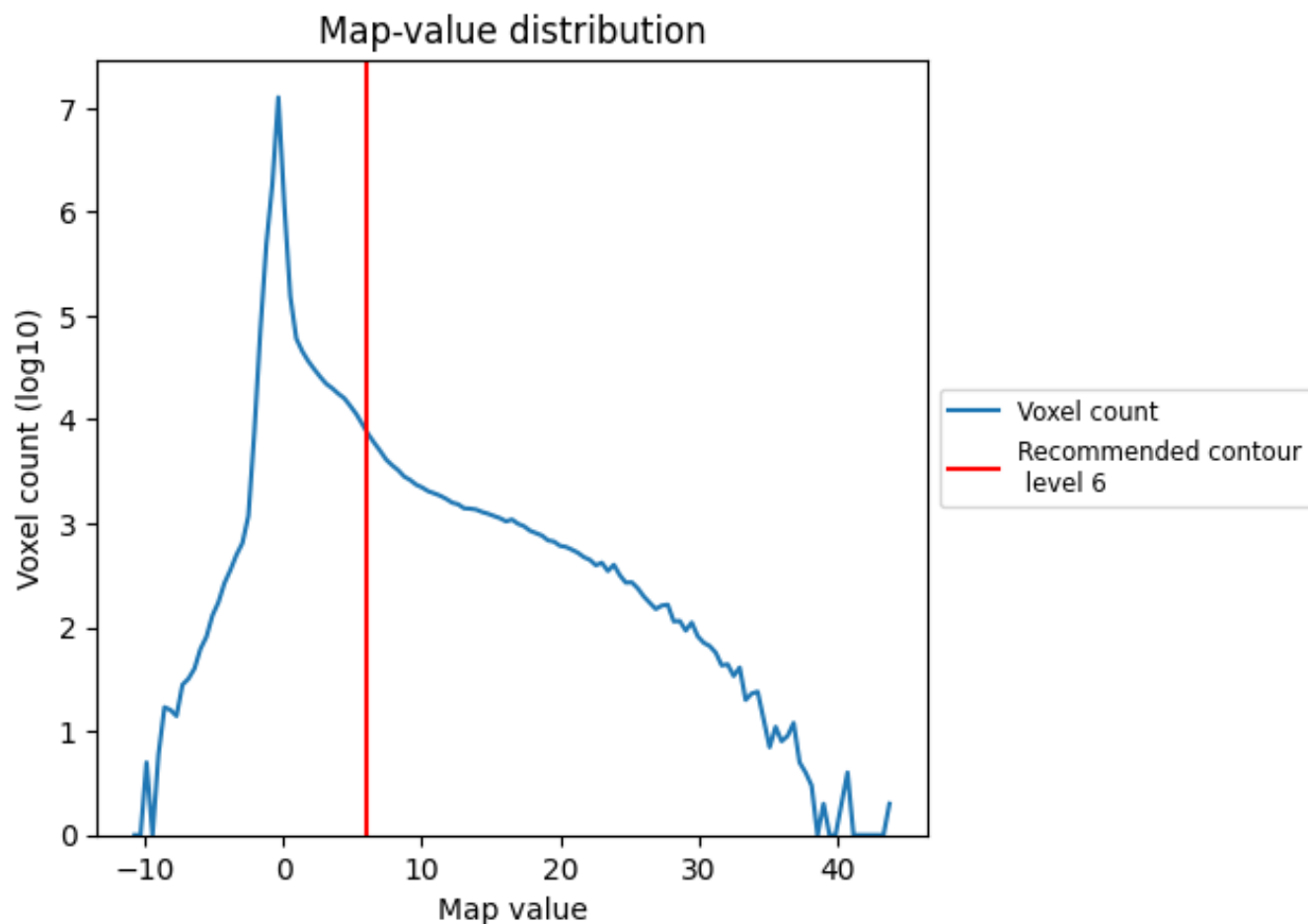
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

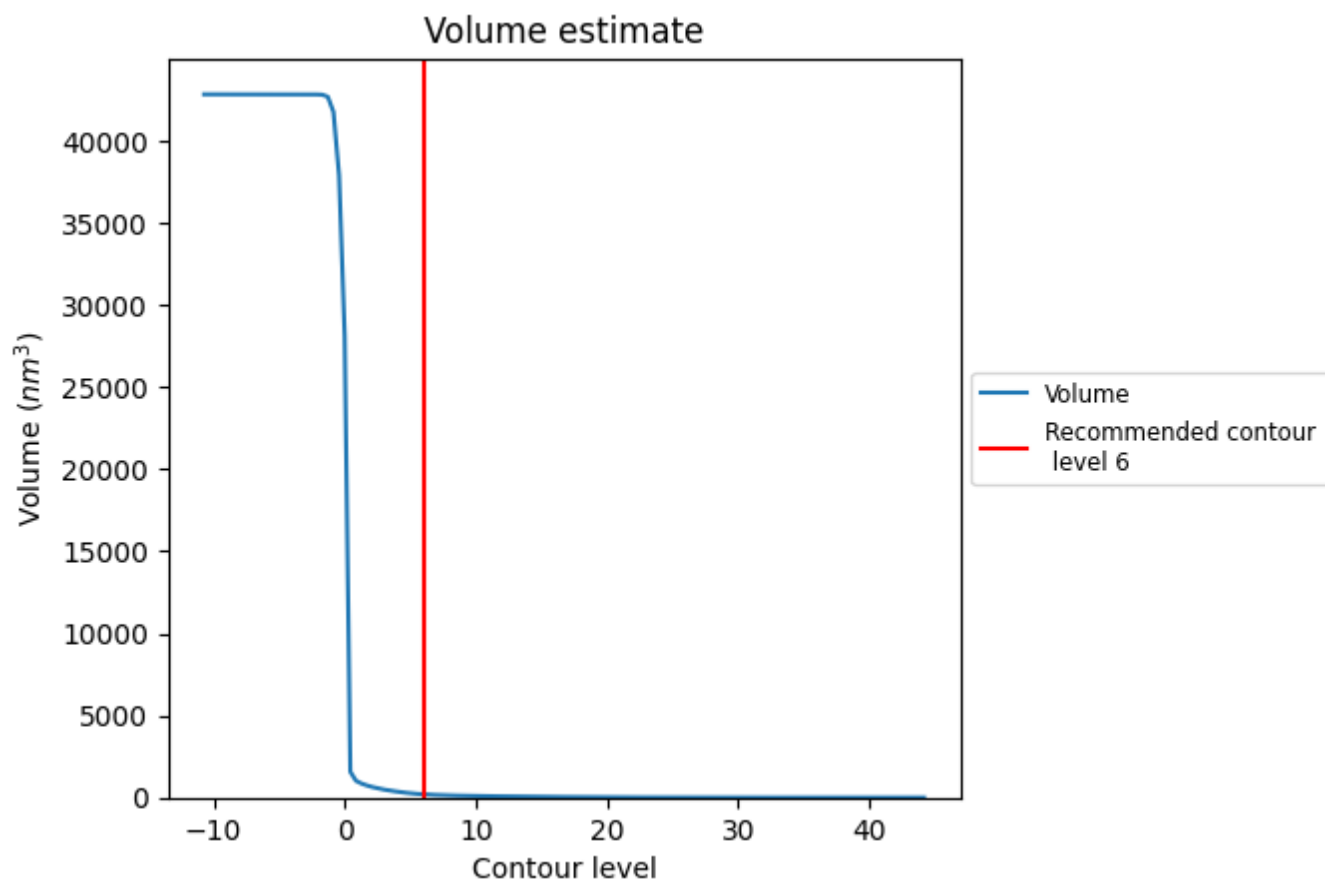
This section contains the results of statistical analysis of the map.

### 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.

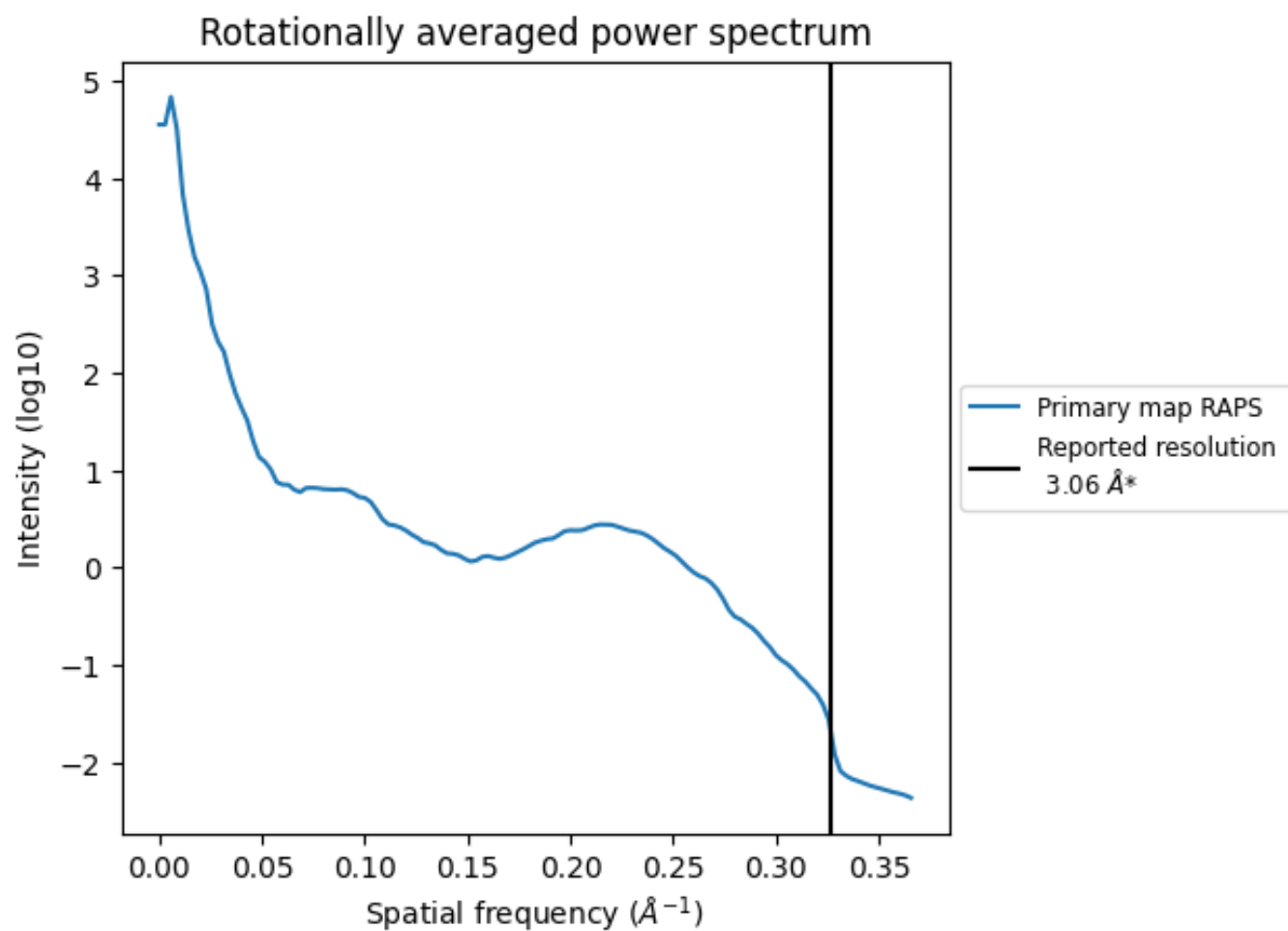
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197  $\text{nm}^3$ ; 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<sup>-1</sup>

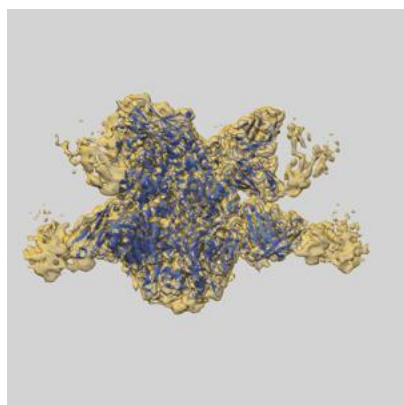
## 8 Fourier-Shell correlation ⓘ

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

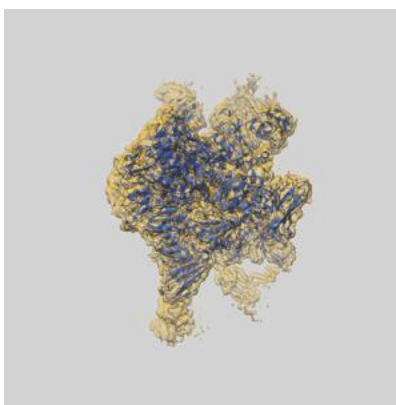
## 9 Map-model fit [i](#)

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

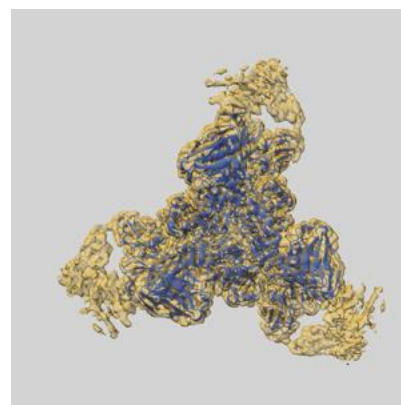
### 9.1 Map-model overlay [i](#)



X



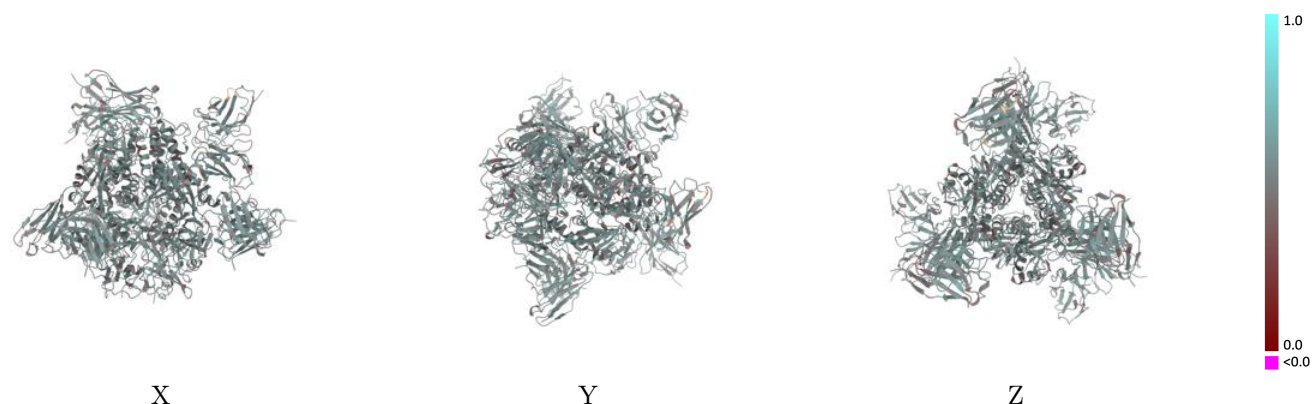
Y



Z

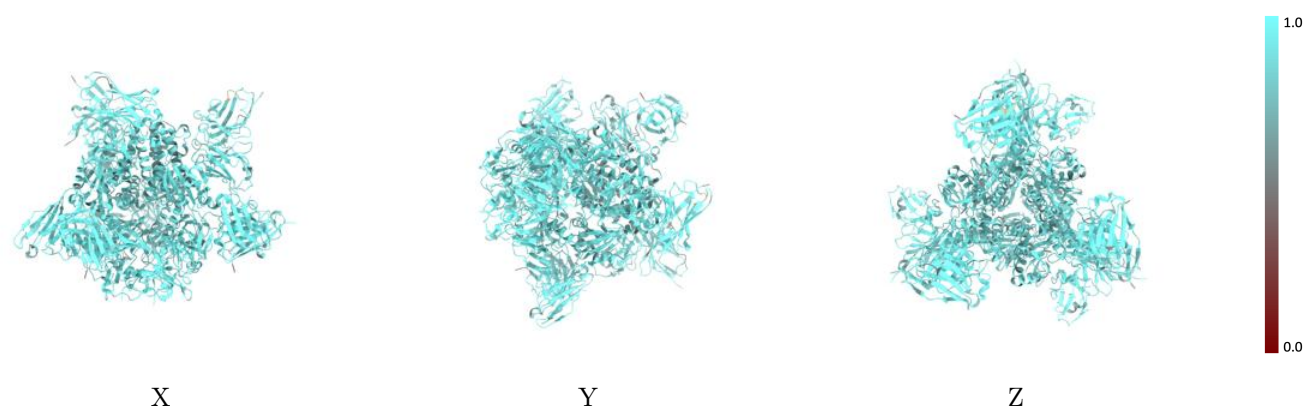
The images above show the 3D surface view of the map at the recommended contour level 6.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



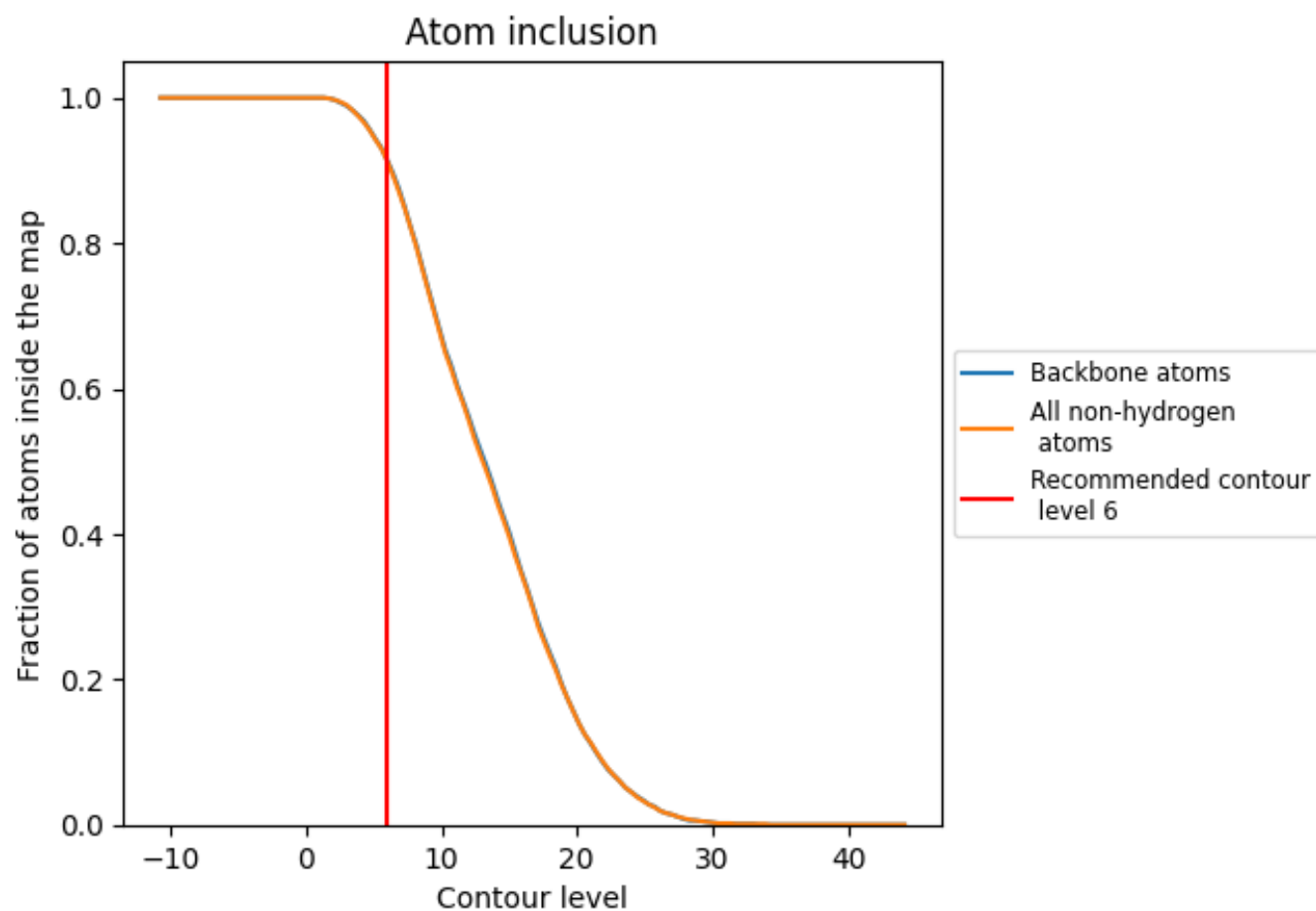
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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

