



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2022 – 09:19 AM EST

PDB ID : 6UDA  
EMDB ID : EMD-20735  
Title : Cryo-EM structure of CH235UCA bound to Man5-enriched CH505.N279K.G  
458Y.SOSIP.664  
Authors : Henderson, R.; Acharya, P.  
Deposited on : 2019-09-19  
Resolution : 4.20 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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

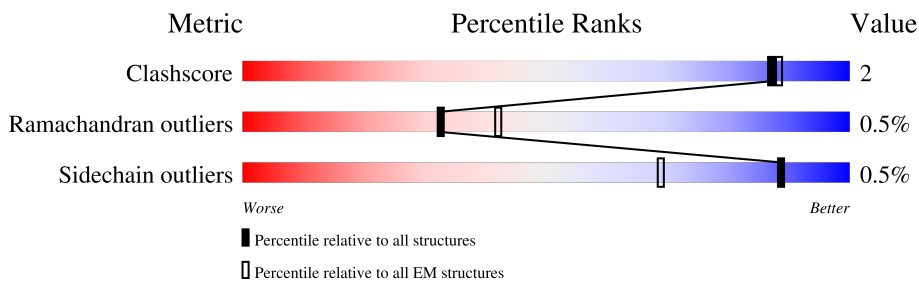
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.20 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	487	
1	E	487	
1	I	487	
2	C	249	
2	G	249	
2	K	249	
3	F	160	
3	J	160	

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Mol	Chain	Length	Quality of chain
3	Z	160	
4	D	234	
4	H	234	
4	L	234	
5	B	4	
5	M	4	
5	N	4	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	605	-	X	X	-
6	NAG	E	605	-	X	X	-
6	NAG	I	605	-	X	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 23733 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 CH505.N279K.G458Y.SOSIP.664 gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	452	3567	2244	624	671	28	0	0
1	E	452	3567	2244	624	671	28	0	0
1	I	452	3567	2244	624	671	28	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7	MET	-	initiating methionine	UNP M4M0W3
A	8	PRO	-	expression tag	UNP M4M0W3
A	9	MET	-	expression tag	UNP M4M0W3
A	10	GLY	-	expression tag	UNP M4M0W3
A	11	SER	-	expression tag	UNP M4M0W3
A	12	LEU	-	expression tag	UNP M4M0W3
A	13	GLN	-	expression tag	UNP M4M0W3
A	14	PRO	-	expression tag	UNP M4M0W3
A	15	LEU	-	expression tag	UNP M4M0W3
A	16	ALA	-	expression tag	UNP M4M0W3
A	17	THR	-	expression tag	UNP M4M0W3
A	18	LEU	-	expression tag	UNP M4M0W3
A	19	TYR	-	expression tag	UNP M4M0W3
A	20	LEU	-	expression tag	UNP M4M0W3
A	21	LEU	-	expression tag	UNP M4M0W3
A	22	GLY	-	expression tag	UNP M4M0W3
A	23	MET	-	expression tag	UNP M4M0W3
A	24	LEU	-	expression tag	UNP M4M0W3
A	25	VAL	-	expression tag	UNP M4M0W3
A	26	ALA	-	expression tag	UNP M4M0W3
A	27	SER	-	expression tag	UNP M4M0W3
A	28	VAL	-	expression tag	UNP M4M0W3
A	29	LEU	-	expression tag	UNP M4M0W3
A	30	ALA	-	expression tag	UNP M4M0W3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	31	ALA	-	expression tag	UNP M4M0W3
A	32	GLU	-	expression tag	UNP M4M0W3
A	33	ASN	-	expression tag	UNP M4M0W3
A	34	LEU	-	expression tag	UNP M4M0W3
A	458	TYR	GLY	engineered mutation	UNP M4M0W3
A	488	LYS	GLU	conflict	UNP M4M0W3
A	489	ILE	VAL	conflict	UNP M4M0W3
A	490	GLU	LYS	conflict	UNP M4M0W3
A	498	ARG	ASN	conflict	UNP M4M0W3
A	499	CYS	ALA	conflict	UNP M4M0W3
A	500	LYS	ARG	conflict	UNP M4M0W3
E	7	MET	-	initiating methionine	UNP M4M0W3
E	8	PRO	-	expression tag	UNP M4M0W3
E	9	MET	-	expression tag	UNP M4M0W3
E	10	GLY	-	expression tag	UNP M4M0W3
E	11	SER	-	expression tag	UNP M4M0W3
E	12	LEU	-	expression tag	UNP M4M0W3
E	13	GLN	-	expression tag	UNP M4M0W3
E	14	PRO	-	expression tag	UNP M4M0W3
E	15	LEU	-	expression tag	UNP M4M0W3
E	16	ALA	-	expression tag	UNP M4M0W3
E	17	THR	-	expression tag	UNP M4M0W3
E	18	LEU	-	expression tag	UNP M4M0W3
E	19	TYR	-	expression tag	UNP M4M0W3
E	20	LEU	-	expression tag	UNP M4M0W3
E	21	LEU	-	expression tag	UNP M4M0W3
E	22	GLY	-	expression tag	UNP M4M0W3
E	23	MET	-	expression tag	UNP M4M0W3
E	24	LEU	-	expression tag	UNP M4M0W3
E	25	VAL	-	expression tag	UNP M4M0W3
E	26	ALA	-	expression tag	UNP M4M0W3
E	27	SER	-	expression tag	UNP M4M0W3
E	28	VAL	-	expression tag	UNP M4M0W3
E	29	LEU	-	expression tag	UNP M4M0W3
E	30	ALA	-	expression tag	UNP M4M0W3
E	31	ALA	-	expression tag	UNP M4M0W3
E	32	GLU	-	expression tag	UNP M4M0W3
E	33	ASN	-	expression tag	UNP M4M0W3
E	34	LEU	-	expression tag	UNP M4M0W3
E	458	TYR	GLY	engineered mutation	UNP M4M0W3
E	488	LYS	GLU	conflict	UNP M4M0W3
E	489	ILE	VAL	conflict	UNP M4M0W3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	490	GLU	LYS	conflict	UNP M4M0W3
E	498	ARG	ASN	conflict	UNP M4M0W3
E	499	CYS	ALA	conflict	UNP M4M0W3
E	500	LYS	ARG	conflict	UNP M4M0W3
I	7	MET	-	initiating methionine	UNP M4M0W3
I	8	PRO	-	expression tag	UNP M4M0W3
I	9	MET	-	expression tag	UNP M4M0W3
I	10	GLY	-	expression tag	UNP M4M0W3
I	11	SER	-	expression tag	UNP M4M0W3
I	12	LEU	-	expression tag	UNP M4M0W3
I	13	GLN	-	expression tag	UNP M4M0W3
I	14	PRO	-	expression tag	UNP M4M0W3
I	15	LEU	-	expression tag	UNP M4M0W3
I	16	ALA	-	expression tag	UNP M4M0W3
I	17	THR	-	expression tag	UNP M4M0W3
I	18	LEU	-	expression tag	UNP M4M0W3
I	19	TYR	-	expression tag	UNP M4M0W3
I	20	LEU	-	expression tag	UNP M4M0W3
I	21	LEU	-	expression tag	UNP M4M0W3
I	22	GLY	-	expression tag	UNP M4M0W3
I	23	MET	-	expression tag	UNP M4M0W3
I	24	LEU	-	expression tag	UNP M4M0W3
I	25	VAL	-	expression tag	UNP M4M0W3
I	26	ALA	-	expression tag	UNP M4M0W3
I	27	SER	-	expression tag	UNP M4M0W3
I	28	VAL	-	expression tag	UNP M4M0W3
I	29	LEU	-	expression tag	UNP M4M0W3
I	30	ALA	-	expression tag	UNP M4M0W3
I	31	ALA	-	expression tag	UNP M4M0W3
I	32	GLU	-	expression tag	UNP M4M0W3
I	33	ASN	-	expression tag	UNP M4M0W3
I	34	LEU	-	expression tag	UNP M4M0W3
I	458	TYR	GLY	engineered mutation	UNP M4M0W3
I	488	LYS	GLU	conflict	UNP M4M0W3
I	489	ILE	VAL	conflict	UNP M4M0W3
I	490	GLU	LYS	conflict	UNP M4M0W3
I	498	ARG	ASN	conflict	UNP M4M0W3
I	499	CYS	ALA	conflict	UNP M4M0W3
I	500	LYS	ARG	conflict	UNP M4M0W3

- Molecule 2 is a protein called CH235 UCA heavy chain Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	220	Total 1645	C 1036	N 276	O 325	S 8	0	0
2	G	220	Total 1645	C 1036	N 276	O 325	S 8	0	0
2	K	220	Total 1645	C 1036	N 276	O 325	S 8	0	0

- Molecule 3 is a protein called CH505.N279K.G458Y.SOSIP.664 gp41.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	126	Total 1001	C 633	N 172	O 190	S 6	0	0
3	F	126	Total 1001	C 633	N 172	O 190	S 6	0	0
3	J	126	Total 1001	C 633	N 172	O 190	S 6	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Z	505	GLY	-	expression tag	UNP Q2N0S5
Z	506	ARG	-	expression tag	UNP Q2N0S5
Z	507	ARG	-	expression tag	UNP Q2N0S5
Z	508	ARG	-	expression tag	UNP Q2N0S5
Z	509	ARG	-	expression tag	UNP Q2N0S5
Z	510	ARG	-	expression tag	UNP Q2N0S5
Z	547L	PRO	ILE	conflict	UNP Q2N0S5
Z	605	CYS	THR	conflict	UNP Q2N0S5
F	505	GLY	-	expression tag	UNP Q2N0S5
F	506	ARG	-	expression tag	UNP Q2N0S5
F	507	ARG	-	expression tag	UNP Q2N0S5
F	508	ARG	-	expression tag	UNP Q2N0S5
F	509	ARG	-	expression tag	UNP Q2N0S5
F	510	ARG	-	expression tag	UNP Q2N0S5
F	547L	PRO	ILE	conflict	UNP Q2N0S5
F	605	CYS	THR	conflict	UNP Q2N0S5
J	505	GLY	-	expression tag	UNP Q2N0S5
J	506	ARG	-	expression tag	UNP Q2N0S5
J	507	ARG	-	expression tag	UNP Q2N0S5
J	508	ARG	-	expression tag	UNP Q2N0S5
J	509	ARG	-	expression tag	UNP Q2N0S5
J	510	ARG	-	expression tag	UNP Q2N0S5
J	547L	PRO	ILE	conflict	UNP Q2N0S5

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Chain	Residue	Modelled	Actual	Comment	Reference
J	605	CYS	THR	conflict	UNP Q2N0S5

- Molecule 4 is a protein called CH235 UCA light chain Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	210	1620	1014	276	325	5	0	0
4	H	210	1620	1014	276	325	5	0	0
4	L	210	1620	1014	276	325	5	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	B	4	50	28	2	20	0	0
5	M	4	50	28	2	20	0	0
5	N	4	50	28	2	20	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



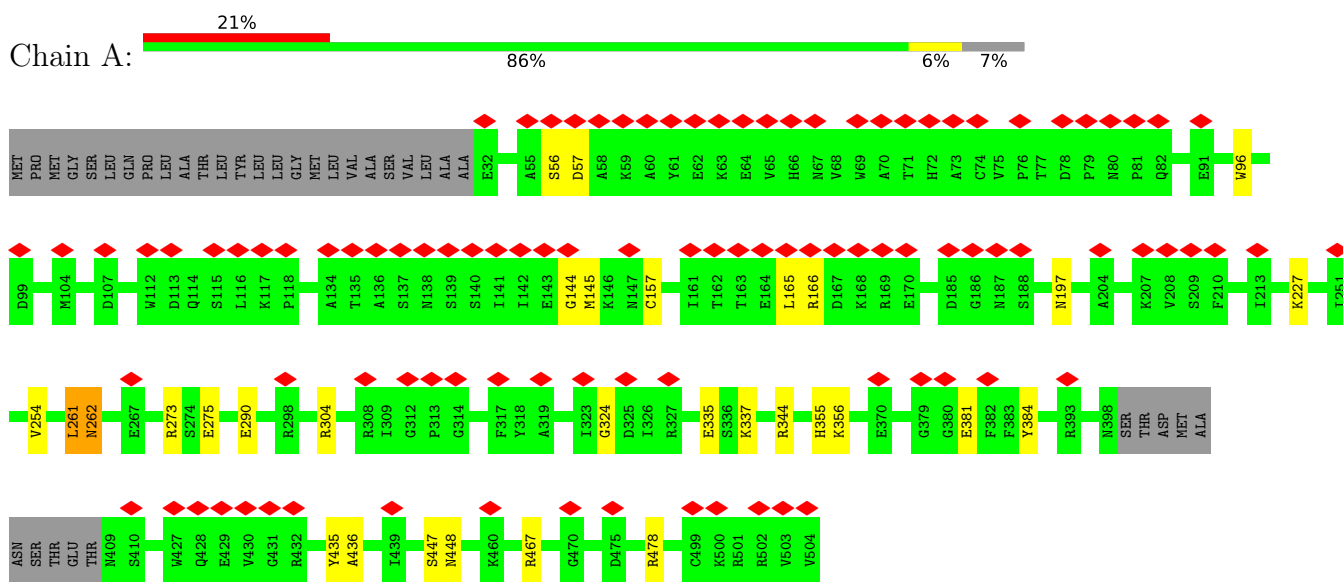


Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	A	1	Total	C	N	O	0
			28	16	2	10	
6	A	1	Total	C	N	O	0
			28	16	2	10	
6	E	1	Total	C	N	O	0
			28	16	2	10	
6	E	1	Total	C	N	O	0
			28	16	2	10	
6	I	1	Total	C	N	O	0
			28	16	2	10	
6	I	1	Total	C	N	O	0
			28	16	2	10	

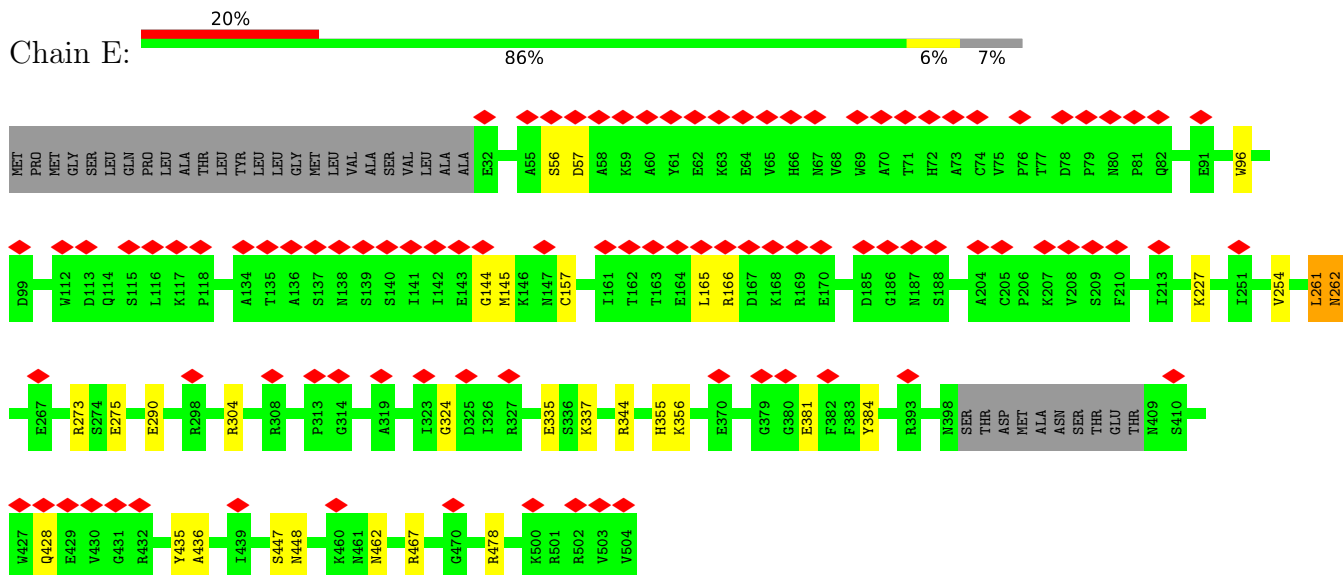
### 3 Residue-property plots

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.

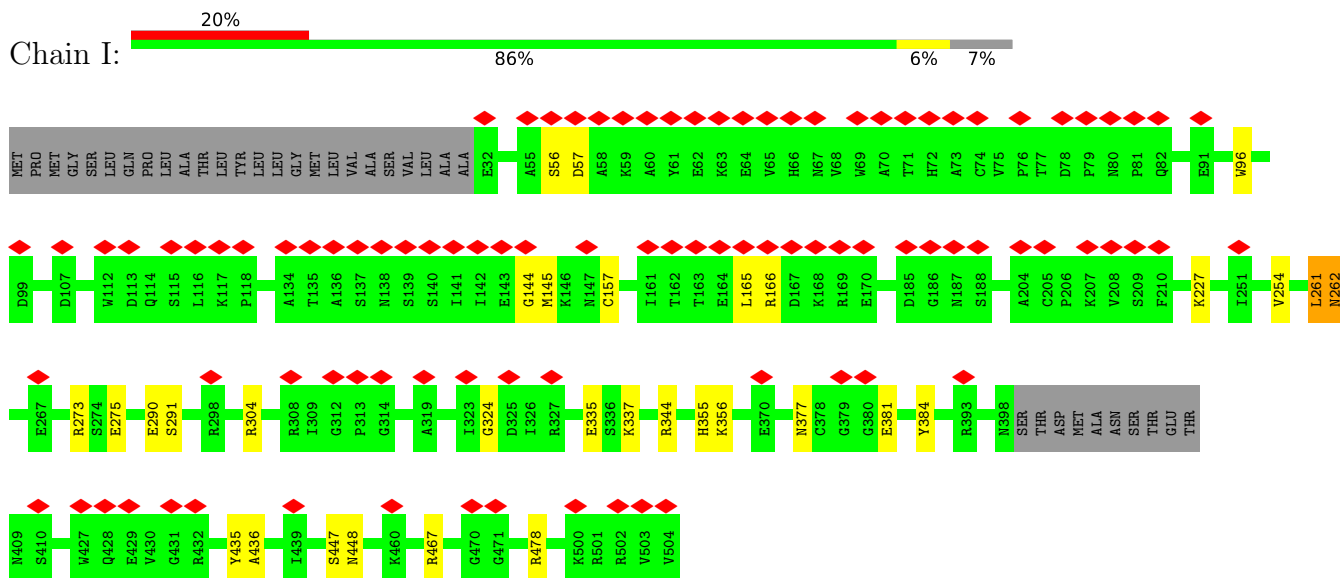
- Molecule 1: CH505.N279K.G458Y.SOSIP.664 gp120



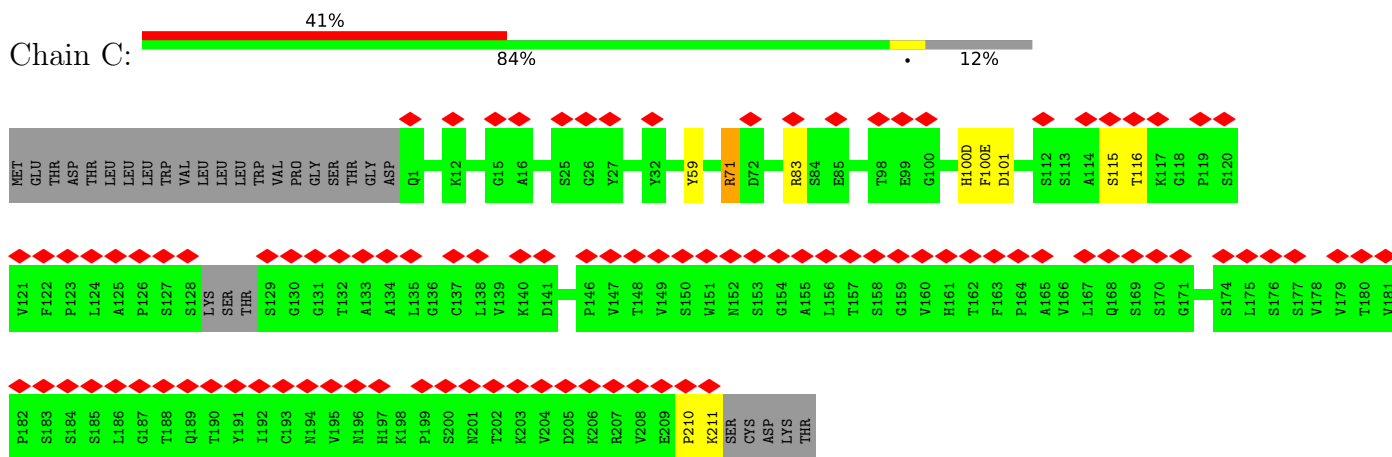
- Molecule 1: CH505.N279K.G458Y.SOSIP.664 gp120



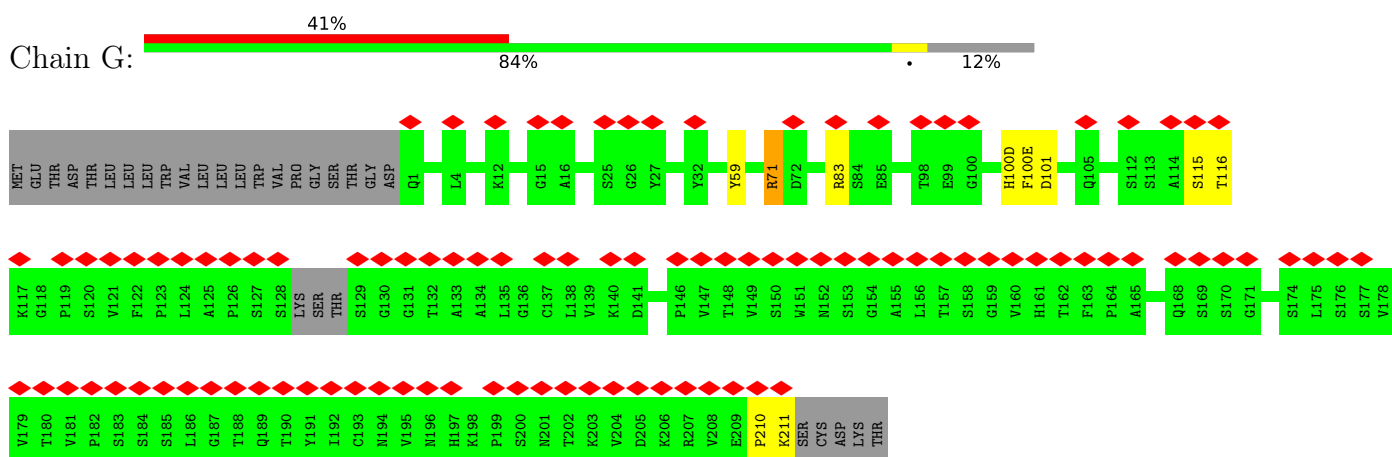
- Molecule 1: CH505.N279K.G458Y.SOSIP.664 gp120



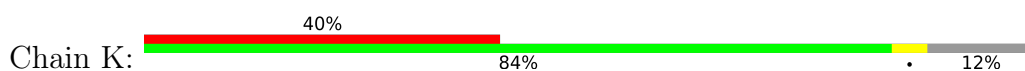
• Molecule 2: CH235 UCA heavy chain Fab

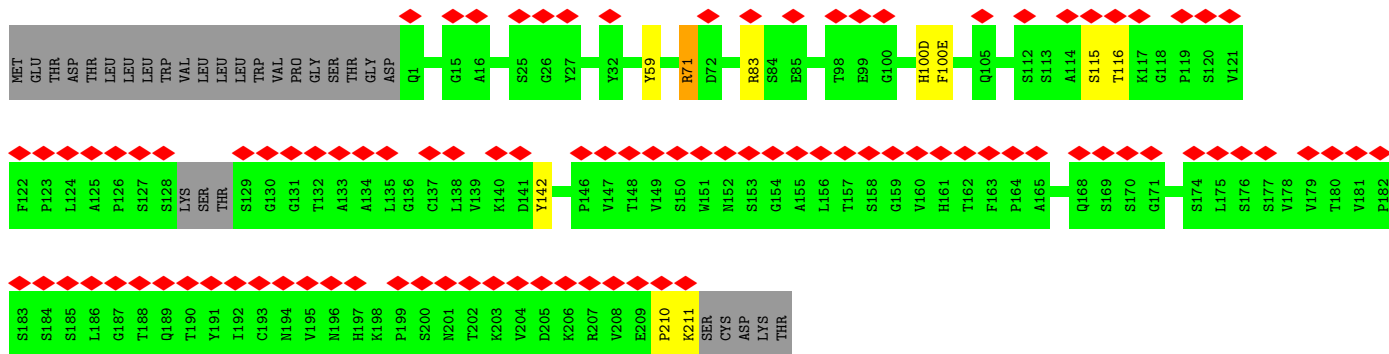


• Molecule 2: CH235 UCA heavy chain Fab

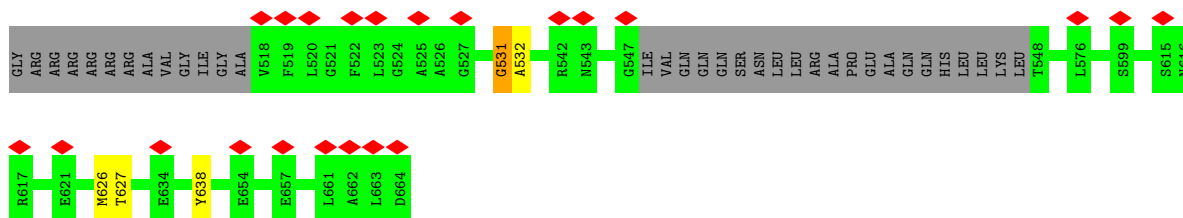
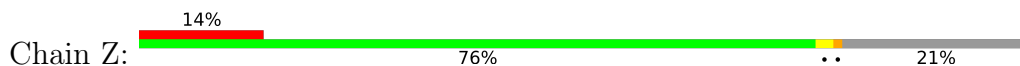


• Molecule 2: CH235 UCA heavy chain Fab

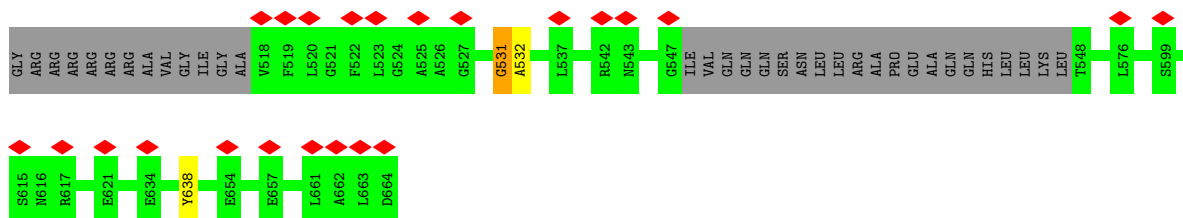
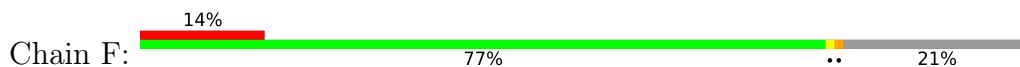




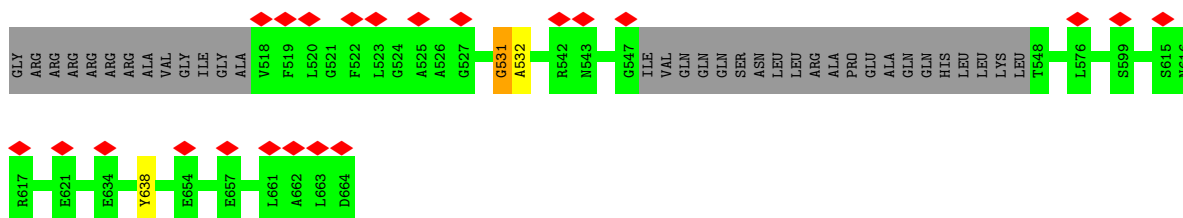
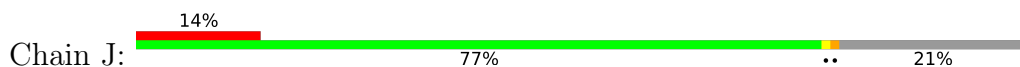
• Molecule 3: CH505.N279K.G458Y.SOSIP.664 gp41



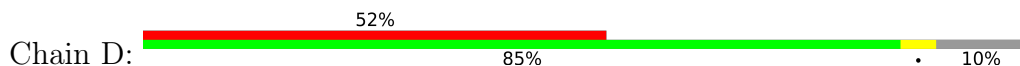
• Molecule 3: CH505.N279K.G458Y.SOSIP.664 gp41

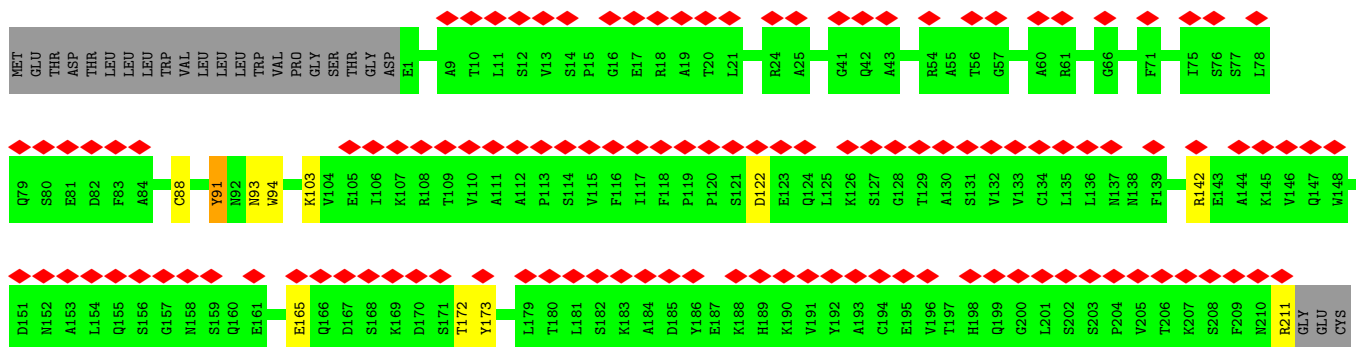


• Molecule 3: CH505.N279K.G458Y.SOSIP.664 gp41

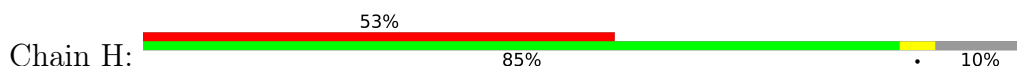


• Molecule 4: CH235 UCA light chain Fab

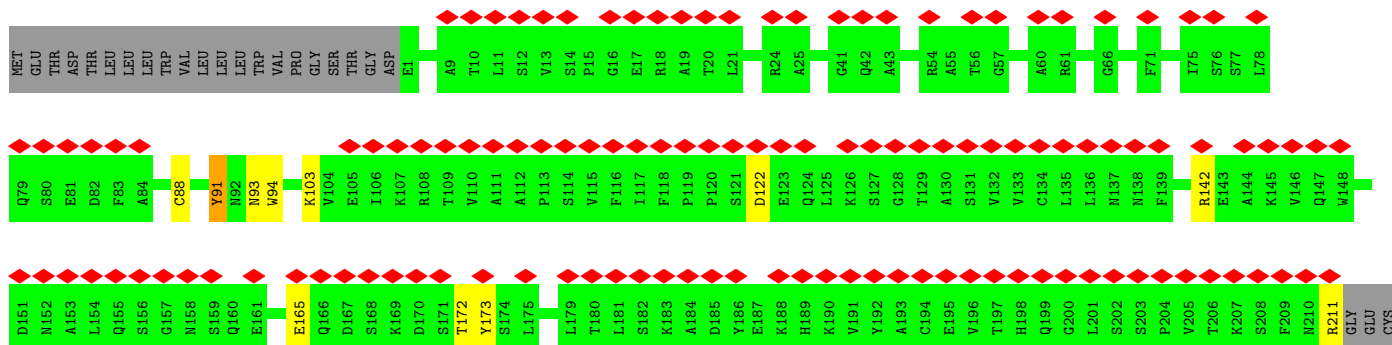
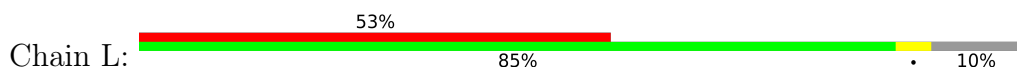




• Molecule 4: CH235 UCA light chain Fab



• Molecule 4: CH235 UCA light chain Fab



• Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	22093	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 ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	2.041	Depositor
Minimum map value	-0.698	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.075	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	345.6, 345.6, 345.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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: MAN, NAG, BMA

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	0.90	4/3641 (0.1%)	0.91	8/4940 (0.2%)
1	E	0.90	4/3641 (0.1%)	0.91	8/4940 (0.2%)
1	I	0.90	4/3641 (0.1%)	0.91	8/4940 (0.2%)
2	C	0.96	1/1684 (0.1%)	0.94	4/2293 (0.2%)
2	G	0.96	1/1684 (0.1%)	0.94	4/2293 (0.2%)
2	K	0.96	1/1684 (0.1%)	0.94	5/2293 (0.2%)
3	F	0.92	0/1019	0.85	2/1382 (0.1%)
3	J	0.92	0/1019	0.85	2/1382 (0.1%)
3	Z	0.92	0/1019	0.85	2/1382 (0.1%)
4	D	0.95	2/1656 (0.1%)	0.91	1/2251 (0.0%)
4	H	0.94	2/1656 (0.1%)	0.91	1/2251 (0.0%)
4	L	0.95	2/1656 (0.1%)	0.91	1/2251 (0.0%)
All	All	0.92	21/24000 (0.1%)	0.91	46/32598 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	I	0	1
All	All	0	3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	91	TYR	CD1-CE1	-6.50	1.29	1.39
4	D	91	TYR	CD1-CE1	-6.49	1.29	1.39
4	H	91	TYR	CD1-CE1	-6.46	1.29	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	381	GLU	CD-OE1	-5.64	1.19	1.25
1	A	381	GLU	CD-OE1	-5.63	1.19	1.25
1	E	381	GLU	CD-OE1	-5.61	1.19	1.25
1	A	157	CYS	CB-SG	5.29	1.91	1.82
1	I	157	CYS	CB-SG	5.28	1.91	1.82
1	E	157	CYS	CB-SG	5.27	1.91	1.82
1	A	254	VAL	CB-CG1	-5.20	1.42	1.52
1	I	254	VAL	CB-CG1	-5.20	1.42	1.52
1	E	254	VAL	CB-CG1	-5.18	1.42	1.52
1	I	335	GLU	CD-OE1	-5.13	1.20	1.25
1	A	335	GLU	CD-OE1	-5.10	1.20	1.25
1	E	335	GLU	CD-OE1	-5.09	1.20	1.25
2	G	59	TYR	CB-CG	-5.05	1.44	1.51
2	C	59	TYR	CB-CG	-5.04	1.44	1.51
4	D	88	CYS	CB-SG	-5.04	1.73	1.81
4	H	88	CYS	CB-SG	-5.03	1.73	1.81
4	L	88	CYS	CB-SG	-5.03	1.73	1.81
2	K	59	TYR	CB-CG	-5.01	1.44	1.51

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	467	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	A	467	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	I	467	ARG	NE-CZ-NH2	-9.20	115.70	120.30
2	G	83	ARG	NE-CZ-NH2	-7.73	116.44	120.30
2	C	83	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	K	83	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	G	71	ARG	NE-CZ-NH2	-7.70	116.45	120.30
2	C	71	ARG	NE-CZ-NH2	-7.68	116.46	120.30
2	K	71	ARG	NE-CZ-NH2	-7.67	116.46	120.30
1	A	273	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	E	273	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	I	273	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	I	344	ARG	NE-CZ-NH2	-7.54	116.53	120.30
1	A	344	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	E	344	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	262	ASN	CB-CA-C	-6.82	96.77	110.40
1	E	262	ASN	CB-CA-C	-6.81	96.78	110.40
1	I	262	ASN	CB-CA-C	-6.81	96.78	110.40
1	A	304	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	I	304	ARG	NE-CZ-NH2	-6.74	116.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	304	ARG	NE-CZ-NH2	-6.73	116.94	120.30
3	J	531	GLY	C-N-CA	6.29	137.43	121.70
3	F	531	GLY	C-N-CA	6.29	137.41	121.70
3	Z	531	GLY	C-N-CA	6.27	137.37	121.70
2	C	100(E)	PHE	N-CA-C	6.05	127.32	111.00
2	G	100(E)	PHE	N-CA-C	6.04	127.31	111.00
2	K	100(E)	PHE	N-CA-C	6.04	127.30	111.00
2	G	71	ARG	NE-CZ-NH1	5.40	123.00	120.30
2	K	71	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	C	71	ARG	NE-CZ-NH1	5.34	122.97	120.30
3	J	638	TYR	CB-CG-CD2	-5.34	117.80	121.00
4	L	142	ARG	NE-CZ-NH1	5.33	122.97	120.30
4	H	142	ARG	NE-CZ-NH1	5.33	122.96	120.30
4	D	142	ARG	NE-CZ-NH1	5.32	122.96	120.30
3	F	638	TYR	CB-CG-CD2	-5.24	117.86	121.00
3	Z	638	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	E	227	LYS	N-CA-C	5.20	125.04	111.00
1	I	227	LYS	N-CA-C	5.19	125.02	111.00
1	A	227	LYS	N-CA-C	5.19	125.02	111.00
1	A	478	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	E	384	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	I	384	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	E	478	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	384	TYR	CB-CG-CD2	-5.11	117.93	121.00
1	I	478	ARG	NE-CZ-NH1	5.08	122.84	120.30
2	K	142	TYR	CB-CG-CD2	-5.04	117.97	121.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	262	ASN	Mainchain
1	E	262	ASN	Mainchain
1	I	262	ASN	Mainchain

## 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	3567	0	3541	19	0
1	E	3567	0	3541	20	0
1	I	3567	0	3541	20	0
2	C	1645	0	1608	6	0
2	G	1645	0	1608	5	0
2	K	1645	0	1608	4	0
3	F	1001	0	978	0	0
3	J	1001	0	978	0	0
3	Z	1001	0	978	1	0
4	D	1620	0	1572	6	0
4	H	1620	0	1572	5	0
4	L	1620	0	1572	5	0
5	B	50	0	43	3	0
5	M	50	0	43	4	0
5	N	50	0	43	3	0
6	A	28	0	24	9	0
6	E	28	0	24	9	0
6	I	28	0	24	9	0
All	All	23733	0	23298	96	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 (96) 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:I:448:ASN:ND2	6:I:605:NAG:C1	1.69	1.55
1:E:448:ASN:ND2	6:E:605:NAG:C1	1.69	1.54
1:A:448:ASN:ND2	6:A:605:NAG:C1	1.69	1.50
1:I:448:ASN:CG	6:I:605:NAG:C1	2.45	0.85
1:A:448:ASN:CG	6:A:605:NAG:C1	2.45	0.85
1:E:448:ASN:CG	6:E:605:NAG:C1	2.45	0.84
1:A:96:TRP:CD1	1:A:275:GLU:OE2	2.35	0.79
1:I:96:TRP:CD1	1:I:275:GLU:OE2	2.35	0.79
1:E:96:TRP:CD1	1:E:275:GLU:OE2	2.35	0.78
1:A:261:LEU:HD23	1:A:261:LEU:N	2.00	0.77
1:E:261:LEU:N	1:E:261:LEU:HD23	2.00	0.77
1:I:261:LEU:N	1:I:261:LEU:HD23	2.00	0.77
5:B:1:NAG:O3	5:B:1:NAG:O7	2.04	0.76
5:M:1:NAG:O7	5:M:1:NAG:O3	2.04	0.75
5:N:1:NAG:O7	5:N:1:NAG:O3	2.04	0.75
1:E:448:ASN:ND2	6:E:605:NAG:C2	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:448:ASN:ND2	6:I:605:NAG:C2	2.50	0.72
1:A:448:ASN:ND2	6:A:605:NAG:C2	2.50	0.70
5:M:2:NAG:H82	5:M:2:NAG:O3	1.99	0.62
5:N:2:NAG:O3	5:N:2:NAG:H82	2.00	0.62
5:B:2:NAG:O3	5:B:2:NAG:H82	1.99	0.62
1:E:261:LEU:HD23	1:E:261:LEU:H	1.68	0.58
1:E:448:ASN:ND2	6:E:605:NAG:C3	2.66	0.58
1:I:261:LEU:HD23	1:I:261:LEU:H	1.68	0.58
1:A:448:ASN:ND2	6:A:605:NAG:C3	2.66	0.58
1:I:448:ASN:ND2	6:I:605:NAG:C5	2.66	0.58
1:E:448:ASN:ND2	6:E:605:NAG:C5	2.66	0.58
1:I:448:ASN:ND2	6:I:605:NAG:C3	2.66	0.58
1:A:448:ASN:ND2	6:A:605:NAG:C5	2.66	0.58
1:I:448:ASN:ND2	6:I:605:NAG:H5	2.19	0.57
1:A:261:LEU:HD23	1:A:261:LEU:H	1.68	0.57
1:E:448:ASN:ND2	6:E:605:NAG:H5	2.19	0.57
1:A:448:ASN:ND2	6:A:605:NAG:H5	2.19	0.56
5:N:1:NAG:HO3	5:N:1:NAG:C7	2.12	0.56
1:I:275:GLU:OE2	1:I:275:GLU:HA	2.06	0.56
1:A:275:GLU:OE2	1:A:275:GLU:HA	2.06	0.54
1:E:275:GLU:OE2	1:E:275:GLU:HA	2.06	0.54
6:E:605:NAG:O4	6:E:605:NAG:O6	2.08	0.50
5:M:1:NAG:HO3	5:M:1:NAG:C7	2.07	0.49
1:E:261:LEU:N	1:E:261:LEU:CD2	2.72	0.48
1:E:56:SER:OG	1:E:57:ASP:N	2.47	0.47
1:A:290:GLU:OE2	1:A:337:LYS:NZ	2.48	0.47
1:I:291:SER:HG	6:I:605:NAG:C7	2.28	0.47
1:A:56:SER:OG	1:A:57:ASP:N	2.47	0.47
1:A:261:LEU:N	1:A:261:LEU:CD2	2.72	0.47
5:M:2:NAG:HO6	5:M:3:BMA:HO2	1.63	0.47
2:K:211:LYS:NZ	4:L:122:ASP:OD2	2.49	0.46
1:I:290:GLU:OE2	1:I:337:LYS:NZ	2.48	0.46
1:A:435:TYR:CG	1:A:436:ALA:N	2.83	0.46
2:C:211:LYS:NZ	4:D:122:ASP:OD2	2.49	0.46
1:I:435:TYR:CG	1:I:436:ALA:N	2.83	0.46
1:I:448:ASN:OD1	6:I:605:NAG:C1	2.64	0.46
2:G:211:LYS:NZ	4:H:122:ASP:OD2	2.49	0.46
1:E:435:TYR:CG	1:E:436:ALA:N	2.83	0.46
1:I:56:SER:OG	1:I:57:ASP:N	2.47	0.46
1:A:448:ASN:OD1	6:A:605:NAG:C1	2.64	0.46
2:G:115:SER:OG	2:G:116:THR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:448:ASN:ND2	6:A:605:NAG:H3	2.32	0.45
1:E:290:GLU:OE2	1:E:337:LYS:NZ	2.48	0.45
4:L:103:LYS:NZ	4:L:165:GLU:OE1	2.49	0.45
2:G:100(D):HIS:HB2	4:H:91:TYR:CZ	2.52	0.44
2:C:100(D):HIS:HB2	4:D:91:TYR:CZ	2.52	0.44
4:D:93:ASN:O	4:D:94:TRP:C	2.55	0.44
1:I:448:ASN:ND2	6:I:605:NAG:H3	2.32	0.44
1:E:448:ASN:OD1	6:E:605:NAG:C1	2.64	0.44
1:E:448:ASN:ND2	6:E:605:NAG:H3	2.32	0.44
1:I:377:ASN:OD1	1:I:377:ASN:N	2.50	0.44
2:K:100(D):HIS:HB2	4:L:91:TYR:CZ	2.52	0.44
1:I:261:LEU:N	1:I:261:LEU:CD2	2.72	0.43
2:C:210:PRO:O	2:C:211:LYS:C	2.56	0.43
2:K:115:SER:OG	2:K:116:THR:N	2.49	0.43
2:G:210:PRO:O	2:G:211:LYS:C	2.56	0.43
4:H:93:ASN:O	4:H:94:TRP:C	2.55	0.43
4:H:103:LYS:NZ	4:H:165:GLU:OE1	2.49	0.43
2:C:115:SER:OG	2:C:116:THR:N	2.49	0.43
4:H:172:THR:OG1	4:H:173:TYR:N	2.52	0.43
1:E:462:ASN:N	1:E:462:ASN:OD1	2.47	0.43
4:L:172:THR:OG1	4:L:173:TYR:N	2.52	0.43
6:A:605:NAG:O4	6:A:605:NAG:O6	2.08	0.42
1:E:355:HIS:CG	1:E:356:LYS:H	2.38	0.42
1:I:355:HIS:CG	1:I:356:LYS:H	2.38	0.42
2:K:210:PRO:O	2:K:211:LYS:C	2.56	0.42
1:A:165:LEU:O	1:A:166:ARG:HB2	2.20	0.42
4:D:172:THR:OG1	4:D:173:TYR:N	2.52	0.42
1:A:355:HIS:CG	1:A:356:LYS:H	2.38	0.42
1:I:165:LEU:O	1:I:166:ARG:HB2	2.20	0.42
2:C:101:ASP:OD1	2:C:101:ASP:N	2.44	0.42
4:L:93:ASN:O	4:L:94:TRP:C	2.55	0.41
1:E:165:LEU:O	1:E:166:ARG:HB2	2.20	0.41
1:E:428:GLN:OE1	1:E:428:GLN:N	2.54	0.41
5:B:2:NAG:O3	5:B:2:NAG:C8	2.68	0.41
2:G:101:ASP:OD1	2:G:101:ASP:N	2.44	0.41
1:A:197:ASN:N	1:A:197:ASN:OD1	2.49	0.41
4:D:103:LYS:NZ	4:D:165:GLU:OE1	2.49	0.40
2:C:100(D):HIS:HB2	4:D:91:TYR:CE1	2.57	0.40
3:Z:626:MET:HB3	3:Z:627:THR:HA	2.04	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	448/487 (92%)	436 (97%)	9 (2%)	3 (1%)	22	62
1	E	448/487 (92%)	436 (97%)	9 (2%)	3 (1%)	22	62
1	I	448/487 (92%)	436 (97%)	9 (2%)	3 (1%)	22	62
2	C	216/249 (87%)	212 (98%)	4 (2%)	0	100	100
2	G	216/249 (87%)	212 (98%)	4 (2%)	0	100	100
2	K	216/249 (87%)	212 (98%)	4 (2%)	0	100	100
3	F	122/160 (76%)	114 (93%)	6 (5%)	2 (2%)	9	45
3	J	122/160 (76%)	114 (93%)	6 (5%)	2 (2%)	9	45
3	Z	122/160 (76%)	114 (93%)	6 (5%)	2 (2%)	9	45
4	D	208/234 (89%)	203 (98%)	5 (2%)	0	100	100
4	H	208/234 (89%)	203 (98%)	5 (2%)	0	100	100
4	L	208/234 (89%)	203 (98%)	5 (2%)	0	100	100
All	All	2982/3390 (88%)	2895 (97%)	72 (2%)	15 (0%)	32	68

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	Z	532	ALA
3	F	532	ALA
3	J	532	ALA
3	Z	531	GLY
3	F	531	GLY
3	J	531	GLY
1	A	324	GLY
1	E	324	GLY
1	I	324	GLY
1	A	145	MET
1	E	145	MET
1	I	145	MET

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Mol	Chain	Res	Type
1	A	144	GLY
1	E	144	GLY
1	I	144	GLY

### 5.3.2 Protein sidechains [i](#)

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	405/433 (94%)	403 (100%)	2 (0%)	88	93
1	E	405/433 (94%)	403 (100%)	2 (0%)	88	93
1	I	405/433 (94%)	403 (100%)	2 (0%)	88	93
2	C	185/213 (87%)	184 (100%)	1 (0%)	88	93
2	G	185/213 (87%)	184 (100%)	1 (0%)	88	93
2	K	185/213 (87%)	184 (100%)	1 (0%)	88	93
3	F	108/135 (80%)	108 (100%)	0	100	100
3	J	108/135 (80%)	108 (100%)	0	100	100
3	Z	108/135 (80%)	108 (100%)	0	100	100
4	D	182/203 (90%)	181 (100%)	1 (0%)	88	93
4	H	182/203 (90%)	181 (100%)	1 (0%)	88	93
4	L	182/203 (90%)	181 (100%)	1 (0%)	88	93
All	All	2640/2952 (89%)	2628 (100%)	12 (0%)	89	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	261	LEU
1	A	447	SER
2	C	71	ARG
4	D	211	ARG
1	E	261	LEU
1	E	447	SER
2	G	71	ARG

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Mol	Chain	Res	Type
4	H	211	ARG
1	I	261	LEU
1	I	447	SER
2	K	71	ARG
4	L	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

12 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
5	NAG	B	1	5	14,14,15	2.50	7 (50%)	17,19,21	3.35	11 (64%)
5	NAG	B	2	5	14,14,15	2.01	5 (35%)	17,19,21	3.46	10 (58%)
5	BMA	B	3	5	11,11,12	0.67	0	15,15,17	2.77	7 (46%)
5	MAN	B	4	5	11,11,12	1.07	0	15,15,17	1.96	5 (33%)
5	NAG	M	1	5	14,14,15	2.51	7 (50%)	17,19,21	3.35	11 (64%)
5	NAG	M	2	5	14,14,15	2.01	5 (35%)	17,19,21	3.46	10 (58%)
5	BMA	M	3	5	11,11,12	0.66	0	15,15,17	2.77	7 (46%)
5	MAN	M	4	5	11,11,12	1.07	0	15,15,17	1.96	5 (33%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	N	1	5	14,14,15	2.51	7 (50%)	17,19,21	3.35	11 (64%)
5	NAG	N	2	5	14,14,15	2.01	5 (35%)	17,19,21	3.46	10 (58%)
5	BMA	N	3	5	11,11,12	0.66	0	15,15,17	2.78	7 (46%)
5	MAN	N	4	5	11,11,12	1.06	0	15,15,17	1.96	5 (33%)

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
5	NAG	B	1	5	-	3/6/23/26	0/1/1/1
5	NAG	B	2	5	-	5/6/23/26	0/1/1/1
5	BMA	B	3	5	-	2/2/19/22	0/1/1/1
5	MAN	B	4	5	-	1/2/19/22	0/1/1/1
5	NAG	M	1	5	-	3/6/23/26	0/1/1/1
5	NAG	M	2	5	-	5/6/23/26	0/1/1/1
5	BMA	M	3	5	-	2/2/19/22	0/1/1/1
5	MAN	M	4	5	-	1/2/19/22	0/1/1/1
5	NAG	N	1	5	-	3/6/23/26	0/1/1/1
5	NAG	N	2	5	-	5/6/23/26	0/1/1/1
5	BMA	N	3	5	-	2/2/19/22	0/1/1/1
5	MAN	N	4	5	-	1/2/19/22	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	N	1	NAG	O5-C1	-4.62	1.36	1.43
5	B	1	NAG	O5-C1	-4.59	1.36	1.43
5	M	1	NAG	O5-C1	-4.57	1.36	1.43
5	M	1	NAG	C2-N2	-4.08	1.39	1.46
5	B	1	NAG	C2-N2	-4.08	1.39	1.46
5	N	1	NAG	C2-N2	-4.04	1.39	1.46
5	B	2	NAG	O5-C1	-3.84	1.37	1.43
5	N	2	NAG	O5-C1	-3.83	1.37	1.43
5	M	2	NAG	O5-C1	-3.81	1.37	1.43
5	N	1	NAG	C3-C2	-3.65	1.44	1.52
5	M	1	NAG	C3-C2	-3.63	1.44	1.52
5	B	1	NAG	C3-C2	-3.62	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	2	NAG	C1-C2	-3.45	1.47	1.52
5	N	2	NAG	C1-C2	-3.42	1.47	1.52
5	B	2	NAG	C1-C2	-3.42	1.47	1.52
5	B	1	NAG	C4-C3	-2.94	1.44	1.52
5	N	1	NAG	C4-C3	-2.92	1.44	1.52
5	M	1	NAG	C4-C3	-2.92	1.44	1.52
5	M	1	NAG	C8-C7	-2.81	1.44	1.50
5	N	1	NAG	C8-C7	-2.81	1.44	1.50
5	B	1	NAG	C8-C7	-2.80	1.44	1.50
5	N	1	NAG	C1-C2	-2.55	1.48	1.52
5	B	2	NAG	C3-C2	-2.52	1.47	1.52
5	N	2	NAG	C3-C2	-2.52	1.47	1.52
5	M	2	NAG	C3-C2	-2.52	1.47	1.52
5	M	1	NAG	C1-C2	-2.50	1.48	1.52
5	B	1	NAG	C1-C2	-2.48	1.48	1.52
5	N	2	NAG	C2-N2	-2.41	1.42	1.46
5	M	2	NAG	C2-N2	-2.41	1.42	1.46
5	B	2	NAG	C2-N2	-2.40	1.42	1.46
5	M	1	NAG	O7-C7	-2.37	1.17	1.23
5	B	1	NAG	O7-C7	-2.35	1.17	1.23
5	N	1	NAG	O7-C7	-2.35	1.17	1.23
5	M	2	NAG	C4-C3	-2.34	1.46	1.52
5	N	2	NAG	C4-C3	-2.33	1.46	1.52
5	B	2	NAG	C4-C3	-2.31	1.46	1.52

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	2	NAG	O4-C4-C5	-7.48	90.74	109.30
5	B	2	NAG	O4-C4-C5	-7.47	90.74	109.30
5	N	2	NAG	O4-C4-C5	-7.46	90.76	109.30
5	N	3	BMA	O5-C5-C6	6.41	117.25	107.20
5	M	3	BMA	O5-C5-C6	6.40	117.24	107.20
5	B	3	BMA	O5-C5-C6	6.39	117.22	107.20
5	M	2	NAG	O4-C4-C3	-6.30	95.78	110.35
5	B	2	NAG	O4-C4-C3	-6.30	95.79	110.35
5	N	2	NAG	O4-C4-C3	-6.29	95.80	110.35
5	M	1	NAG	O5-C1-C2	-5.37	102.81	111.29
5	B	1	NAG	O5-C1-C2	-5.36	102.82	111.29
5	N	1	NAG	O5-C1-C2	-5.36	102.83	111.29
5	B	1	NAG	C1-C2-N2	-5.17	101.66	110.49
5	M	1	NAG	C1-C2-N2	-5.16	101.68	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	N	1	NAG	C1-C2-N2	-5.14	101.70	110.49
5	B	2	NAG	C1-O5-C5	-5.08	105.31	112.19
5	M	2	NAG	C1-O5-C5	-5.08	105.31	112.19
5	N	2	NAG	C1-O5-C5	-5.07	105.32	112.19
5	M	1	NAG	O3-C3-C4	-5.06	98.65	110.35
5	N	1	NAG	O3-C3-C4	-5.06	98.65	110.35
5	B	1	NAG	O3-C3-C4	-5.05	98.67	110.35
5	N	1	NAG	C8-C7-N2	4.97	124.52	116.10
5	M	1	NAG	C8-C7-N2	4.95	124.47	116.10
5	B	1	NAG	C8-C7-N2	4.94	124.47	116.10
5	N	1	NAG	O7-C7-C8	-4.89	112.98	122.06
5	M	1	NAG	O7-C7-C8	-4.88	112.99	122.06
5	B	1	NAG	O7-C7-C8	-4.88	113.00	122.06
5	M	2	NAG	C1-C2-N2	-4.85	102.21	110.49
5	N	2	NAG	C1-C2-N2	-4.84	102.23	110.49
5	B	2	NAG	C1-C2-N2	-4.83	102.23	110.49
5	B	1	NAG	C2-N2-C7	-4.43	116.59	122.90
5	N	2	NAG	O5-C5-C6	4.43	114.15	107.20
5	M	1	NAG	C2-N2-C7	-4.42	116.61	122.90
5	N	1	NAG	C2-N2-C7	-4.41	116.63	122.90
5	M	2	NAG	O5-C5-C6	4.41	114.11	107.20
5	B	2	NAG	O5-C5-C6	4.38	114.07	107.20
5	N	3	BMA	O3-C3-C2	-4.19	101.98	109.99
5	M	3	BMA	O3-C3-C2	-4.18	101.98	109.99
5	B	3	BMA	O3-C3-C2	-4.17	102.00	109.99
5	B	1	NAG	O4-C4-C3	-3.81	101.53	110.35
5	M	1	NAG	O4-C4-C3	-3.81	101.53	110.35
5	N	1	NAG	O4-C4-C3	-3.80	101.55	110.35
5	N	3	BMA	C1-C2-C3	3.78	114.31	109.67
5	M	3	BMA	C1-C2-C3	3.74	114.26	109.67
5	B	3	BMA	C1-C2-C3	3.73	114.25	109.67
5	B	4	MAN	O3-C3-C2	3.71	117.10	109.99
5	N	4	MAN	O3-C3-C2	3.71	117.10	109.99
5	M	4	MAN	O3-C3-C2	3.70	117.08	109.99
5	N	4	MAN	C2-C3-C4	-3.63	104.61	110.89
5	M	4	MAN	C2-C3-C4	-3.62	104.62	110.89
5	B	4	MAN	C2-C3-C4	-3.62	104.62	110.89
5	N	3	BMA	O5-C1-C2	-3.57	105.25	110.77
5	M	3	BMA	O5-C1-C2	-3.56	105.28	110.77
5	B	3	BMA	O5-C1-C2	-3.51	105.35	110.77
5	M	2	NAG	O3-C3-C2	-3.06	103.13	109.47
5	N	2	NAG	O3-C3-C2	-3.06	103.13	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2	NAG	O3-C3-C2	-3.04	103.17	109.47
5	B	1	NAG	O3-C3-C2	-3.03	103.19	109.47
5	M	1	NAG	O3-C3-C2	-3.02	103.23	109.47
5	N	2	NAG	C3-C4-C5	-3.01	104.87	110.24
5	B	2	NAG	C3-C4-C5	-3.01	104.87	110.24
5	M	2	NAG	C3-C4-C5	-3.01	104.88	110.24
5	N	1	NAG	O3-C3-C2	-3.00	103.26	109.47
5	M	3	BMA	O2-C2-C3	2.77	115.69	110.14
5	N	3	BMA	O2-C2-C3	2.76	115.67	110.14
5	B	3	BMA	O2-C2-C3	2.75	115.66	110.14
5	M	4	MAN	O5-C1-C2	-2.72	106.58	110.77
5	N	4	MAN	O5-C1-C2	-2.70	106.60	110.77
5	B	4	MAN	O5-C1-C2	-2.70	106.61	110.77
5	N	1	NAG	C4-C3-C2	-2.63	107.17	111.02
5	M	1	NAG	C4-C3-C2	-2.63	107.17	111.02
5	B	1	NAG	C4-C3-C2	-2.62	107.17	111.02
5	B	2	NAG	C4-C3-C2	-2.61	107.19	111.02
5	N	4	MAN	O5-C5-C6	2.60	111.28	107.20
5	M	2	NAG	C4-C3-C2	-2.60	107.21	111.02
5	M	4	MAN	O5-C5-C6	2.58	111.24	107.20
5	B	4	MAN	O5-C5-C6	2.57	111.24	107.20
5	N	2	NAG	C4-C3-C2	-2.57	107.25	111.02
5	M	3	BMA	C3-C4-C5	-2.46	105.85	110.24
5	N	3	BMA	C3-C4-C5	-2.45	105.86	110.24
5	B	3	BMA	C3-C4-C5	-2.44	105.88	110.24
5	B	4	MAN	C3-C4-C5	-2.30	106.14	110.24
5	M	4	MAN	C3-C4-C5	-2.29	106.16	110.24
5	N	4	MAN	C3-C4-C5	-2.27	106.19	110.24
5	M	2	NAG	O3-C3-C4	-2.19	105.28	110.35
5	N	2	NAG	O3-C3-C4	-2.19	105.29	110.35
5	B	2	NAG	O3-C3-C4	-2.19	105.29	110.35
5	N	1	NAG	C1-O5-C5	2.15	115.11	112.19
5	M	1	NAG	C3-C4-C5	-2.15	106.40	110.24
5	B	1	NAG	C3-C4-C5	-2.15	106.41	110.24
5	N	1	NAG	C3-C4-C5	-2.14	106.42	110.24
5	B	1	NAG	C1-O5-C5	2.14	115.08	112.19
5	M	1	NAG	C1-O5-C5	2.13	115.08	112.19
5	B	3	BMA	O4-C4-C5	-2.08	104.13	109.30
5	N	3	BMA	O4-C4-C5	-2.08	104.14	109.30
5	M	3	BMA	O4-C4-C5	-2.07	104.17	109.30
5	B	2	NAG	O5-C5-C4	2.04	115.79	110.83
5	N	2	NAG	O5-C5-C4	2.03	115.76	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	2	NAG	O5-C5-C4	2.03	115.76	110.83

There are no chirality outliers.

All (33) torsion outliers are listed below:

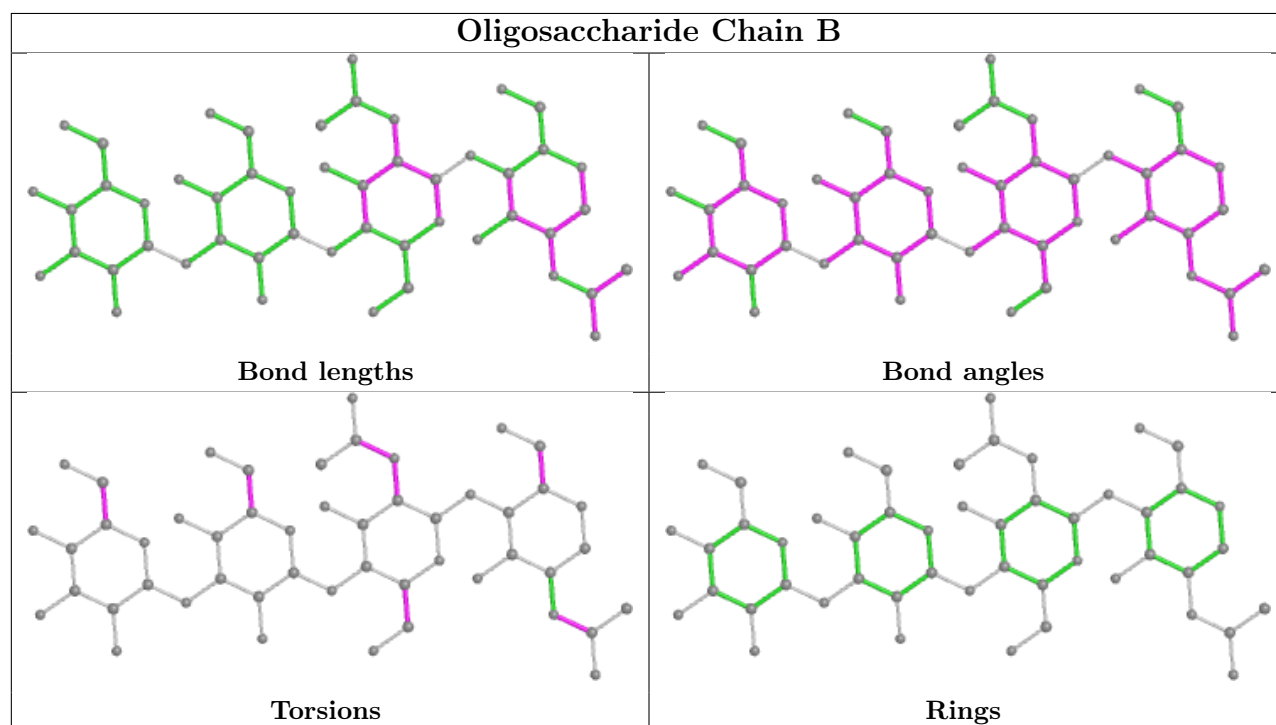
Mol	Chain	Res	Type	Atoms
5	B	2	NAG	C3-C2-N2-C7
5	B	2	NAG	C8-C7-N2-C2
5	B	2	NAG	O7-C7-N2-C2
5	M	2	NAG	C3-C2-N2-C7
5	M	2	NAG	C8-C7-N2-C2
5	M	2	NAG	O7-C7-N2-C2
5	N	2	NAG	C3-C2-N2-C7
5	N	2	NAG	C8-C7-N2-C2
5	N	2	NAG	O7-C7-N2-C2
5	B	3	BMA	C4-C5-C6-O6
5	M	3	BMA	C4-C5-C6-O6
5	N	3	BMA	C4-C5-C6-O6
5	B	2	NAG	O5-C5-C6-O6
5	M	2	NAG	O5-C5-C6-O6
5	N	2	NAG	O5-C5-C6-O6
5	B	3	BMA	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	N	3	BMA	O5-C5-C6-O6
5	B	1	NAG	O5-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	N	1	NAG	O5-C5-C6-O6
5	B	2	NAG	C4-C5-C6-O6
5	M	2	NAG	C4-C5-C6-O6
5	N	2	NAG	C4-C5-C6-O6
5	B	1	NAG	O7-C7-N2-C2
5	M	1	NAG	O7-C7-N2-C2
5	N	1	NAG	O7-C7-N2-C2
5	B	1	NAG	C8-C7-N2-C2
5	M	1	NAG	C8-C7-N2-C2
5	N	1	NAG	C8-C7-N2-C2
5	M	4	MAN	C4-C5-C6-O6
5	B	4	MAN	C4-C5-C6-O6
5	N	4	MAN	C4-C5-C6-O6

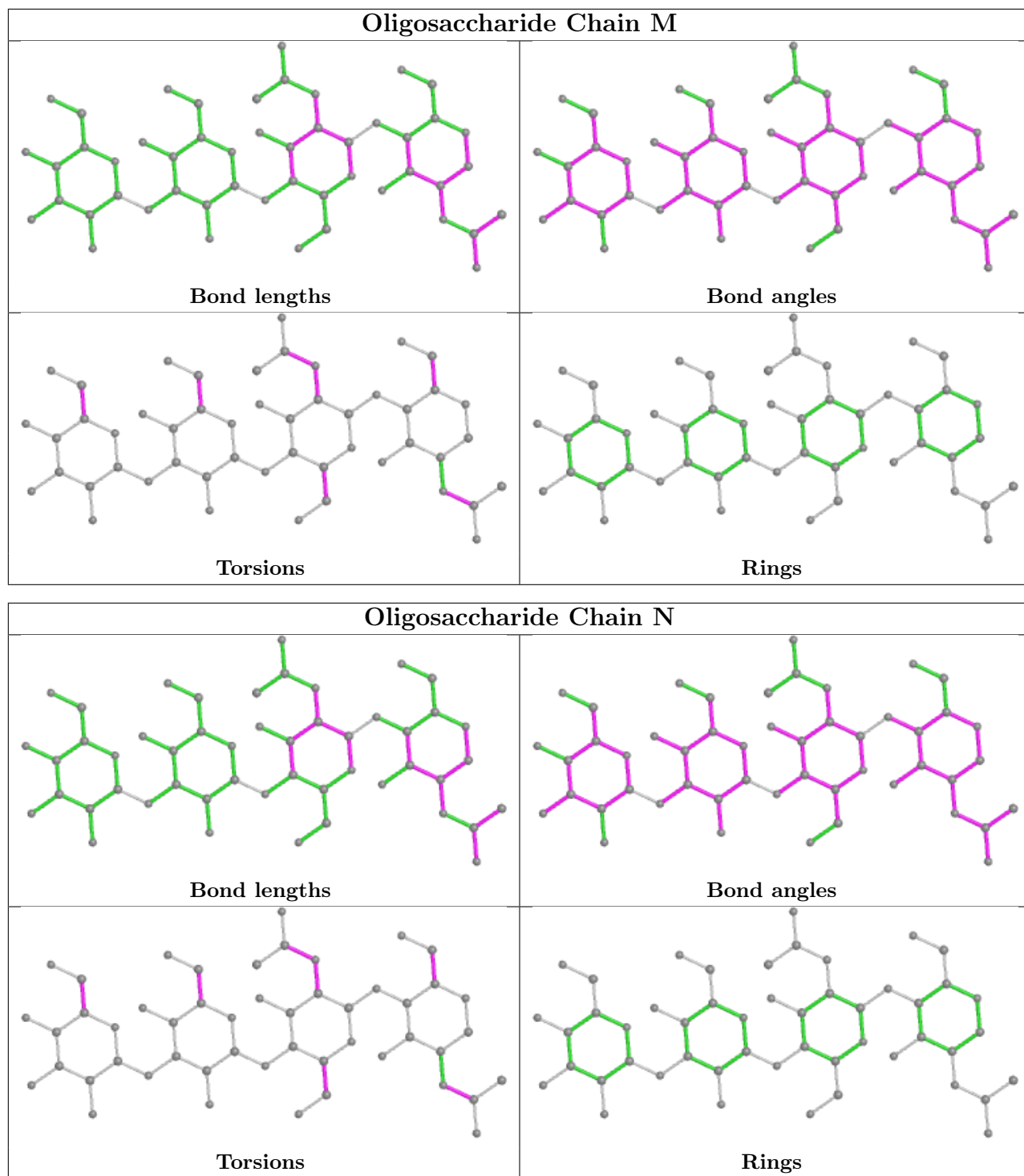
There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	1	NAG	2	0
5	N	1	NAG	2	0
5	M	2	NAG	2	0
5	N	2	NAG	1	0
5	B	1	NAG	1	0
5	M	3	BMA	1	0
5	B	2	NAG	2	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](#)

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
6	NAG	I	605	-	14,14,15	3.43	9 (64%)	17,19,21	5.50	11 (64%)
6	NAG	E	605	-	14,14,15	3.43	9 (64%)	17,19,21	5.50	11 (64%)
6	NAG	E	606	-	14,14,15	0.27	0	17,19,21	0.66	0
6	NAG	I	606	-	14,14,15	0.27	0	17,19,21	0.66	0
6	NAG	A	605	-	14,14,15	3.43	9 (64%)	17,19,21	5.50	11 (64%)
6	NAG	A	606	-	14,14,15	0.28	0	17,19,21	0.66	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
6	NAG	I	605	-	-	5/6/23/26	0/1/1/1
6	NAG	E	605	-	-	5/6/23/26	0/1/1/1
6	NAG	E	606	-	-	0/6/23/26	0/1/1/1
6	NAG	I	606	-	-	0/6/23/26	0/1/1/1
6	NAG	A	605	-	-	5/6/23/26	0/1/1/1
6	NAG	A	606	-	-	0/6/23/26	0/1/1/1

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	605	NAG	O5-C5	-6.28	1.30	1.43
6	E	605	NAG	O5-C5	-6.27	1.30	1.43
6	A	605	NAG	O5-C5	-6.25	1.30	1.43
6	I	605	NAG	C1-C2	-5.97	1.43	1.52
6	E	605	NAG	C1-C2	-5.96	1.43	1.52
6	A	605	NAG	C1-C2	-5.95	1.43	1.52
6	A	605	NAG	C4-C5	-5.80	1.40	1.53
6	E	605	NAG	C4-C5	-5.76	1.40	1.53
6	I	605	NAG	C4-C5	-5.75	1.41	1.53
6	A	605	NAG	C3-C2	-3.83	1.44	1.52
6	I	605	NAG	C3-C2	-3.82	1.44	1.52
6	E	605	NAG	C3-C2	-3.81	1.44	1.52
6	A	605	NAG	O5-C1	-3.16	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	605	NAG	O5-C1	-3.13	1.38	1.43
6	I	605	NAG	O5-C1	-3.13	1.38	1.43
6	A	605	NAG	C4-C3	-2.89	1.45	1.52
6	E	605	NAG	C4-C3	-2.88	1.45	1.52
6	I	605	NAG	C4-C3	-2.88	1.45	1.52
6	E	605	NAG	O4-C4	-2.79	1.36	1.43
6	I	605	NAG	O4-C4	-2.77	1.36	1.43
6	A	605	NAG	O4-C4	-2.75	1.36	1.43
6	I	605	NAG	C2-N2	-2.50	1.42	1.46
6	E	605	NAG	C2-N2	-2.47	1.42	1.46
6	A	605	NAG	C2-N2	-2.45	1.42	1.46
6	I	605	NAG	O3-C3	-2.30	1.37	1.43
6	A	605	NAG	O3-C3	-2.30	1.37	1.43
6	E	605	NAG	O3-C3	-2.28	1.37	1.43

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	605	NAG	O4-C4-C5	-10.82	82.43	109.30
6	E	605	NAG	O4-C4-C5	-10.81	82.47	109.30
6	A	605	NAG	O4-C4-C5	-10.80	82.47	109.30
6	A	605	NAG	C1-C2-N2	-9.37	94.49	110.49
6	E	605	NAG	C1-C2-N2	-9.37	94.49	110.49
6	I	605	NAG	C1-C2-N2	-9.36	94.49	110.49
6	I	605	NAG	O4-C4-C3	-7.86	92.19	110.35
6	A	605	NAG	O4-C4-C3	-7.85	92.20	110.35
6	E	605	NAG	O4-C4-C3	-7.84	92.21	110.35
6	I	605	NAG	O6-C6-C5	-7.10	86.94	111.29
6	E	605	NAG	O6-C6-C5	-7.08	86.99	111.29
6	A	605	NAG	O6-C6-C5	-7.08	87.01	111.29
6	A	605	NAG	O3-C3-C4	-6.62	95.05	110.35
6	E	605	NAG	O3-C3-C4	-6.61	95.06	110.35
6	I	605	NAG	O3-C3-C4	-6.61	95.07	110.35
6	I	605	NAG	C2-N2-C7	6.34	131.93	122.90
6	A	605	NAG	C2-N2-C7	6.33	131.92	122.90
6	E	605	NAG	C2-N2-C7	6.32	131.90	122.90
6	E	605	NAG	O3-C3-C2	-6.13	96.78	109.47
6	I	605	NAG	O3-C3-C2	-6.12	96.80	109.47
6	A	605	NAG	O3-C3-C2	-6.12	96.81	109.47
6	E	605	NAG	O5-C1-C2	-5.30	102.92	111.29
6	A	605	NAG	O5-C1-C2	-5.29	102.93	111.29
6	I	605	NAG	O5-C1-C2	-5.29	102.94	111.29

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	605	NAG	C4-C3-C2	-4.88	103.87	111.02
6	E	605	NAG	C4-C3-C2	-4.87	103.88	111.02
6	I	605	NAG	C4-C3-C2	-4.87	103.89	111.02
6	E	605	NAG	C8-C7-N2	-2.92	111.16	116.10
6	A	605	NAG	C8-C7-N2	-2.90	111.19	116.10
6	I	605	NAG	C8-C7-N2	-2.89	111.20	116.10
6	E	605	NAG	O7-C7-C8	2.75	127.16	122.06
6	A	605	NAG	O7-C7-C8	2.74	127.15	122.06
6	I	605	NAG	O7-C7-C8	2.74	127.15	122.06

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	605	NAG	C3-C2-N2-C7
6	A	605	NAG	C8-C7-N2-C2
6	A	605	NAG	O7-C7-N2-C2
6	E	605	NAG	C3-C2-N2-C7
6	E	605	NAG	C8-C7-N2-C2
6	E	605	NAG	O7-C7-N2-C2
6	I	605	NAG	C3-C2-N2-C7
6	I	605	NAG	C8-C7-N2-C2
6	I	605	NAG	O7-C7-N2-C2
6	A	605	NAG	O5-C5-C6-O6
6	E	605	NAG	O5-C5-C6-O6
6	I	605	NAG	O5-C5-C6-O6
6	A	605	NAG	C4-C5-C6-O6
6	E	605	NAG	C4-C5-C6-O6
6	I	605	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	I	605	NAG	9	0
6	E	605	NAG	9	0
6	A	605	NAG	9	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

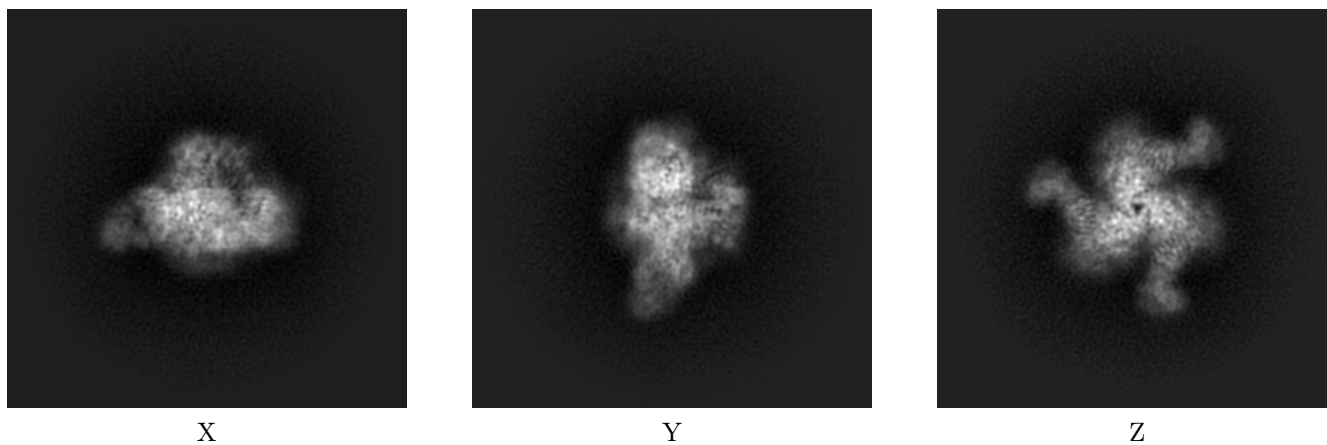
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20735. 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](#)

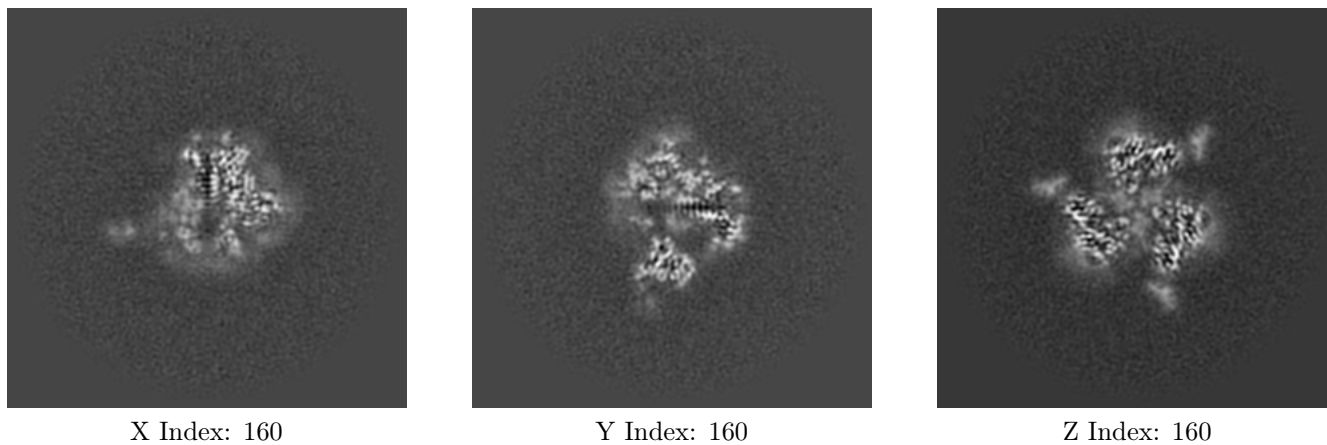
#### 6.1.1 Primary map



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

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

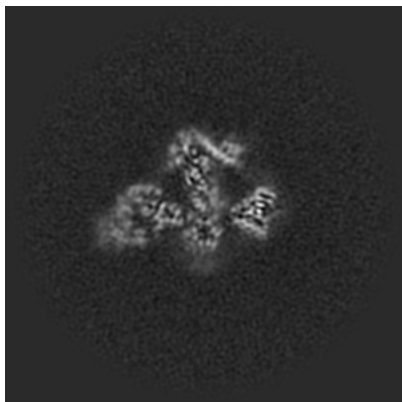
#### 6.2.1 Primary map



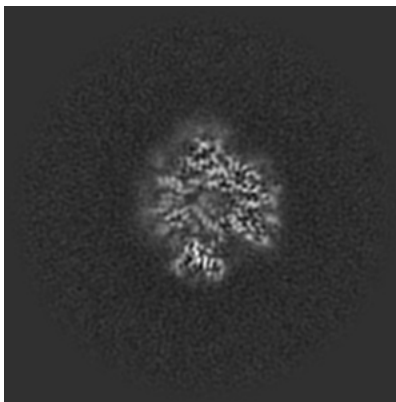
The images above show central slices of the map in three orthogonal directions.

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

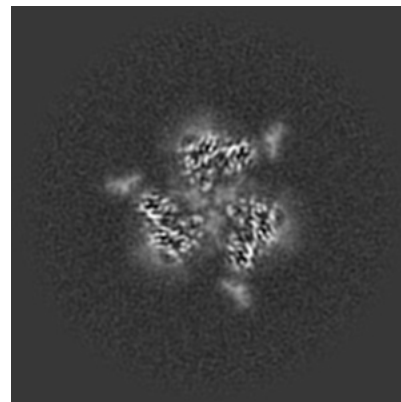
### 6.3.1 Primary map



X Index: 175



Y Index: 151

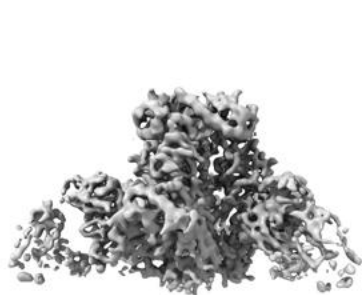


Z Index: 160

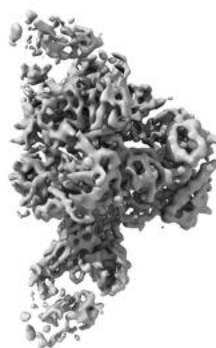
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

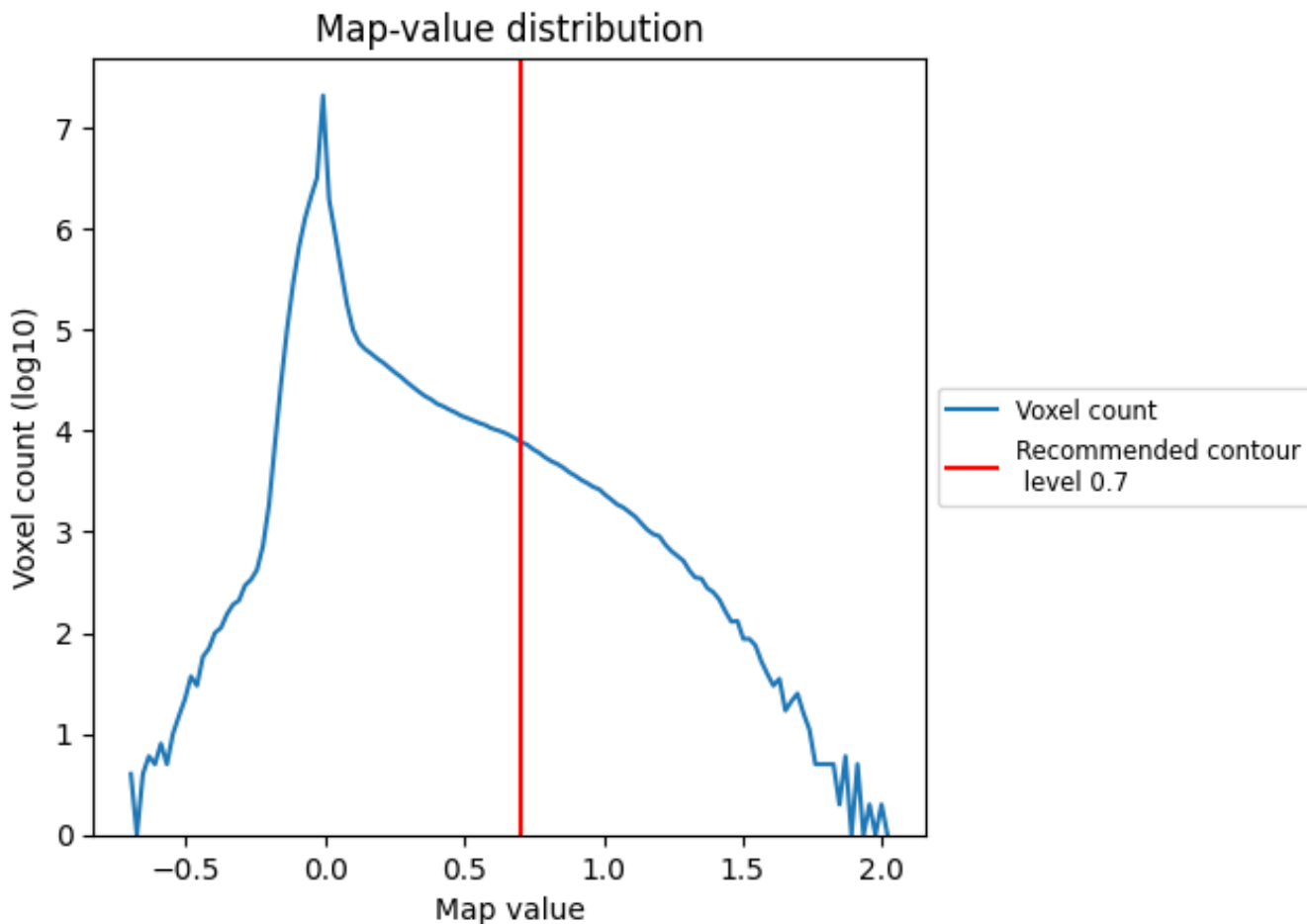
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

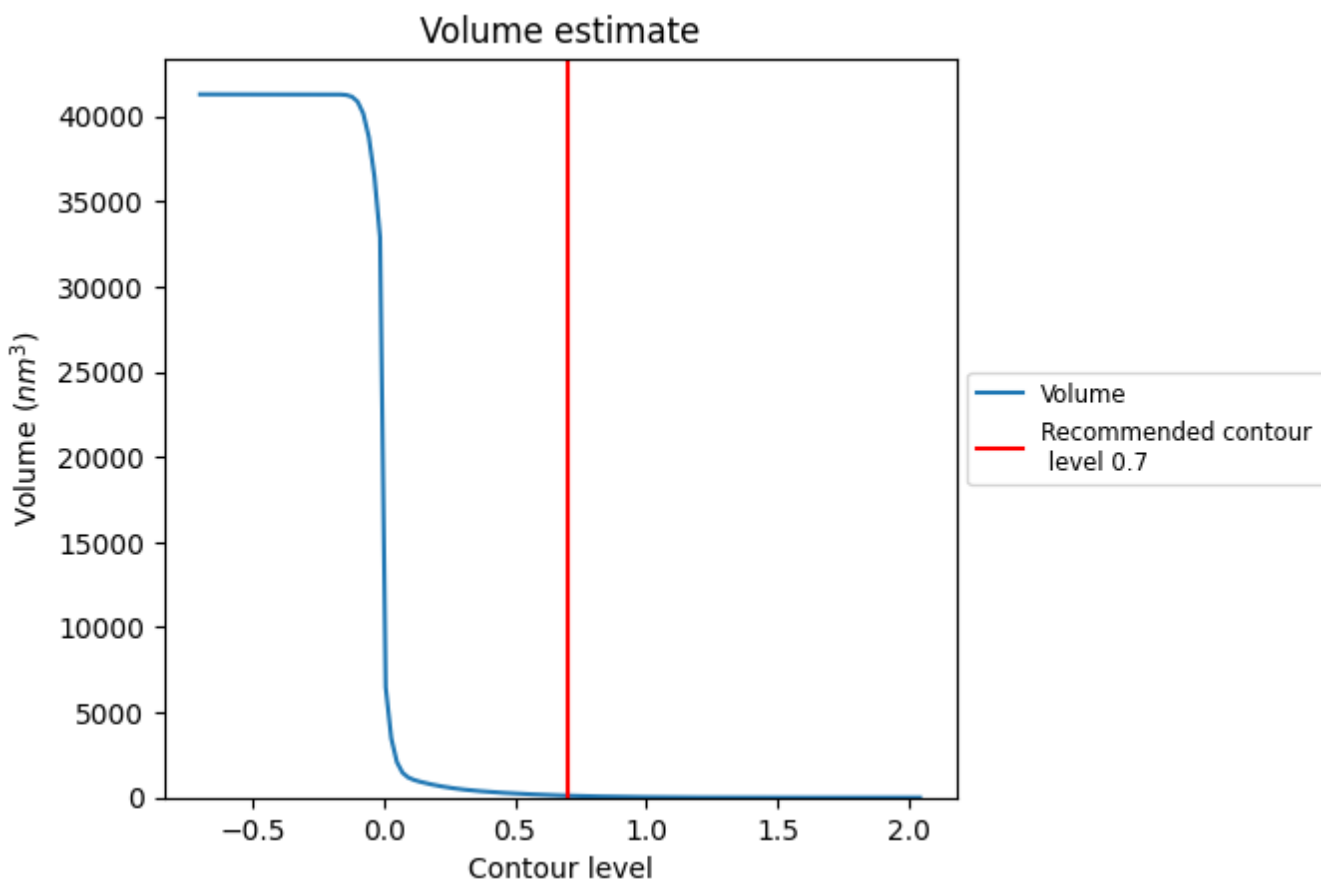
This section contains the results of statistical analysis of the map.

### 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](#)

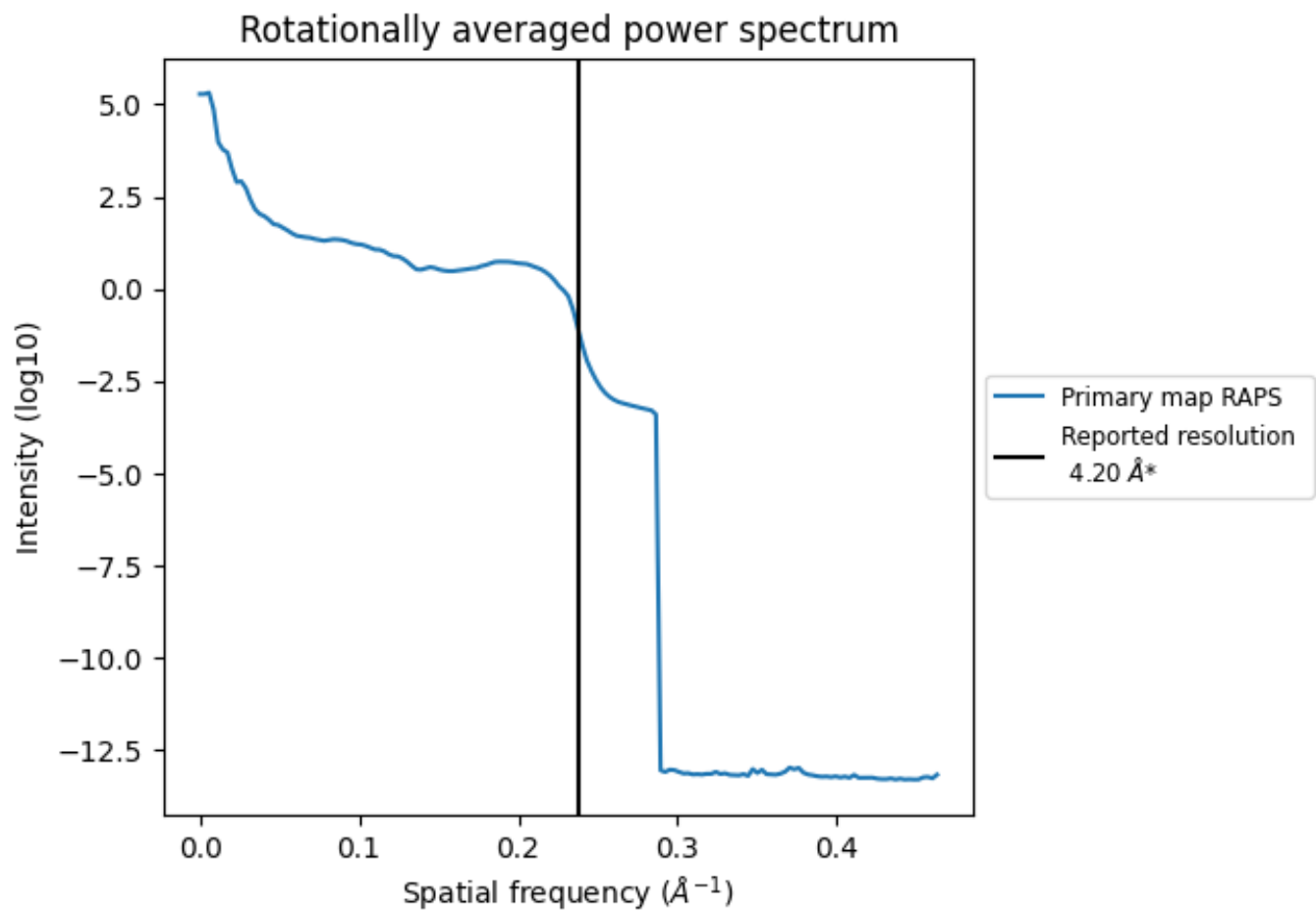


The volume at the recommended contour level is  $111 \text{ nm}^3$ ; this corresponds to an approximate mass of 100 kDa.

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.238 Å<sup>-1</sup>

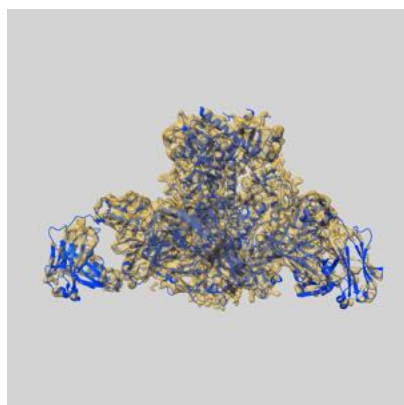
## 8 Fourier-Shell correlation

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

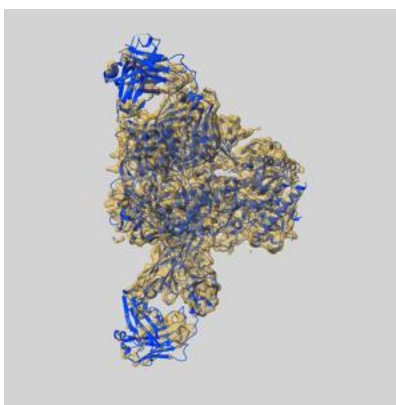
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20735 and PDB model 6UDA. Per-residue inclusion information can be found in section 3 on page 10.

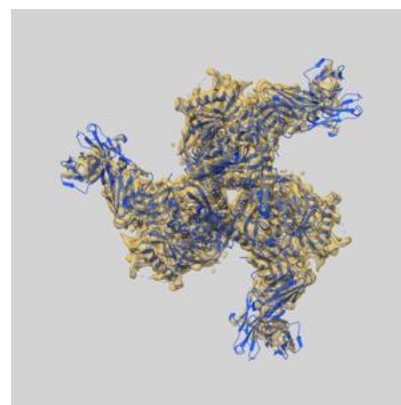
### 9.1 Map-model overlay [i](#)



X



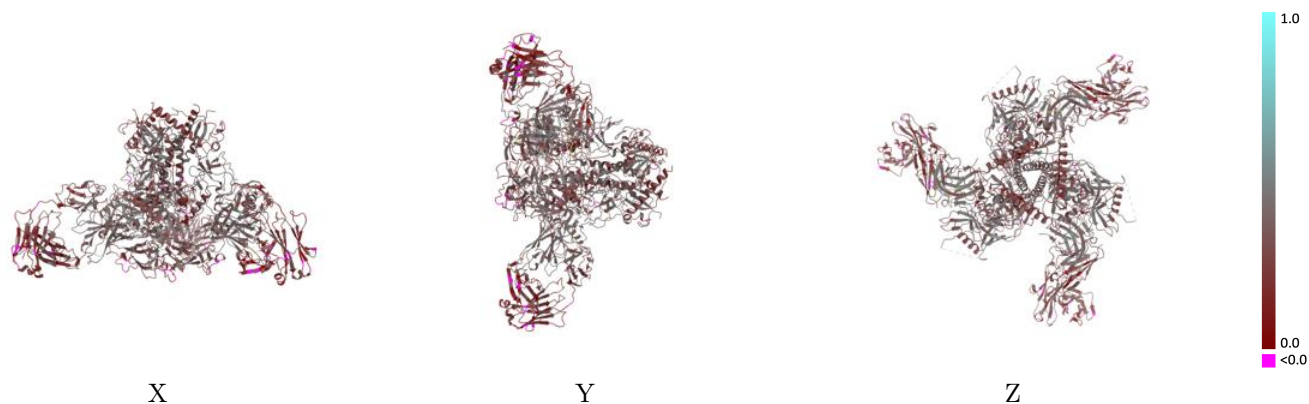
Y



Z

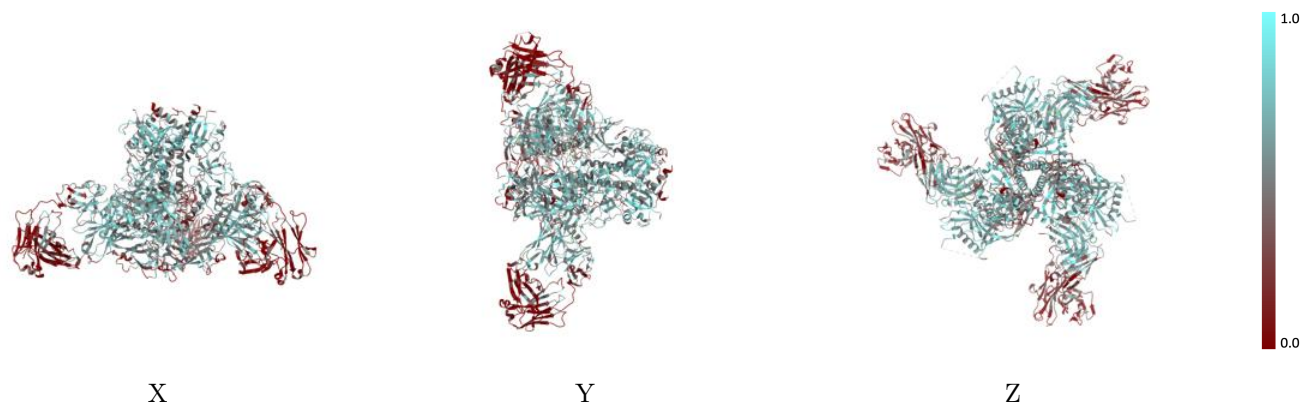
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



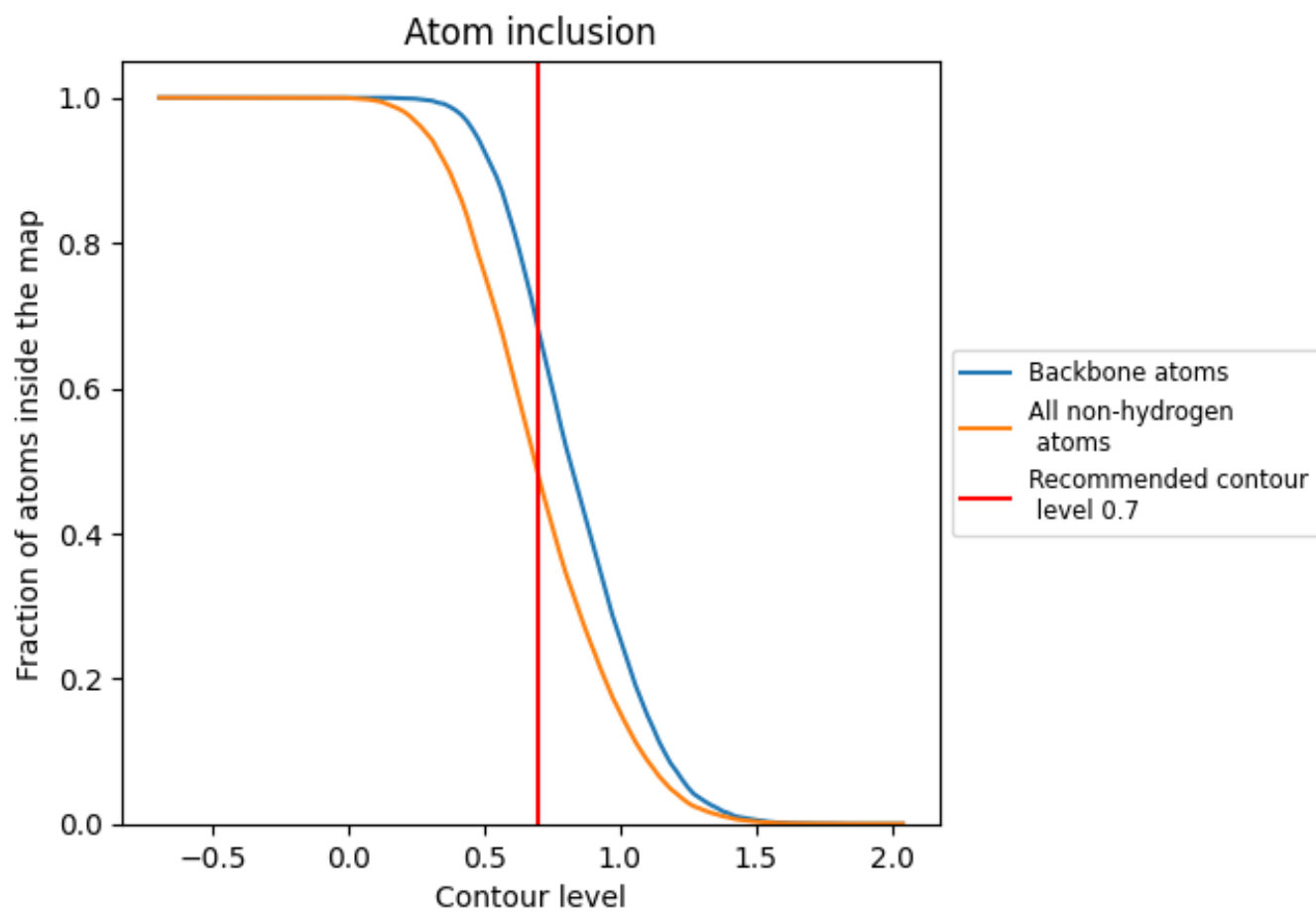
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 68% of all backbone atoms, 48% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4773	 0.3250
A	 0.5463	 0.3510
B	 0.3800	 0.4590
C	 0.4079	 0.3210
D	 0.3344	 0.2720
E	 0.5454	 0.3500
F	 0.5759	 0.3210
G	 0.4110	 0.3200
H	 0.3312	 0.2720
I	 0.5502	 0.3510
J	 0.5780	 0.3200
K	 0.4104	 0.3190
L	 0.3294	 0.2720
M	 0.4000	 0.4820
N	 0.4000	 0.4740
Z	 0.5770	 0.3190

