wwPDB EM Validation Summary Report

Nov 14, 2022 – 09:37 PM EST

PDB ID	:	7KFE
EMDB ID	:	EMD-22851
Title	:	Bundibugyo virus GP (mucin deleted) bound to antibody Fab BDBV-329
Authors	:	Murin, C.D.; Ward, A.B.
Deposited on	:	2020-10-13
Resolution	:	6.60 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

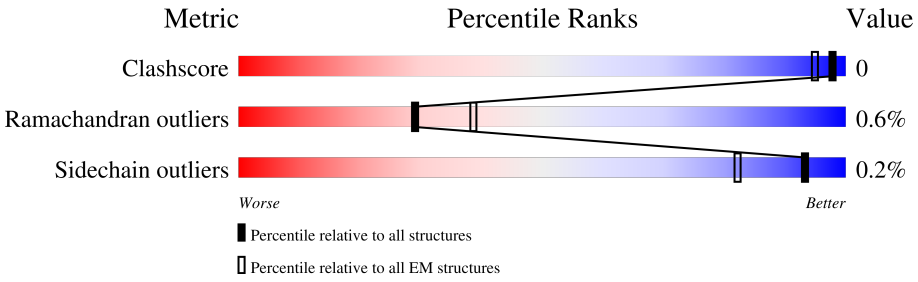
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 6.60 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	G	244	22% 54% · 43%
1	H	244	12% 56% · 43%
2	I	215	26% 47% · 50%
2	J	215	21% 47% · 50%
3	A	343	· 46% · 50%
3	B	343	· 58% 6% 36%
3	C	343	· 60% · 36%
4	D	177	8% 62% · 35%

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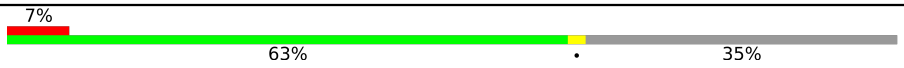
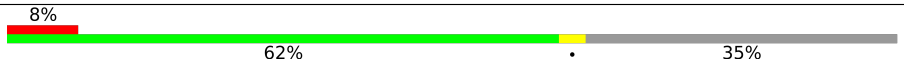
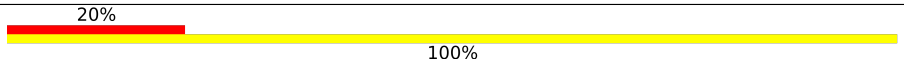
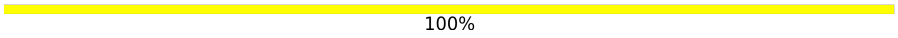
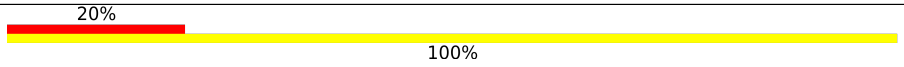
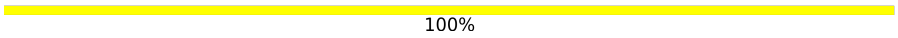
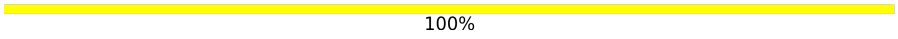
Mol	Chain	Length	Quality of chain
4	E	177	
4	F	177	
5	K	5	
5	M	5	
5	O	5	
6	L	2	
6	N	2	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11538 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 Antibody BDBV-329 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	H	140	Total	C	N	O	S	0	0
			1073	683	186	199	5		
1	G	140	Total	C	N	O	S	0	0
			1073	683	186	199	5		

- Molecule 2 is a protein called Antibody BDBV-329 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	J	108	Total	C	N	O	S	0	0
			810	507	138	162	3		
2	I	108	Total	C	N	O	S	0	0
			810	507	138	162	3		

- Molecule 3 is a protein called Spike glycoprotein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	170	Total	C	N	O	S	0	0
			1313	836	223	249	5		
3	B	219	Total	C	N	O	S	0	0
			1728	1108	292	322	6		
3	C	219	Total	C	N	O	S	0	0
			1728	1108	292	322	6		

There are 93 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	313	ILE	-	expression tag	UNP A0A510C2V9
A	314	ASP	-	expression tag	UNP A0A510C2V9
A	315	ILE	-	expression tag	UNP A0A510C2V9
A	316	SER	-	expression tag	UNP A0A510C2V9
A	317	GLU	-	expression tag	UNP A0A510C2V9
A	318	SER	-	expression tag	UNP A0A510C2V9
A	319	THR	-	expression tag	UNP A0A510C2V9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	320	GLU	-	expression tag	UNP A0A510C2V9
A	321	PRO	-	expression tag	UNP A0A510C2V9
A	322	GLY	-	expression tag	UNP A0A510C2V9
A	323	PRO	-	expression tag	UNP A0A510C2V9
A	324	LEU	-	expression tag	UNP A0A510C2V9
A	325	THR	-	expression tag	UNP A0A510C2V9
A	326	ASN	-	expression tag	UNP A0A510C2V9
A	327	THR	-	expression tag	UNP A0A510C2V9
A	328	THR	-	expression tag	UNP A0A510C2V9
A	329	ARG	-	expression tag	UNP A0A510C2V9
A	330	GLY	-	expression tag	UNP A0A510C2V9
A	331	ALA	-	expression tag	UNP A0A510C2V9
A	332	ALA	-	expression tag	UNP A0A510C2V9
A	333	ASN	-	expression tag	UNP A0A510C2V9
A	334	LEU	-	expression tag	UNP A0A510C2V9
A	335	LEU	-	expression tag	UNP A0A510C2V9
A	336	THR	-	expression tag	UNP A0A510C2V9
A	337	GLY	-	expression tag	UNP A0A510C2V9
A	338	SER	-	expression tag	UNP A0A510C2V9
A	339	ARG	-	expression tag	UNP A0A510C2V9
A	340	ARG	-	expression tag	UNP A0A510C2V9
A	341	THR	-	expression tag	UNP A0A510C2V9
A	342	ARG	-	expression tag	UNP A0A510C2V9
A	343	ARG	-	expression tag	UNP A0A510C2V9
B	313	ILE	-	expression tag	UNP A0A510C2V9
B	314	ASP	-	expression tag	UNP A0A510C2V9
B	315	ILE	-	expression tag	UNP A0A510C2V9
B	316	SER	-	expression tag	UNP A0A510C2V9
B	317	GLU	-	expression tag	UNP A0A510C2V9
B	318	SER	-	expression tag	UNP A0A510C2V9
B	319	THR	-	expression tag	UNP A0A510C2V9
B	320	GLU	-	expression tag	UNP A0A510C2V9
B	321	PRO	-	expression tag	UNP A0A510C2V9
B	322	GLY	-	expression tag	UNP A0A510C2V9
B	323	PRO	-	expression tag	UNP A0A510C2V9
B	324	LEU	-	expression tag	UNP A0A510C2V9
B	325	THR	-	expression tag	UNP A0A510C2V9
B	326	ASN	-	expression tag	UNP A0A510C2V9
B	327	THR	-	expression tag	UNP A0A510C2V9
B	328	THR	-	expression tag	UNP A0A510C2V9
B	329	ARG	-	expression tag	UNP A0A510C2V9
B	330	GLY	-	expression tag	UNP A0A510C2V9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	331	ALA	-	expression tag	UNP A0A510C2V9
B	332	ALA	-	expression tag	UNP A0A510C2V9
B	333	ASN	-	expression tag	UNP A0A510C2V9
B	334	LEU	-	expression tag	UNP A0A510C2V9
B	335	LEU	-	expression tag	UNP A0A510C2V9
B	336	THR	-	expression tag	UNP A0A510C2V9
B	337	GLY	-	expression tag	UNP A0A510C2V9
B	338	SER	-	expression tag	UNP A0A510C2V9
B	339	ARG	-	expression tag	UNP A0A510C2V9
B	340	ARG	-	expression tag	UNP A0A510C2V9
B	341	THR	-	expression tag	UNP A0A510C2V9
B	342	ARG	-	expression tag	UNP A0A510C2V9
B	343	ARG	-	expression tag	UNP A0A510C2V9
C	313	ILE	-	expression tag	UNP A0A510C2V9
C	314	ASP	-	expression tag	UNP A0A510C2V9
C	315	ILE	-	expression tag	UNP A0A510C2V9
C	316	SER	-	expression tag	UNP A0A510C2V9
C	317	GLU	-	expression tag	UNP A0A510C2V9
C	318	SER	-	expression tag	UNP A0A510C2V9
C	319	THR	-	expression tag	UNP A0A510C2V9
C	320	GLU	-	expression tag	UNP A0A510C2V9
C	321	PRO	-	expression tag	UNP A0A510C2V9
C	322	GLY	-	expression tag	UNP A0A510C2V9
C	323	PRO	-	expression tag	UNP A0A510C2V9
C	324	LEU	-	expression tag	UNP A0A510C2V9
C	325	THR	-	expression tag	UNP A0A510C2V9
C	326	ASN	-	expression tag	UNP A0A510C2V9
C	327	THR	-	expression tag	UNP A0A510C2V9
C	328	THR	-	expression tag	UNP A0A510C2V9
C	329	ARG	-	expression tag	UNP A0A510C2V9
C	330	GLY	-	expression tag	UNP A0A510C2V9
C	331	ALA	-	expression tag	UNP A0A510C2V9
C	332	ALA	-	expression tag	UNP A0A510C2V9
C	333	ASN	-	expression tag	UNP A0A510C2V9
C	334	LEU	-	expression tag	UNP A0A510C2V9
C	335	LEU	-	expression tag	UNP A0A510C2V9
C	336	THR	-	expression tag	UNP A0A510C2V9
C	337	GLY	-	expression tag	UNP A0A510C2V9
C	338	SER	-	expression tag	UNP A0A510C2V9
C	339	ARG	-	expression tag	UNP A0A510C2V9
C	340	ARG	-	expression tag	UNP A0A510C2V9
C	341	THR	-	expression tag	UNP A0A510C2V9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	342	ARG	-	expression tag	UNP A0A510C2V9
C	343	ARG	-	expression tag	UNP A0A510C2V9

- Molecule 4 is a protein called Envelope glycoprotein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	115	Total	C	N	O	S	0	0
			912	579	159	168	6		
4	E	115	Total	C	N	O	S	0	0
			912	579	159	168	6		
4	F	115	Total	C	N	O	S	0	0
			912	579	159	168	6		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	641	VAL	-	expression tag	UNP B8XCN0
D	642	GLU	-	expression tag	UNP B8XCN0
D	643	VAL	-	expression tag	UNP B8XCN0
D	644	ASP	-	expression tag	UNP B8XCN0
D	645	ASP	-	expression tag	UNP B8XCN0
D	646	ASP	-	expression tag	UNP B8XCN0
D	647	ASP	-	expression tag	UNP B8XCN0
D	648	LYS	-	expression tag	UNP B8XCN0
D	649	ALA	-	expression tag	UNP B8XCN0
D	650	GLY	-	expression tag	UNP B8XCN0
D	651	TRP	-	expression tag	UNP B8XCN0
D	652	SER	-	expression tag	UNP B8XCN0
D	653	HIS	-	expression tag	UNP B8XCN0
D	654	PRO	-	expression tag	UNP B8XCN0
D	655	GLN	-	expression tag	UNP B8XCN0
D	656	PHE	-	expression tag	UNP B8XCN0
D	657	GLU	-	expression tag	UNP B8XCN0
D	658	LYS	-	expression tag	UNP B8XCN0
D	659	GLY	-	expression tag	UNP B8XCN0
D	660	GLY	-	expression tag	UNP B8XCN0
D	661	GLY	-	expression tag	UNP B8XCN0
D	662	SER	-	expression tag	UNP B8XCN0
D	663	GLY	-	expression tag	UNP B8XCN0
D	664	GLY	-	expression tag	UNP B8XCN0
D	665	GLY	-	expression tag	UNP B8XCN0
D	666	SER	-	expression tag	UNP B8XCN0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	667	GLY	-	expression tag	UNP B8XCN0
D	668	GLY	-	expression tag	UNP B8XCN0
D	669	GLY	-	expression tag	UNP B8XCN0
D	670	SER	-	expression tag	UNP B8XCN0
D	671	TRP	-	expression tag	UNP B8XCN0
D	672	SER	-	expression tag	UNP B8XCN0
D	673	HIS	-	expression tag	UNP B8XCN0
D	674	PRO	-	expression tag	UNP B8XCN0
D	675	GLN	-	expression tag	UNP B8XCN0
D	676	PHE	-	expression tag	UNP B8XCN0
D	677	GLU	-	expression tag	UNP B8XCN0
D	678	LYS	-	expression tag	UNP B8XCN0
E	641	VAL	-	expression tag	UNP B8XCN0
E	642	GLU	-	expression tag	UNP B8XCN0
E	643	VAL	-	expression tag	UNP B8XCN0
E	644	ASP	-	expression tag	UNP B8XCN0
E	645	ASP	-	expression tag	UNP B8XCN0
E	646	ASP	-	expression tag	UNP B8XCN0
E	647	ASP	-	expression tag	UNP B8XCN0
E	648	LYS	-	expression tag	UNP B8XCN0
E	649	ALA	-	expression tag	UNP B8XCN0
E	650	GLY	-	expression tag	UNP B8XCN0
E	651	TRP	-	expression tag	UNP B8XCN0
E	652	SER	-	expression tag	UNP B8XCN0
E	653	HIS	-	expression tag	UNP B8XCN0
E	654	PRO	-	expression tag	UNP B8XCN0
E	655	GLN	-	expression tag	UNP B8XCN0
E	656	PHE	-	expression tag	UNP B8XCN0
E	657	GLU	-	expression tag	UNP B8XCN0
E	658	LYS	-	expression tag	UNP B8XCN0
E	659	GLY	-	expression tag	UNP B8XCN0
E	660	GLY	-	expression tag	UNP B8XCN0
E	661	GLY	-	expression tag	UNP B8XCN0
E	662	SER	-	expression tag	UNP B8XCN0
E	663	GLY	-	expression tag	UNP B8XCN0
E	664	GLY	-	expression tag	UNP B8XCN0
E	665	GLY	-	expression tag	UNP B8XCN0
E	666	SER	-	expression tag	UNP B8XCN0
E	667	GLY	-	expression tag	UNP B8XCN0
E	668	GLY	-	expression tag	UNP B8XCN0
E	669	GLY	-	expression tag	UNP B8XCN0
E	670	SER	-	expression tag	UNP B8XCN0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	671	TRP	-	expression tag	UNP B8XCN0
E	672	SER	-	expression tag	UNP B8XCN0
E	673	HIS	-	expression tag	UNP B8XCN0
E	674	PRO	-	expression tag	UNP B8XCN0
E	675	GLN	-	expression tag	UNP B8XCN0
E	676	PHE	-	expression tag	UNP B8XCN0
E	677	GLU	-	expression tag	UNP B8XCN0
E	678	LYS	-	expression tag	UNP B8XCN0
F	641	VAL	-	expression tag	UNP B8XCN0
F	642	GLU	-	expression tag	UNP B8XCN0
F	643	VAL	-	expression tag	UNP B8XCN0
F	644	ASP	-	expression tag	UNP B8XCN0
F	645	ASP	-	expression tag	UNP B8XCN0
F	646	ASP	-	expression tag	UNP B8XCN0
F	647	ASP	-	expression tag	UNP B8XCN0
F	648	LYS	-	expression tag	UNP B8XCN0
F	649	ALA	-	expression tag	UNP B8XCN0
F	650	GLY	-	expression tag	UNP B8XCN0
F	651	TRP	-	expression tag	UNP B8XCN0
F	652	SER	-	expression tag	UNP B8XCN0
F	653	HIS	-	expression tag	UNP B8XCN0
F	654	PRO	-	expression tag	UNP B8XCN0
F	655	GLN	-	expression tag	UNP B8XCN0
F	656	PHE	-	expression tag	UNP B8XCN0
F	657	GLU	-	expression tag	UNP B8XCN0
F	658	LYS	-	expression tag	UNP B8XCN0
F	659	GLY	-	expression tag	UNP B8XCN0
F	660	GLY	-	expression tag	UNP B8XCN0
F	661	GLY	-	expression tag	UNP B8XCN0
F	662	SER	-	expression tag	UNP B8XCN0
F	663	GLY	-	expression tag	UNP B8XCN0
F	664	GLY	-	expression tag	UNP B8XCN0
F	665	GLY	-	expression tag	UNP B8XCN0
F	666	SER	-	expression tag	UNP B8XCN0
F	667	GLY	-	expression tag	UNP B8XCN0
F	668	GLY	-	expression tag	UNP B8XCN0
F	669	GLY	-	expression tag	UNP B8XCN0
F	670	SER	-	expression tag	UNP B8XCN0
F	671	TRP	-	expression tag	UNP B8XCN0
F	672	SER	-	expression tag	UNP B8XCN0
F	673	HIS	-	expression tag	UNP B8XCN0
F	674	PRO	-	expression tag	UNP B8XCN0

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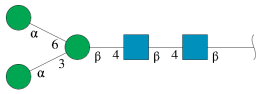
Chain	Residue	Modelled	Actual	Comment	Reference
F	675	GLN	-	expression tag	UNP B8XCN0
F	676	PHE	-	expression tag	UNP B8XCN0
F	677	GLU	-	expression tag	UNP B8XCN0
F	678	LYS	-	expression tag	UNP B8XCN0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

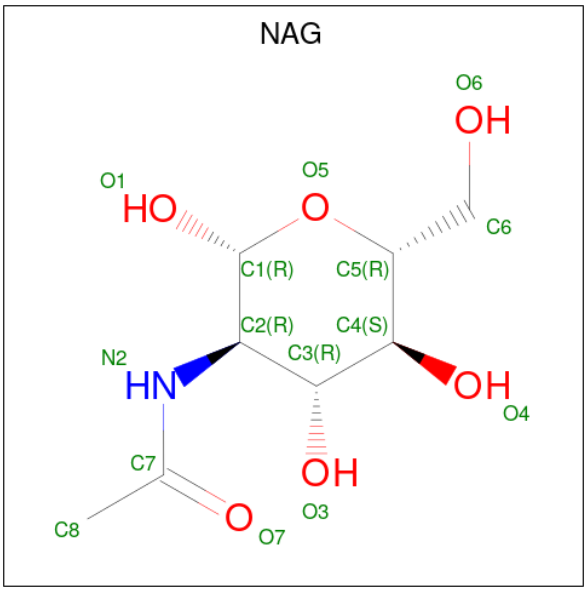


Mol	Chain	Residues	Atoms				AltConf	Trace
5	K	5	Total	C	N	O	0	0
			61	34	2	25		
5	M	5	Total	C	N	O	0	0
			61	34	2	25		
5	O	5	Total	C	N	O	0	0
			61	34	2	25		

- 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	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		

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



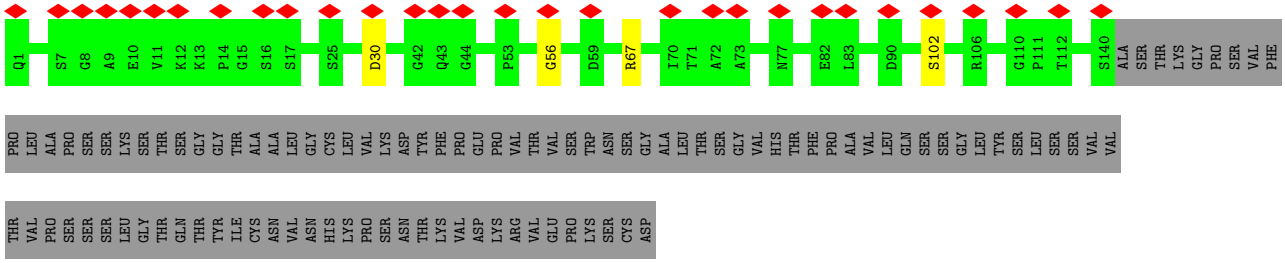
Mol	Chain	Residues	Atoms				AltConf
7	B	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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.

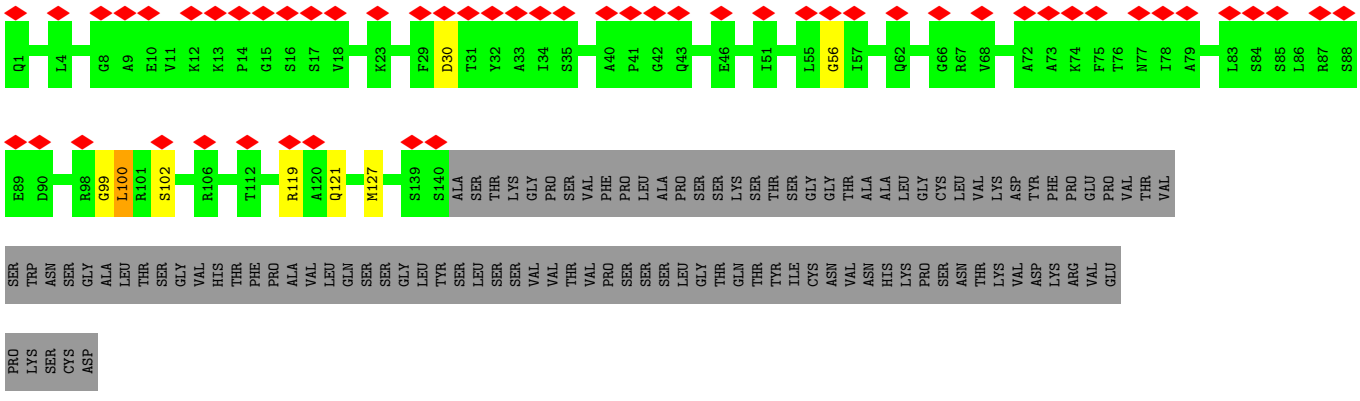
• Molecule 1: Antibody BDBV-329 heavy chain

Chain H:



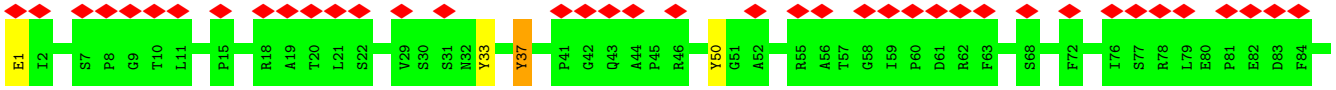
• Molecule 1: Antibody BDBV-329 heavy chain

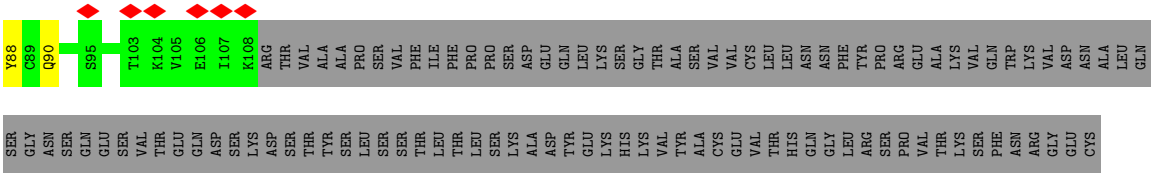
Chain G:



• Molecule 2: Antibody BDBV-329 light chain

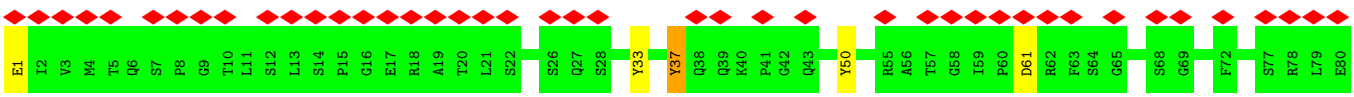
Chain J:

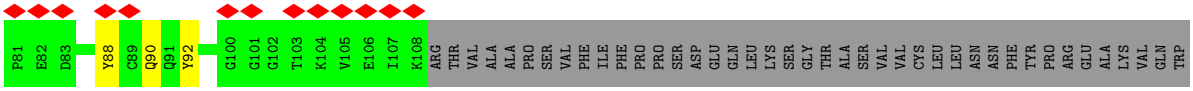




• Molecule 2: Antibody BDBV-329 light chain

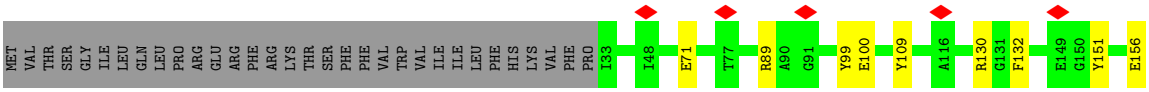
Chain I:

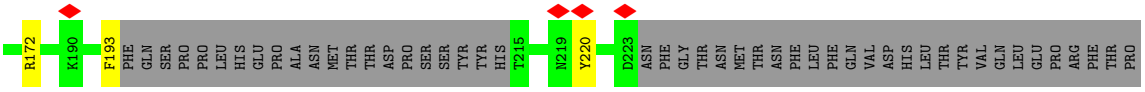




• Molecule 3: Spike glycoprotein 1

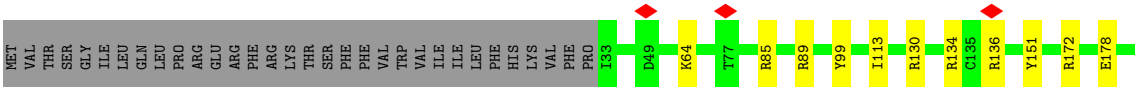
Chain A:

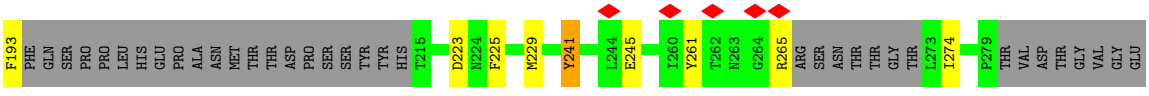




• Molecule 3: Spike glycoprotein 1

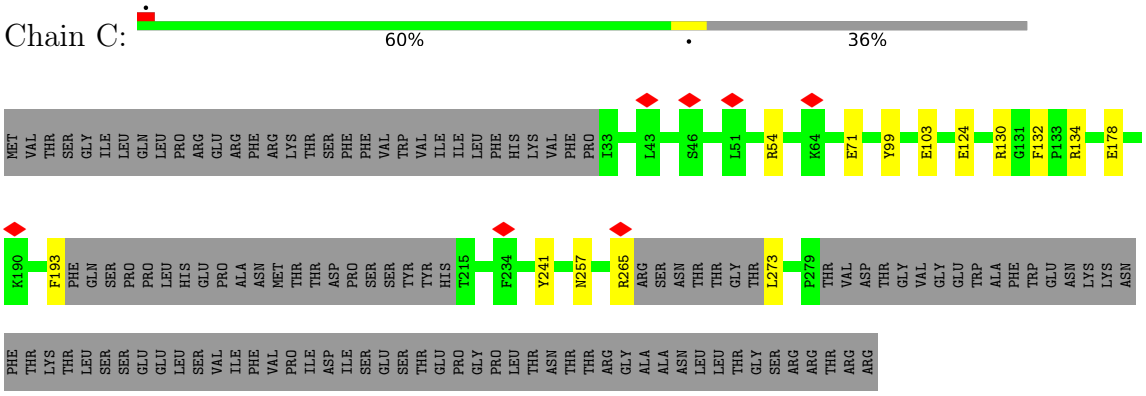
Chain B:





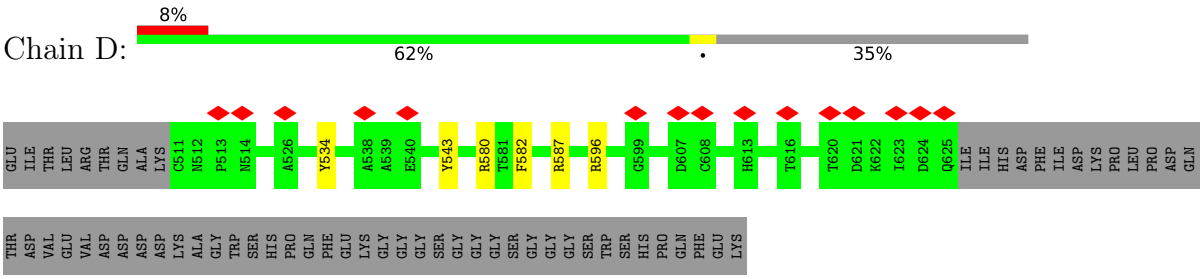
• Molecule 3: Spike glycoprotein 1

Chain C:



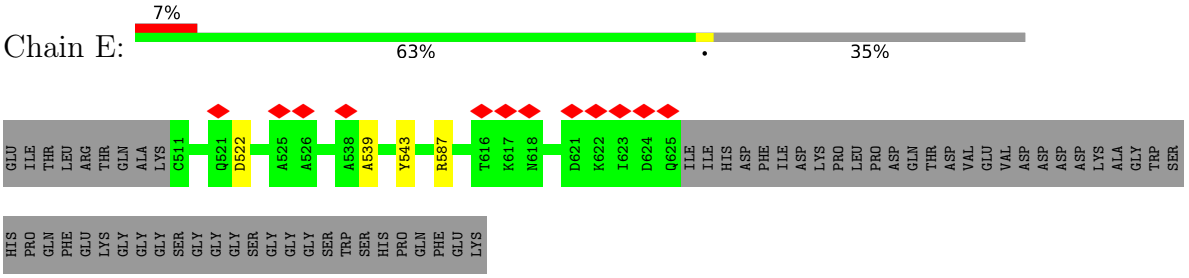
• Molecule 4: Envelope glycoprotein 2

Chain D:



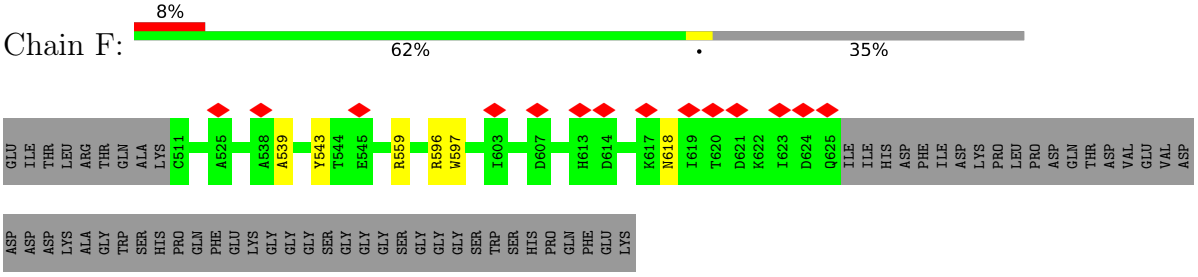
• Molecule 4: Envelope glycoprotein 2

Chain E:



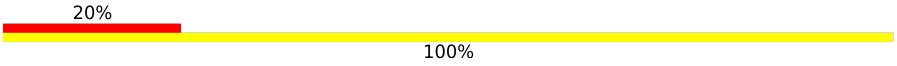
• Molecule 4: Envelope glycoprotein 2

Chain F:



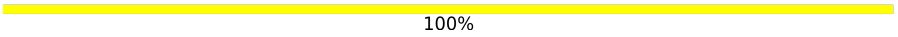
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



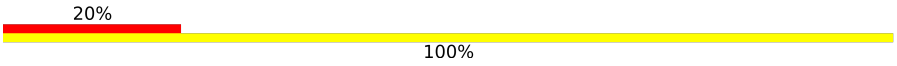
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



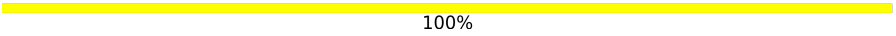
• Molecule 5: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



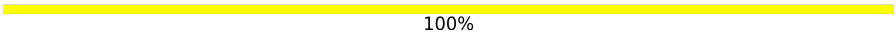
• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



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

Chain N:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45640	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.116	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0289	Depositor
Map size (Å)	331.19998, 331.19998, 331.19998	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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, BMA, MAN

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	G	1.02	0/1100	1.03	2/1494 (0.1%)
1	H	1.02	0/1100	1.06	3/1494 (0.2%)
2	I	1.11	5/829 (0.6%)	0.99	2/1124 (0.2%)
2	J	1.10	4/829 (0.5%)	0.99	1/1124 (0.1%)
3	A	1.22	10/1343 (0.7%)	1.07	9/1824 (0.5%)
3	B	1.24	11/1770 (0.6%)	1.10	12/2407 (0.5%)
3	C	1.23	16/1770 (0.9%)	0.99	3/2407 (0.1%)
4	D	1.06	0/935	0.99	5/1274 (0.4%)
4	E	1.08	2/935 (0.2%)	0.96	2/1274 (0.2%)
4	F	1.13	5/935 (0.5%)	0.98	3/1274 (0.2%)
All	All	1.14	53/11546 (0.5%)	1.03	42/15696 (0.3%)

The worst 5 of 53 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	178	GLU	CG-CD	-8.28	1.39	1.51
3	A	193	PHE	CG-CD1	7.59	1.50	1.38
3	B	193	PHE	CG-CD2	7.18	1.49	1.38
3	C	193	PHE	CG-CD1	7.14	1.49	1.38
3	B	193	PHE	CG-CD1	6.96	1.49	1.38

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	67	ARG	NE-CZ-NH2	-11.50	114.55	120.30
3	B	151	TYR	CB-CG-CD1	-10.27	114.84	121.00
3	A	151	TYR	CB-CG-CD1	-9.97	115.02	121.00
4	F	543	TYR	CB-CG-CD1	-9.71	115.17	121.00
3	B	99	TYR	CB-CG-CD1	-8.76	115.75	121.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1073	0	1059	3	0
1	H	1073	0	1059	0	0
2	I	810	0	785	2	0
2	J	810	0	785	1	0
3	A	1313	0	1289	0	0
3	B	1728	0	1691	3	0
3	C	1728	0	1691	0	0
4	D	912	0	876	0	0
4	E	912	0	876	1	0
4	F	912	0	876	0	0
5	K	61	0	52	0	0
5	M	61	0	52	0	0
5	O	61	0	52	0	0
6	L	28	0	24	0	0
6	N	28	0	25	0	0
7	B	14	0	13	0	0
7	C	14	0	13	0	0
All	All	11538	0	11218	9	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 0.

The worst 5 of 9 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:G:99:GLY:O	1:G:100:LEU:HB3	2.13	0.49
2:J:37:TYR:CZ	2:J:88:TYR:HB2	2.48	0.48
3:B:113:ILE:HG23	3:B:225:PHE:CZ	2.48	0.48
2:I:37:TYR:CZ	2:I:88:TYR:HB2	2.50	0.47
2:I:61:ASP:OD1	2:I:61:ASP:N	2.48	0.46

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	G	138/244 (57%)	130 (94%)	5 (4%)	3 (2%)	6 35
1	H	138/244 (57%)	129 (94%)	7 (5%)	2 (1%)	11 46
2	I	106/215 (49%)	105 (99%)	1 (1%)	0	100 100
2	J	106/215 (49%)	105 (99%)	1 (1%)	0	100 100
3	A	166/343 (48%)	160 (96%)	6 (4%)	0	100 100
3	B	213/343 (62%)	208 (98%)	5 (2%)	0	100 100
3	C	213/343 (62%)	207 (97%)	6 (3%)	0	100 100
4	D	113/177 (64%)	106 (94%)	6 (5%)	1 (1%)	17 57
4	E	113/177 (64%)	108 (96%)	4 (4%)	1 (1%)	17 57
4	F	113/177 (64%)	107 (95%)	5 (4%)	1 (1%)	17 57
All	All	1419/2478 (57%)	1365 (96%)	46 (3%)	8 (1%)	29 66

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	102	SER
1	G	102	SER
1	H	30	ASP
1	G	30	ASP
1	G	100	LEU

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	G	111/201 (55%)	111 (100%)	0	100 100
1	H	111/201 (55%)	111 (100%)	0	100 100
2	I	88/184 (48%)	88 (100%)	0	100 100
2	J	88/184 (48%)	88 (100%)	0	100 100
3	A	143/303 (47%)	143 (100%)	0	100 100
3	B	190/303 (63%)	189 (100%)	1 (0%)	88 93
3	C	190/303 (63%)	189 (100%)	1 (0%)	88 93
4	D	96/146 (66%)	96 (100%)	0	100 100
4	E	96/146 (66%)	96 (100%)	0	100 100
4	F	96/146 (66%)	95 (99%)	1 (1%)	76 86
All	All	1209/2117 (57%)	1206 (100%)	3 (0%)	93 96

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

Mol	Chain	Res	Type
3	B	229	MET
3	C	257	ASN
4	F	618	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	6	GLN

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)

19 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	K	1	4,5	14,14,15	2.18	5 (35%)	17,19,21	1.39	3 (17%)
5	NAG	K	2	5	14,14,15	2.05	6 (42%)	17,19,21	0.99	2 (11%)
5	BMA	K	3	5	11,11,12	1.40	2 (18%)	15,15,17	0.62	0
5	MAN	K	4	5	11,11,12	2.04	6 (54%)	15,15,17	0.72	0
5	MAN	K	5	5	11,11,12	1.91	5 (45%)	15,15,17	0.74	0
6	NAG	L	1	6,3	14,14,15	2.15	6 (42%)	17,19,21	6.83	2 (11%)
6	NAG	L	2	6	14,14,15	2.01	7 (50%)	17,19,21	1.90	3 (17%)
5	NAG	M	1	4,5	14,14,15	2.30	5 (35%)	17,19,21	1.30	3 (17%)
5	NAG	M	2	5	14,14,15	2.10	7 (50%)	17,19,21	1.03	1 (5%)
5	BMA	M	3	5	11,11,12	1.48	3 (27%)	15,15,17	0.64	0
5	MAN	M	4	5	11,11,12	2.00	6 (54%)	15,15,17	0.70	0
5	MAN	M	5	5	11,11,12	1.93	5 (45%)	15,15,17	0.68	0
6	NAG	N	1	6,3	14,14,15	2.24	6 (42%)	17,19,21	1.98	3 (17%)
6	NAG	N	2	6	14,14,15	1.97	5 (35%)	17,19,21	0.99	2 (11%)
5	NAG	O	1	4,5	14,14,15	2.27	6 (42%)	17,19,21	1.18	2 (11%)
5	NAG	O	2	5	14,14,15	2.03	7 (50%)	17,19,21	0.99	0
5	BMA	O	3	5	11,11,12	1.42	2 (18%)	15,15,17	0.63	0
5	MAN	O	4	5	11,11,12	1.99	6 (54%)	15,15,17	0.72	0
5	MAN	O	5	5	11,11,12	1.94	5 (45%)	15,15,17	0.70	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
5	NAG	K	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	K	2	5	-	0/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1
5	MAN	K	5	5	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	1	6,3	-	1/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1
5	NAG	M	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	M	2	5	-	1/6/23/26	0/1/1/1
5	BMA	M	3	5	-	0/2/19/22	0/1/1/1
5	MAN	M	4	5	-	0/2/19/22	0/1/1/1
5	MAN	M	5	5	-	0/2/19/22	0/1/1/1
6	NAG	N	1	6,3	-	2/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
5	NAG	O	1	4,5	-	0/6/23/26	0/1/1/1
5	NAG	O	2	5	-	1/6/23/26	0/1/1/1
5	BMA	O	3	5	-	0/2/19/22	0/1/1/1
5	MAN	O	4	5	-	0/2/19/22	0/1/1/1
5	MAN	O	5	5	-	0/2/19/22	0/1/1/1

The worst 5 of 100 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1	NAG	C1-C2	6.21	1.61	1.52
5	O	1	NAG	C1-C2	6.01	1.61	1.52
5	K	1	NAG	C1-C2	5.65	1.60	1.52
6	N	1	NAG	C1-C2	5.57	1.60	1.52
5	K	2	NAG	C1-C2	4.97	1.59	1.52

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	1	NAG	C2-N2-C7	27.82	162.52	122.90
6	L	2	NAG	C8-C7-N2	6.15	126.51	116.10
6	N	1	NAG	C8-C7-N2	6.06	126.36	116.10
6	N	1	NAG	O7-C7-N2	-3.41	115.67	121.95
6	L	2	NAG	O7-C7-N2	-3.24	116.00	121.95

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	L	1	NAG	C3-C2-N2-C7
6	L	2	NAG	C8-C7-N2-C2
6	L	2	NAG	O7-C7-N2-C2
6	N	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

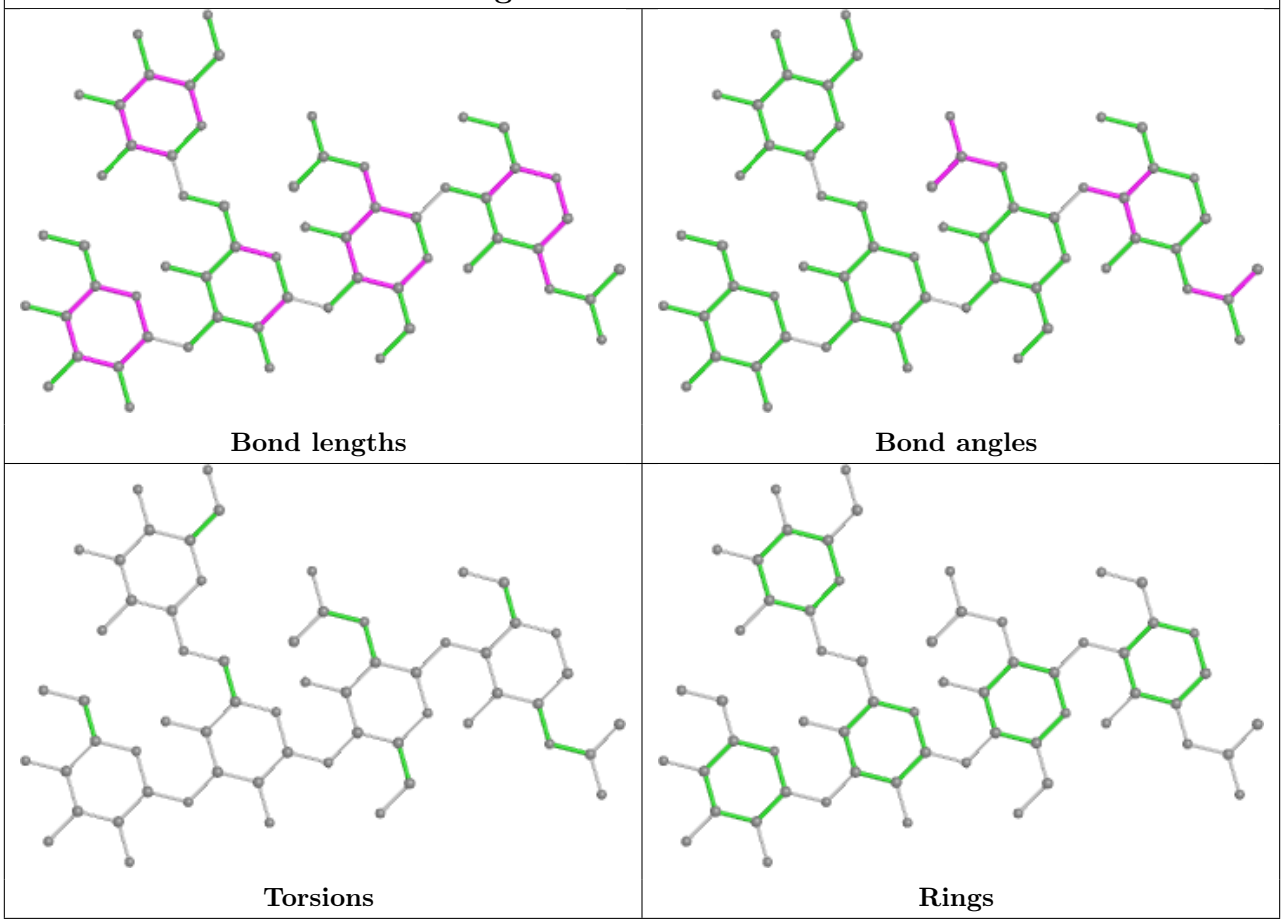
Mol	Chain	Res	Type	Atoms
6	N	1	NAG	O7-C7-N2-C2

There are no ring outliers.

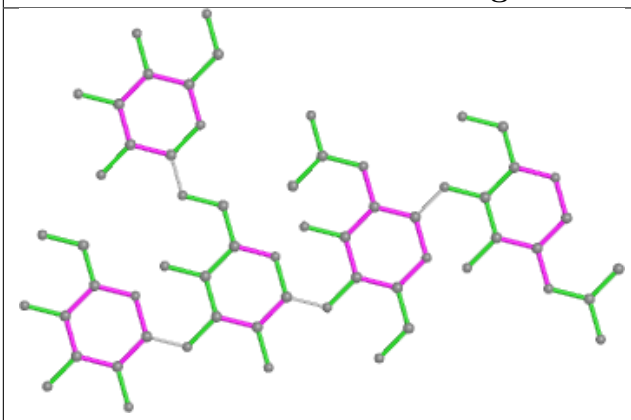
No monomer is involved in short contacts.

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

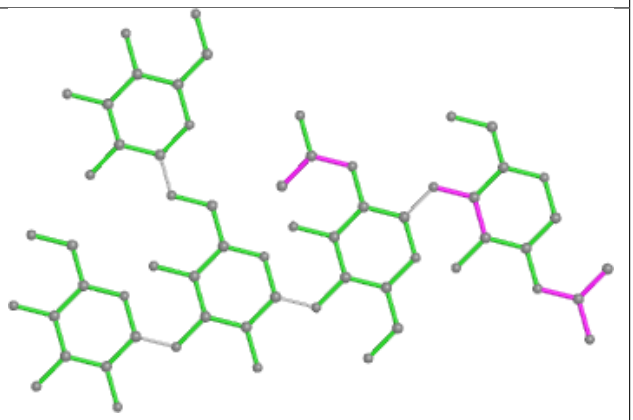
Oligosaccharide Chain K



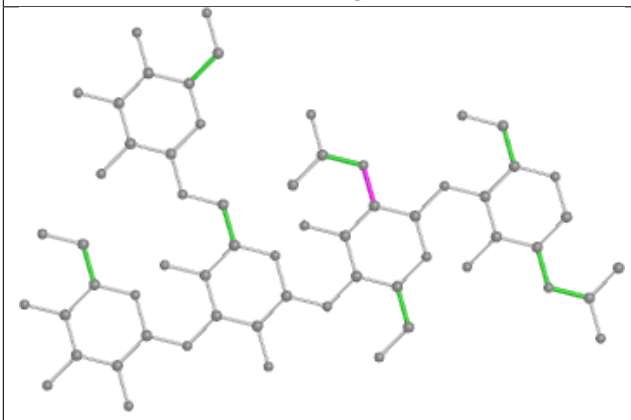
Oligosaccharide Chain M



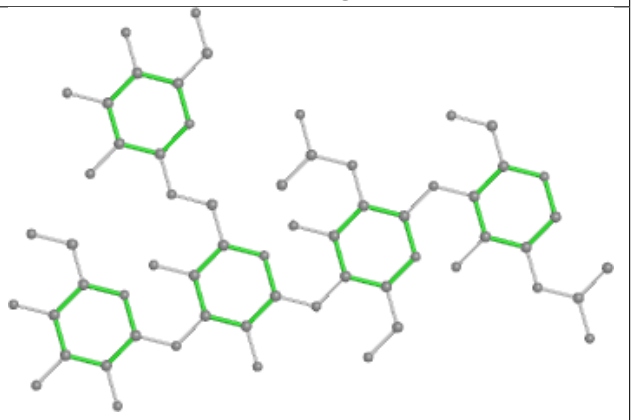
Bond lengths



Bond angles

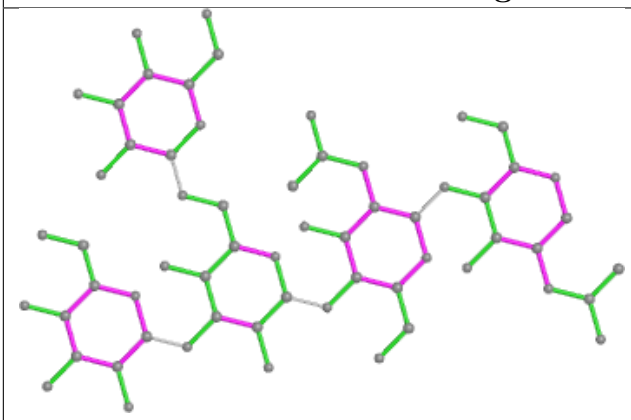


Torsions

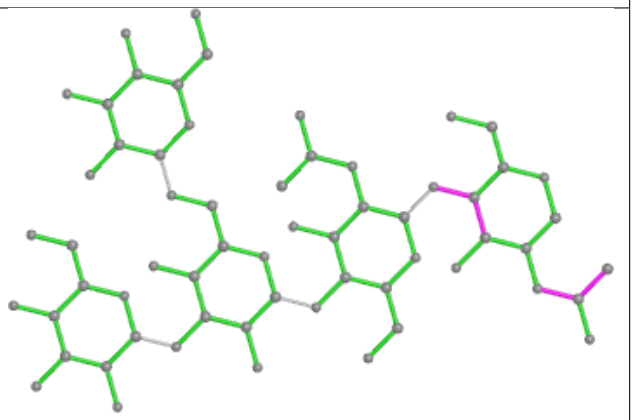


Rings

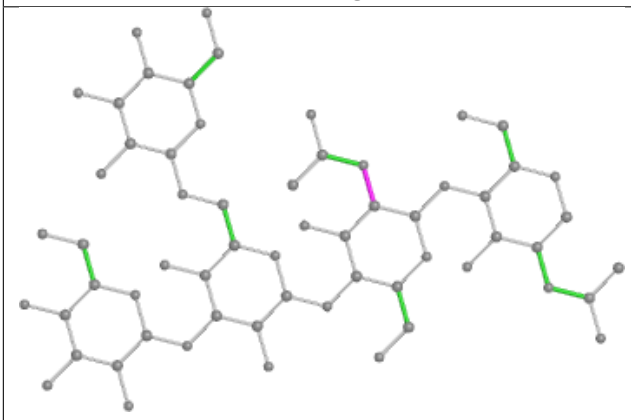
Oligosaccharide Chain O



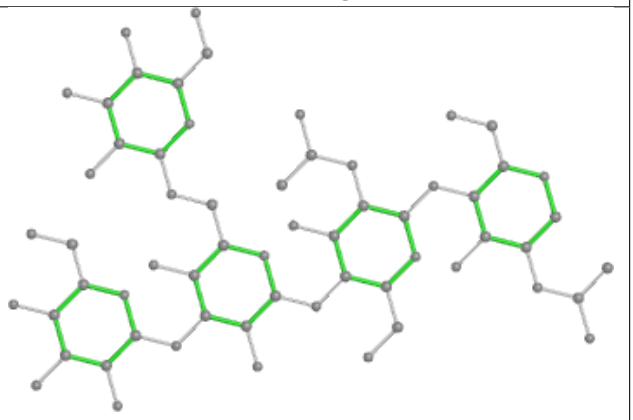
Bond lengths



Bond angles

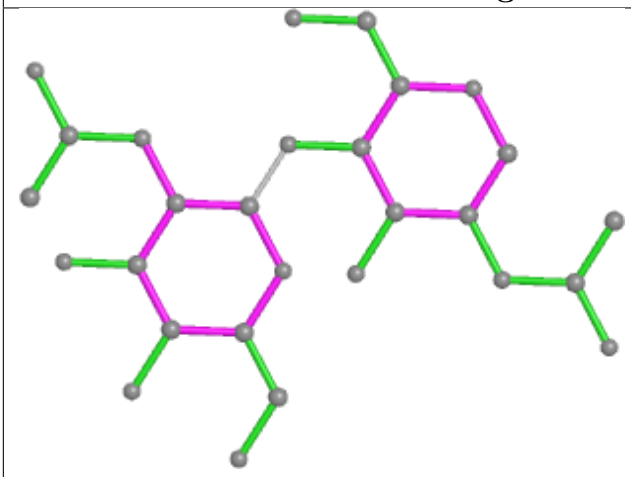


Torsions

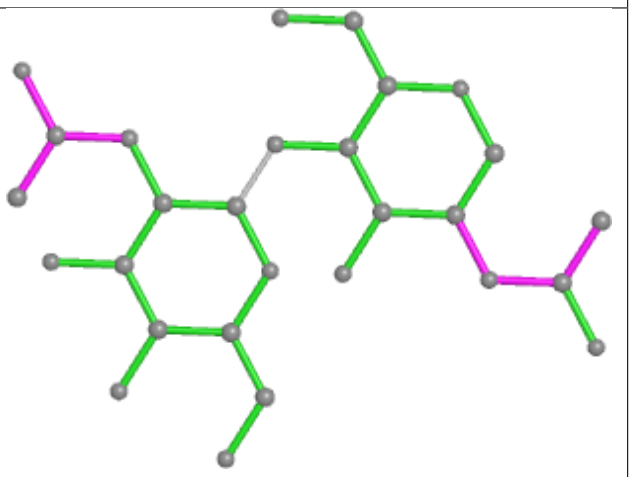


Rings

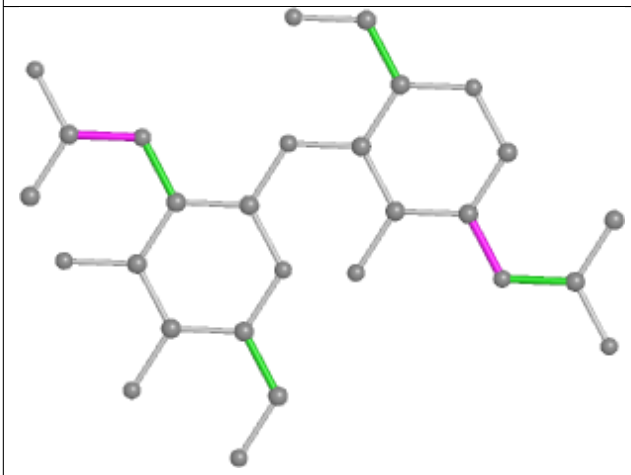
Oligosaccharide Chain L



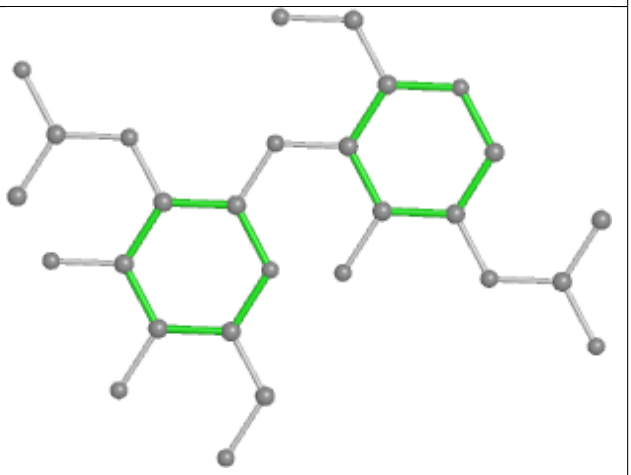
Bond lengths



Bond angles

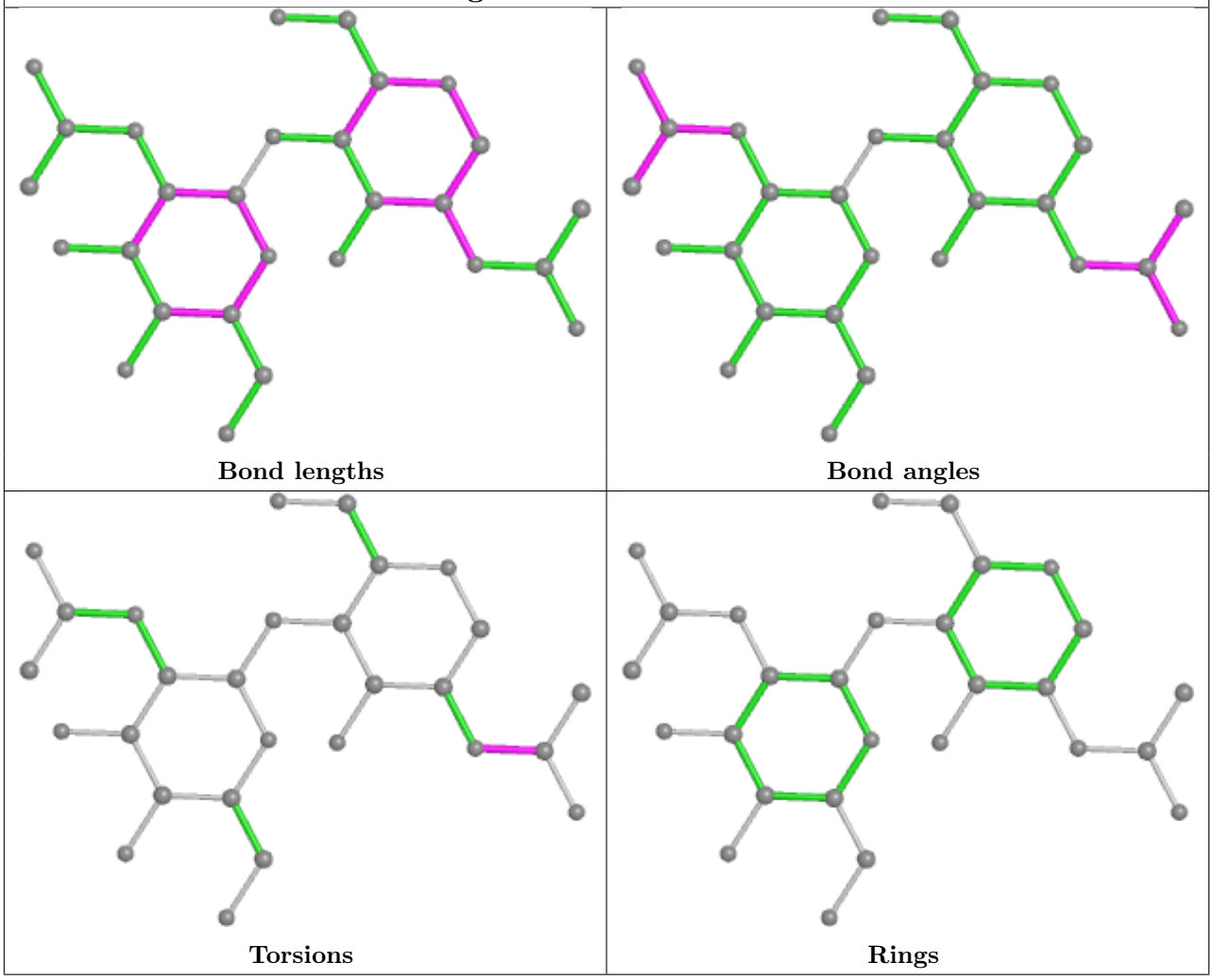


Torsions



Rings

Oligosaccharide Chain N



5.6 Ligand geometry (i)

2 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	401	3	14,14,15	2.18	5 (35%)	17,19,21	0.93	1 (5%)
7	NAG	B	401	3	14,14,15	2.16	5 (35%)	17,19,21	0.94	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	401	3	-	0/6/23/26	0/1/1/1
7	NAG	B	401	3	-	0/6/23/26	0/1/1/1

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	401	NAG	C1-C2	5.48	1.60	1.52
7	B	401	NAG	C1-C2	5.30	1.60	1.52
7	B	401	NAG	O5-C5	3.21	1.50	1.43
7	C	401	NAG	O5-C5	3.06	1.49	1.43
7	B	401	NAG	O5-C1	2.78	1.48	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	401	NAG	C8-C7-N2	2.03	119.54	116.10
7	C	401	NAG	C8-C7-N2	2.01	119.50	116.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.

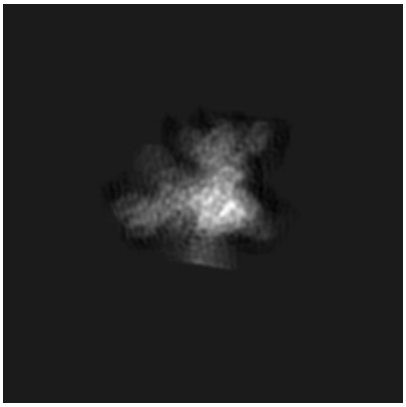
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22851. These allow visual inspection of the internal detail of the map and identification of artifacts.

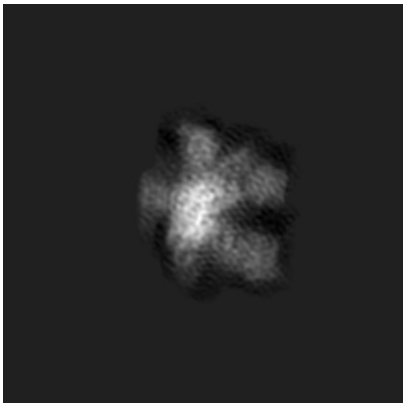
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

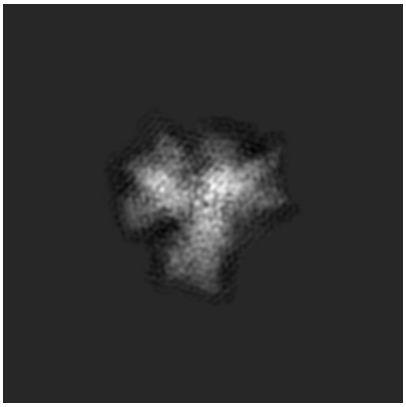
6.1.1 Primary map



X



Y

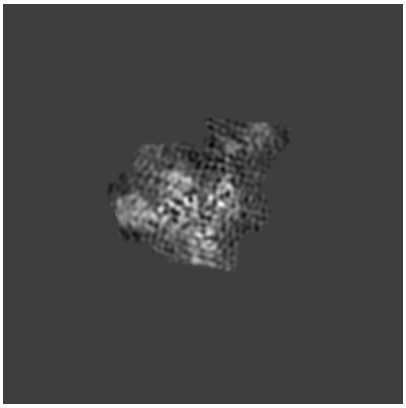


Z

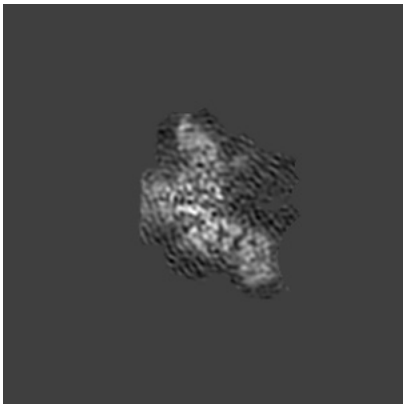
The images above show the map projected in three orthogonal directions.

6.2 Central slices

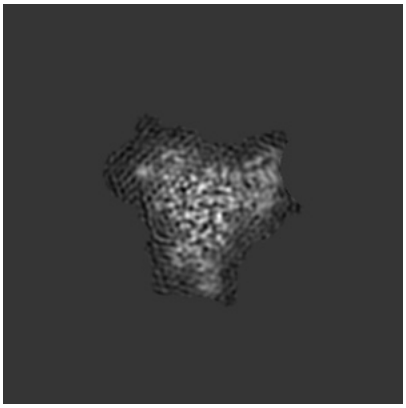
6.2.1 Primary map



X Index: 144



Y Index: 144

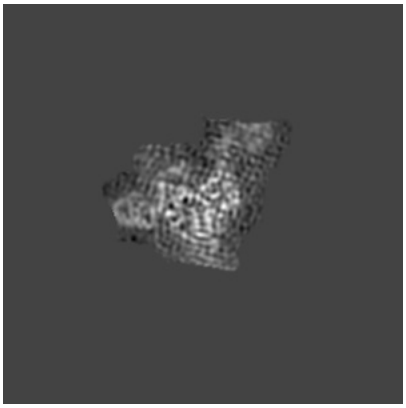


Z Index: 144

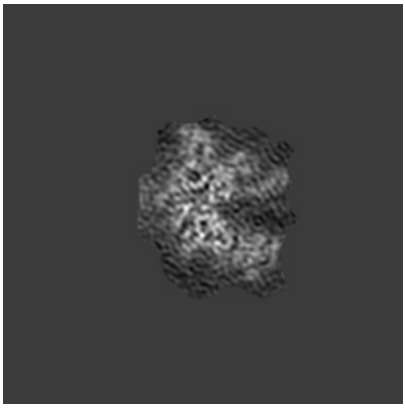
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

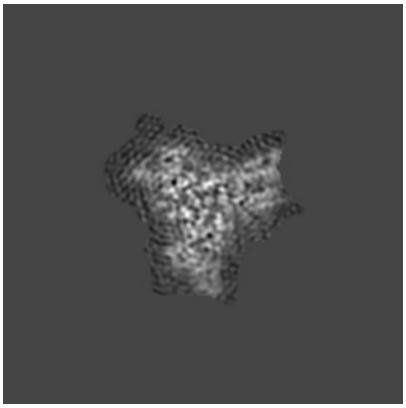
6.3.1 Primary map



X Index: 149



Y Index: 153



Z Index: 142

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 0.0289. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

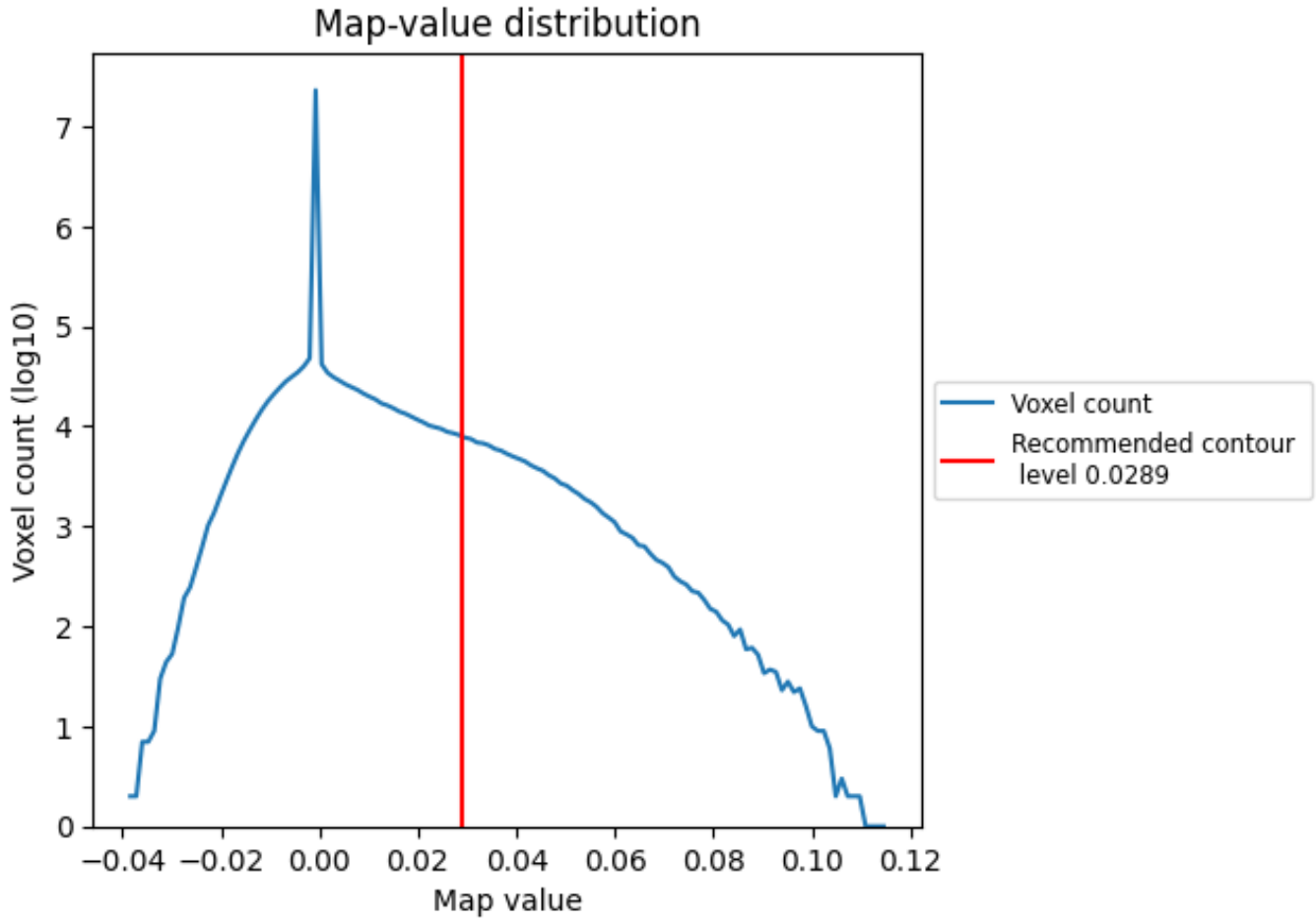
6.5 Mask visualisation (i)

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

7 Map analysis

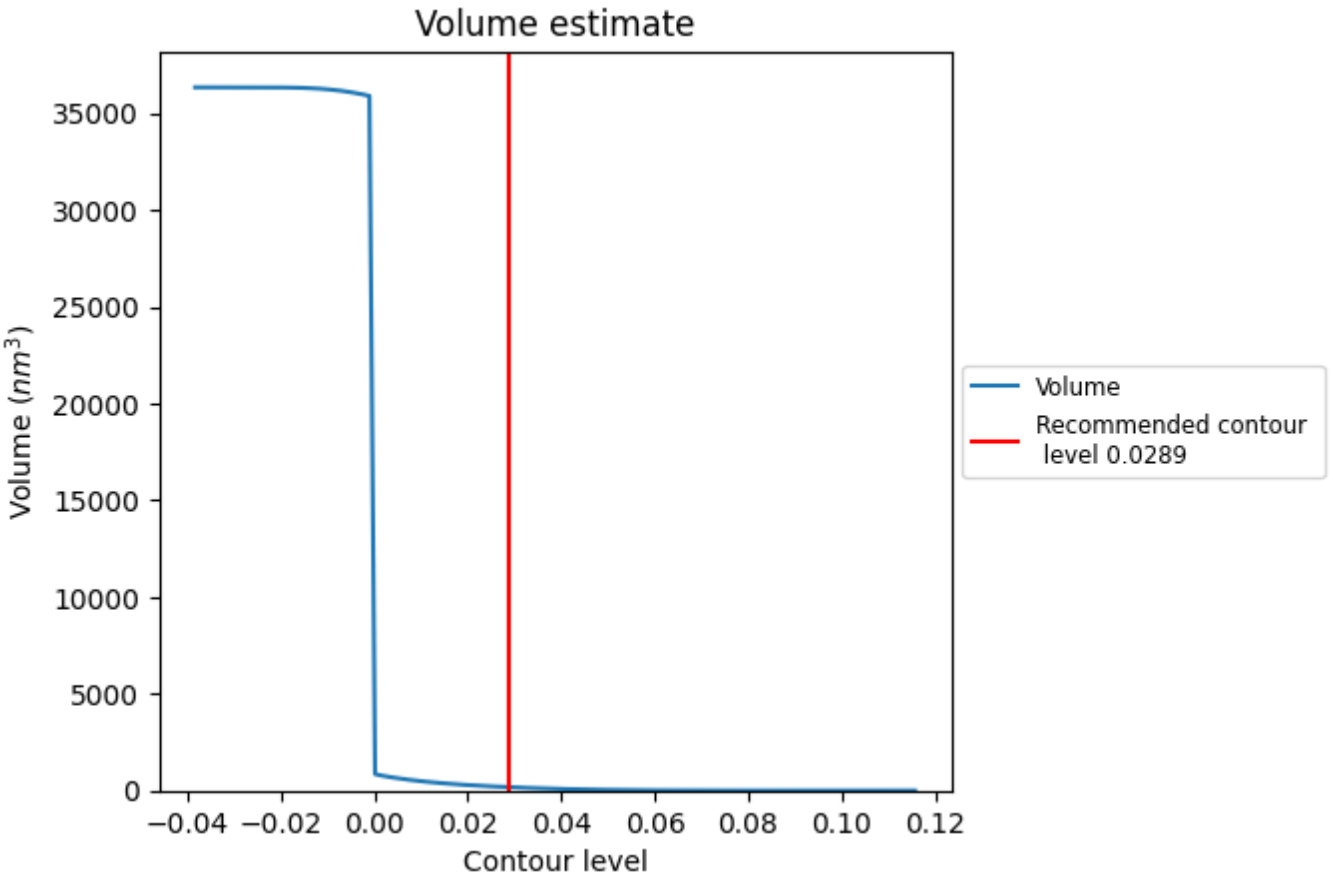
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

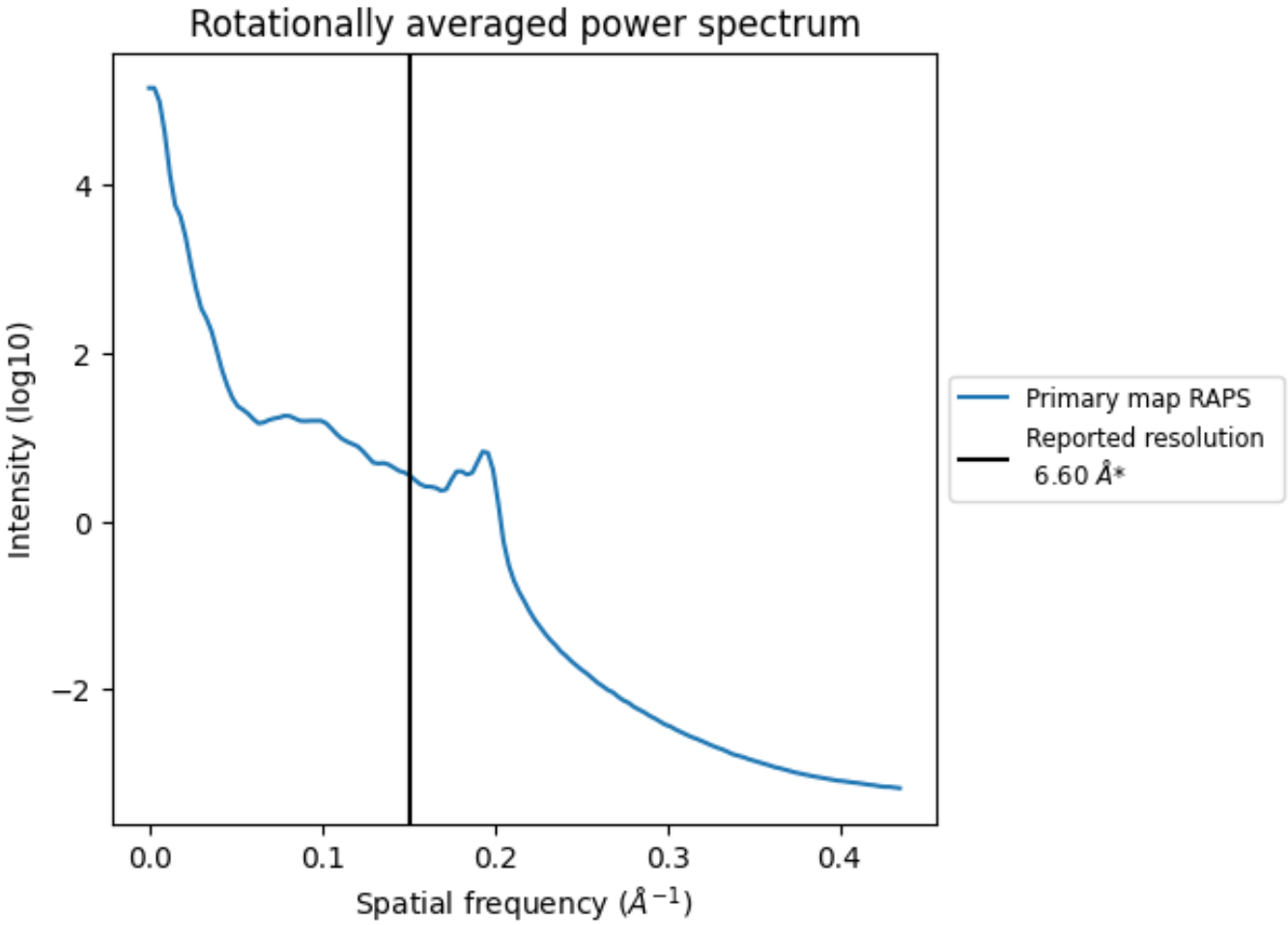
7.2 Volume estimate (i)



The volume at the recommended contour level is 176 nm^3; this corresponds to an approximate mass of 159 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)

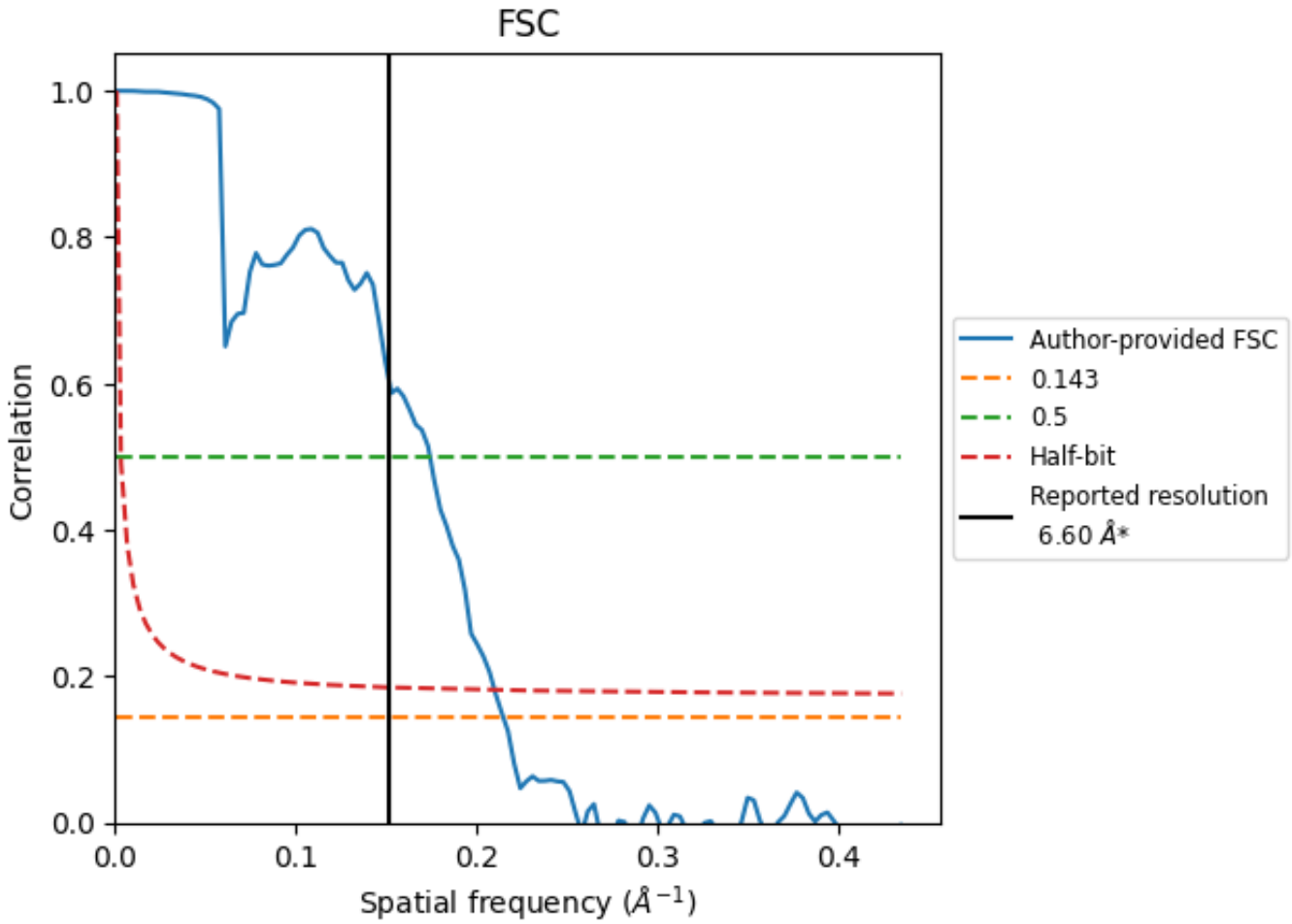


*Reported resolution corresponds to spatial frequency of 0.152 $Å^{-1}$

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates (i)

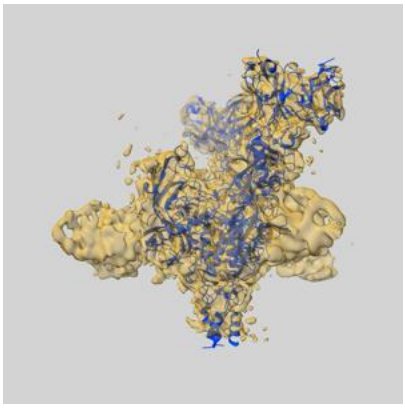
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	4.66	5.74	4.76
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from author-provided FSC intersecting FSC 0.143 CUT-OFF 4.66 differs from the reported value 6.6 by more than 10 %

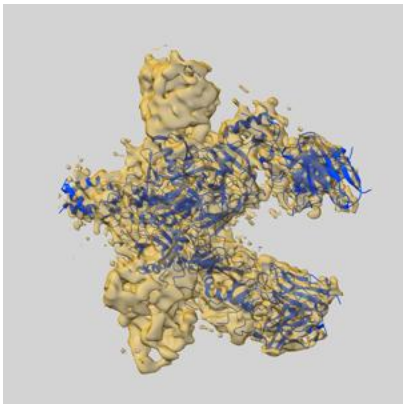
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-22851 and PDB model 7KFE. Per-residue inclusion information can be found in section 3 on page 12.

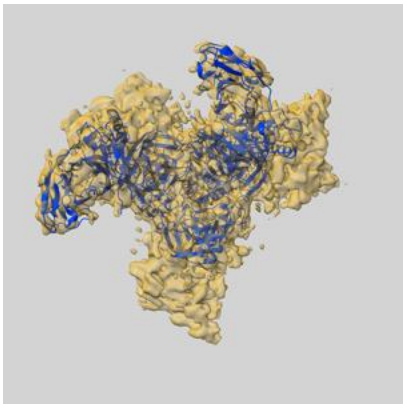
9.1 Map-model overlay



X



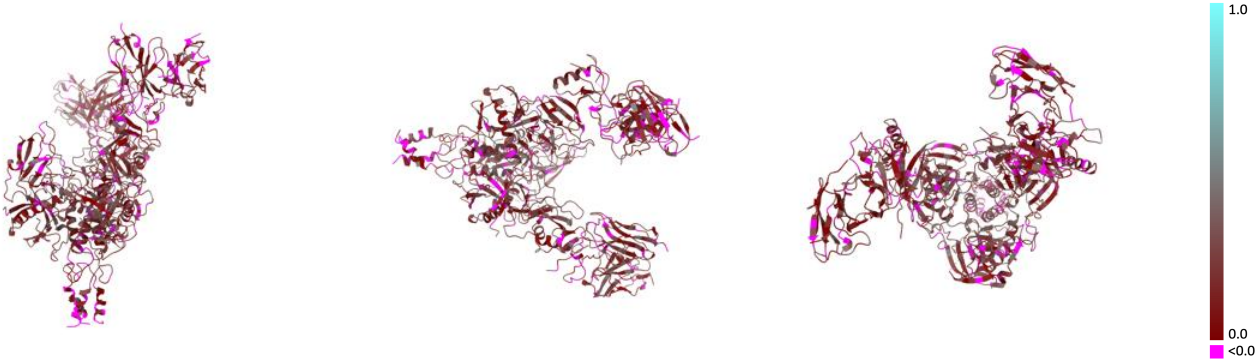
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0289 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

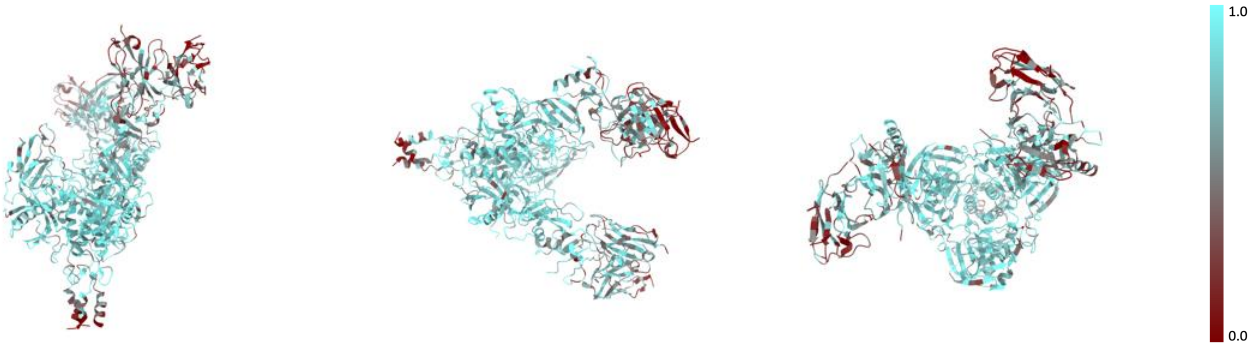
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

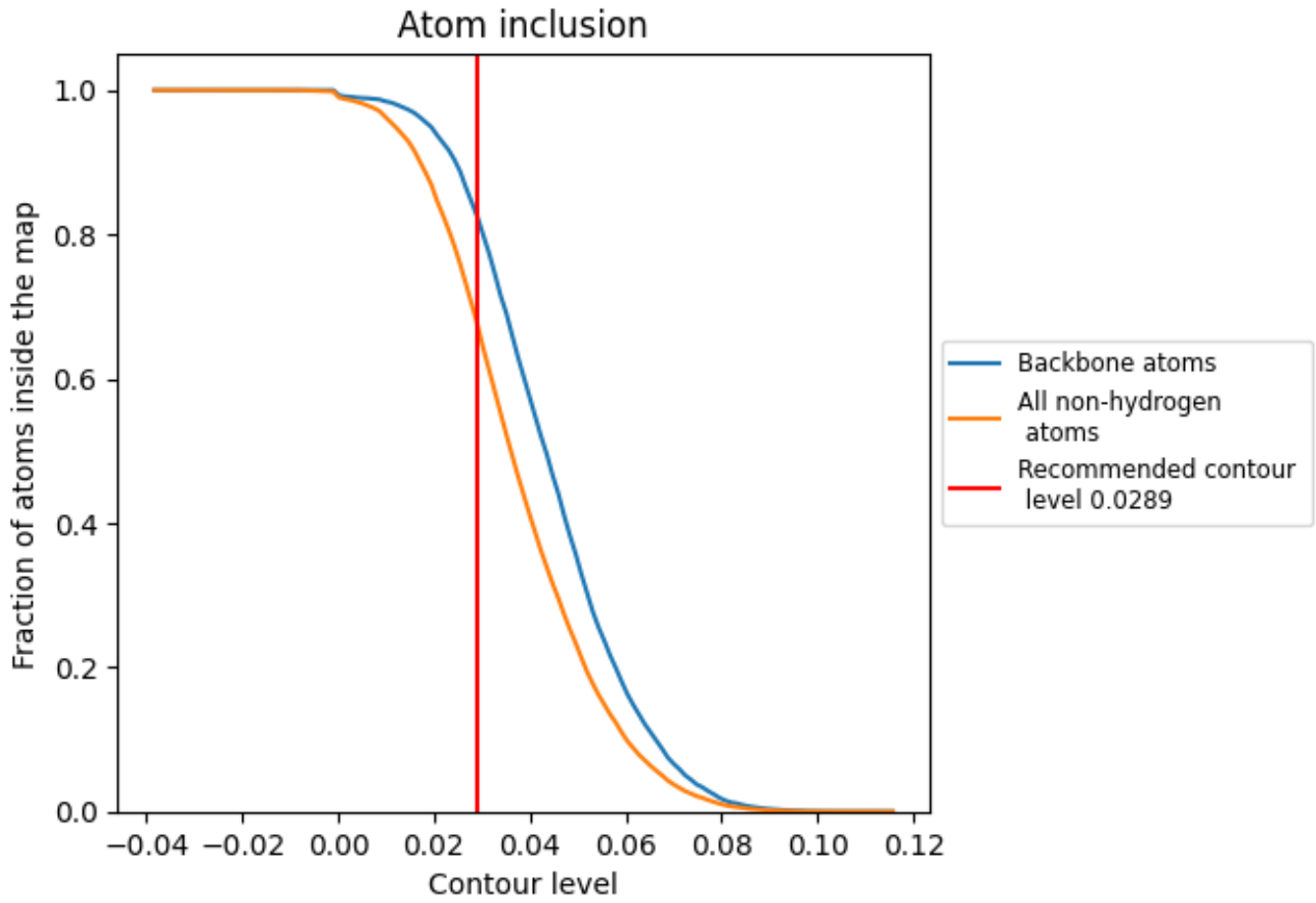
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0289).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 68% 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 (0.0289) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6785	0.1710
A	0.7725	0.1910
B	0.7661	0.1950
C	0.7883	0.2050
D	0.7330	0.1720
E	0.7754	0.1760
F	0.7385	0.1580
G	0.4875	0.1170
H	0.6149	0.1460
I	0.3704	0.1240
J	0.5082	0.1490
K	0.6885	0.2710
L	0.5357	0.2050
M	0.6557	0.2920
N	0.6786	0.2070
O	0.6885	0.2870